



## Full wwPDB EM Validation Report ⓘ

Jul 24, 2024 – 04:24 PM JST

PDB ID : 8XVT  
EMDB ID : EMD-38718  
Title : The core subcomplex of human NuA4/TIP60 complex  
Authors : Chen, K.; Wang, L.; Yu, Z.; Yu, J.; Ren, Y.; Wang, Q.; Xu, Y.  
Deposited on : 2024-01-15  
Resolution : 3.20 Å (reported)  
Based on initial model : 6IGM

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:

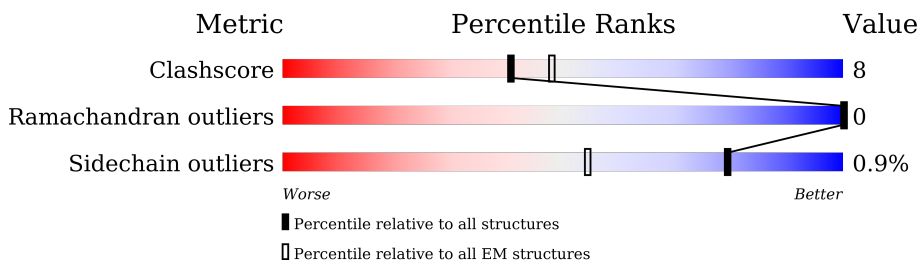
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.20 Å.

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



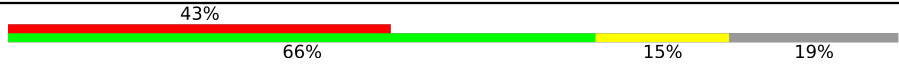
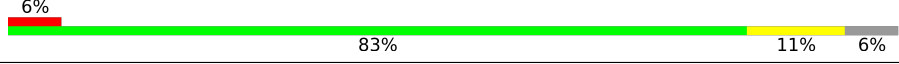
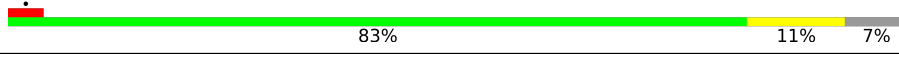
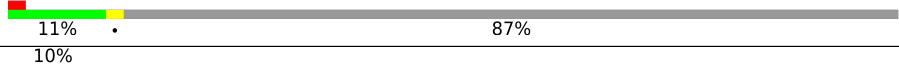

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	456	 79% 14% 7%
1	C	456	 75% 16% 9%
1	E	456	 83% 12% 5%
2	B	463	 6% 73% 13% 14%
2	D	463	 77% 14% 8%
2	F	463	 74% 16% 10%
3	G	467	 7% 36% 7% 57%
4	H	3123	 9% 23% 73%

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Mol	Chain	Length	Quality of chain
5	I	429	
5	J	429	
6	K	375	
7	M	813	
8	N	364	

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
9	ADP	A	501	-	-	X	-
9	ADP	B	501	-	-	X	-
9	ADP	C	501	-	-	X	-
9	ADP	D	501	-	-	X	-
9	ADP	E	501	-	-	X	-
9	ADP	F	501	-	-	X	-
9	ADP	I	501	-	-	X	-
9	ADP	K	401	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 38987 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 RuvB-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	426	Total	C	N	O	S	0	0
			3279	2067	563	633	16		
1	C	416	Total	C	N	O	S	0	0
			3210	2027	552	616	15		
1	E	435	Total	C	N	O	S	0	0
			3344	2106	574	647	17		

- Molecule 2 is a protein called RuvB-like 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	399	Total	C	N	O	S	0	0
			3101	1940	541	605	15		
2	D	427	Total	C	N	O	S	0	0
			3315	2069	584	646	16		
2	F	417	Total	C	N	O	S	0	0
			3242	2025	570	631	16		

- Molecule 3 is a protein called DNA methyltransferase 1-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	G	201	Total	C	N	O	S	0	0
			1717	1093	316	305	3		

- Molecule 4 is a protein called Isoform 2 of E1A-binding protein p400.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	H	841	Total	C	N	O	S	0	0
			6900	4393	1253	1220	34		

- Molecule 5 is a protein called Actin-like protein 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	I	349	Total 2715	C 1716	N 459	O 519	S 21	0	0
5	J	403	Total 3139	C 1984	N 535	O 597	S 23	0	0

- Molecule 6 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	K	350	Total 2733	C 1736	N 458	O 519	S 20	0	0

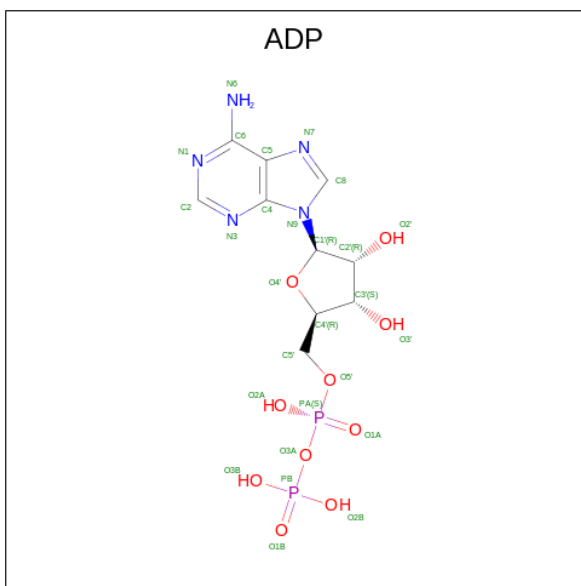
- Molecule 7 is a protein called Isoform 2 of Enhancer of polycomb homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	M	106	Total 861	C 541	N 166	O 149	S 5	0	0

- Molecule 8 is a protein called Vacuolar protein sorting-associated protein 72 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	N	150	Total 1188	C 764	N 213	O 208	S 3	0	0

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).

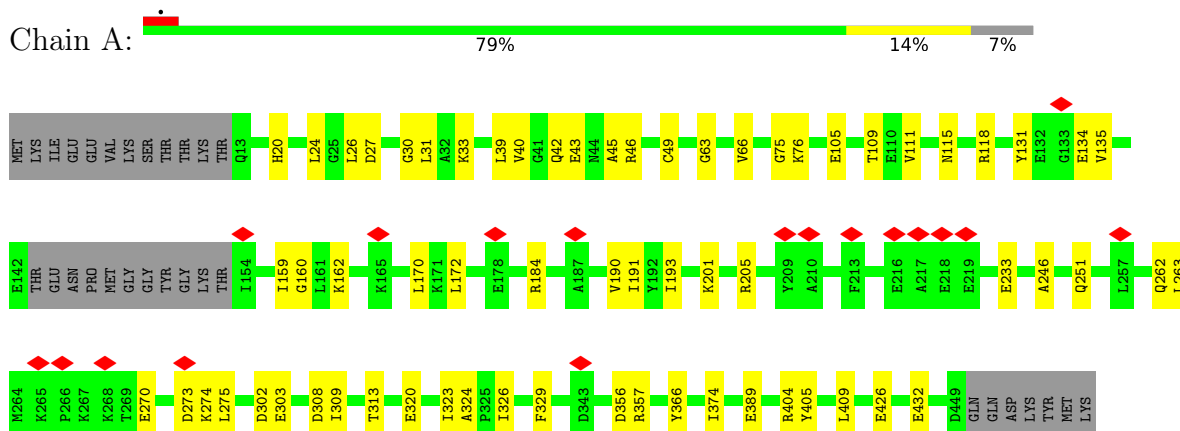


Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total 27	C 10	N 5	O 10	P 2	0
9	B	1	Total 27	C 10	N 5	O 10	P 2	0
9	C	1	Total 27	C 10	N 5	O 10	P 2	0
9	D	1	Total 27	C 10	N 5	O 10	P 2	0
9	E	1	Total 27	C 10	N 5	O 10	P 2	0
9	F	1	Total 27	C 10	N 5	O 10	P 2	0
9	I	1	Total 27	C 10	N 5	O 10	P 2	0
9	J	1	Total 27	C 10	N 5	O 10	P 2	0
9	K	1	Total 27	C 10	N 5	O 10	P 2	0

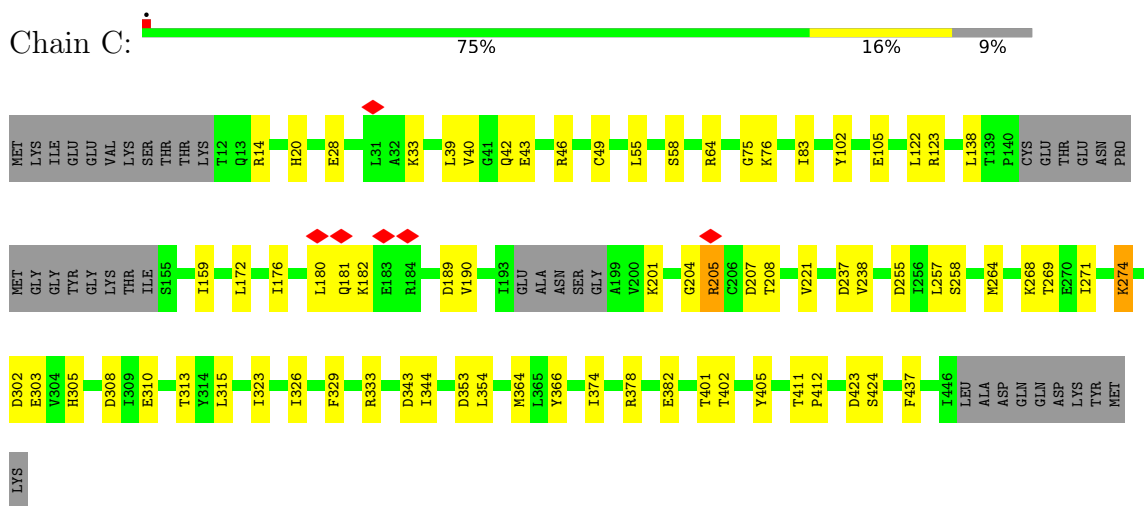
### 3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

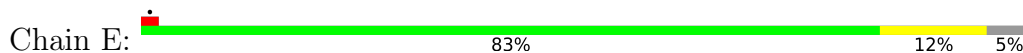
- Molecule 1: RuvB-like 1

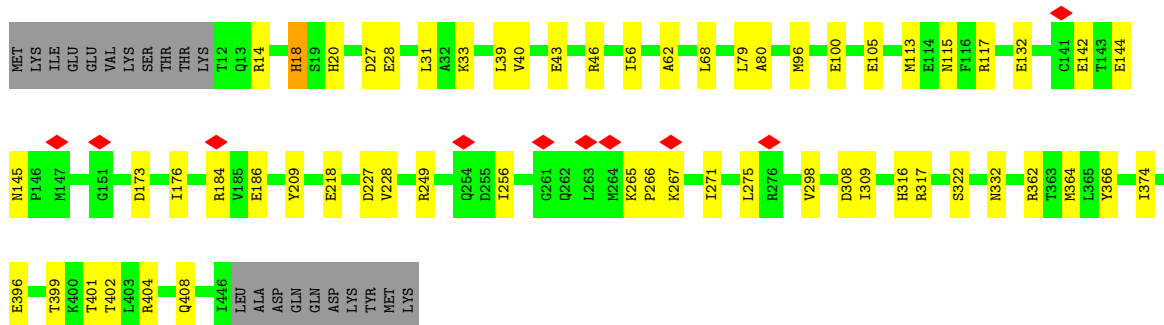


- Molecule 1: RuvB-like 1

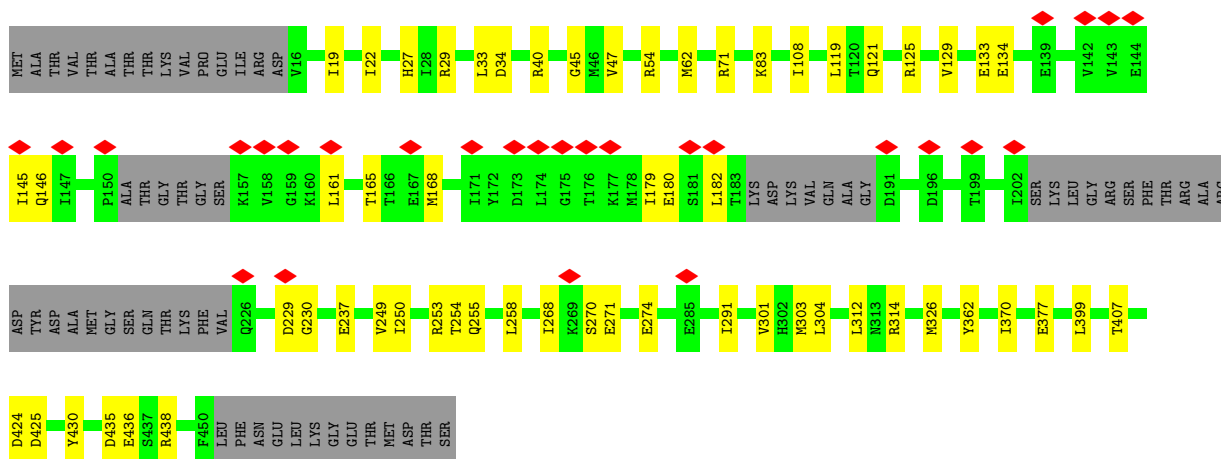
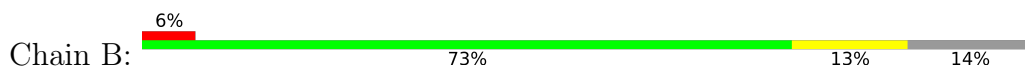


- Molecule 1: RuvB-like 1

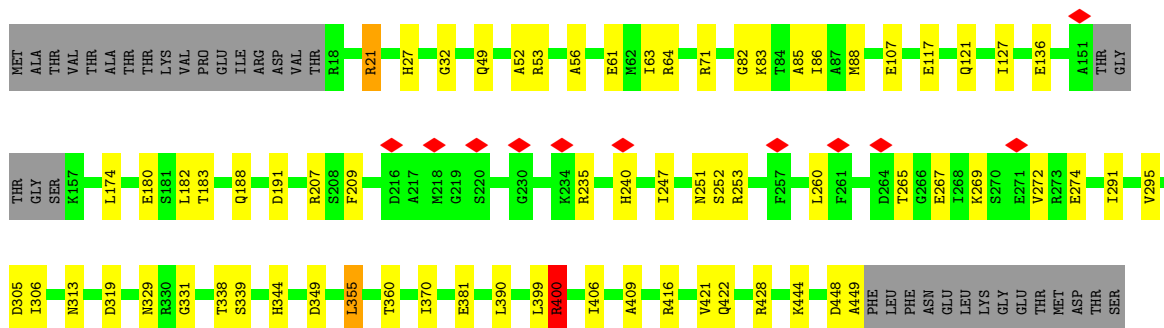
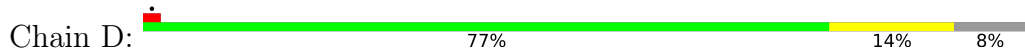




• Molecule 2: RuvB-like 2



• Molecule 2: RuvB-like 2



• Molecule 2: RuvB-like 2



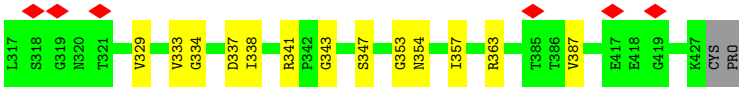




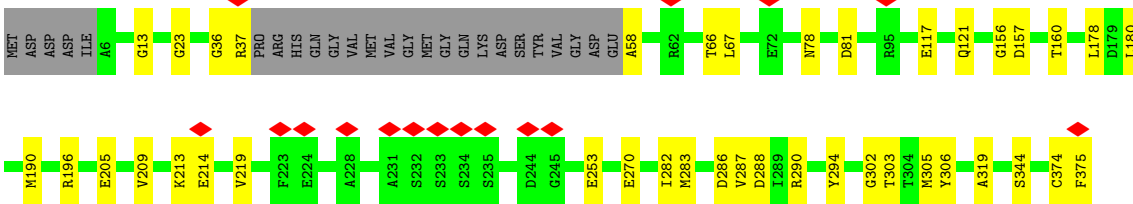
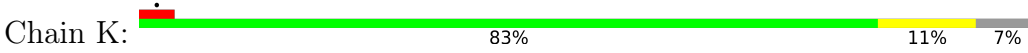




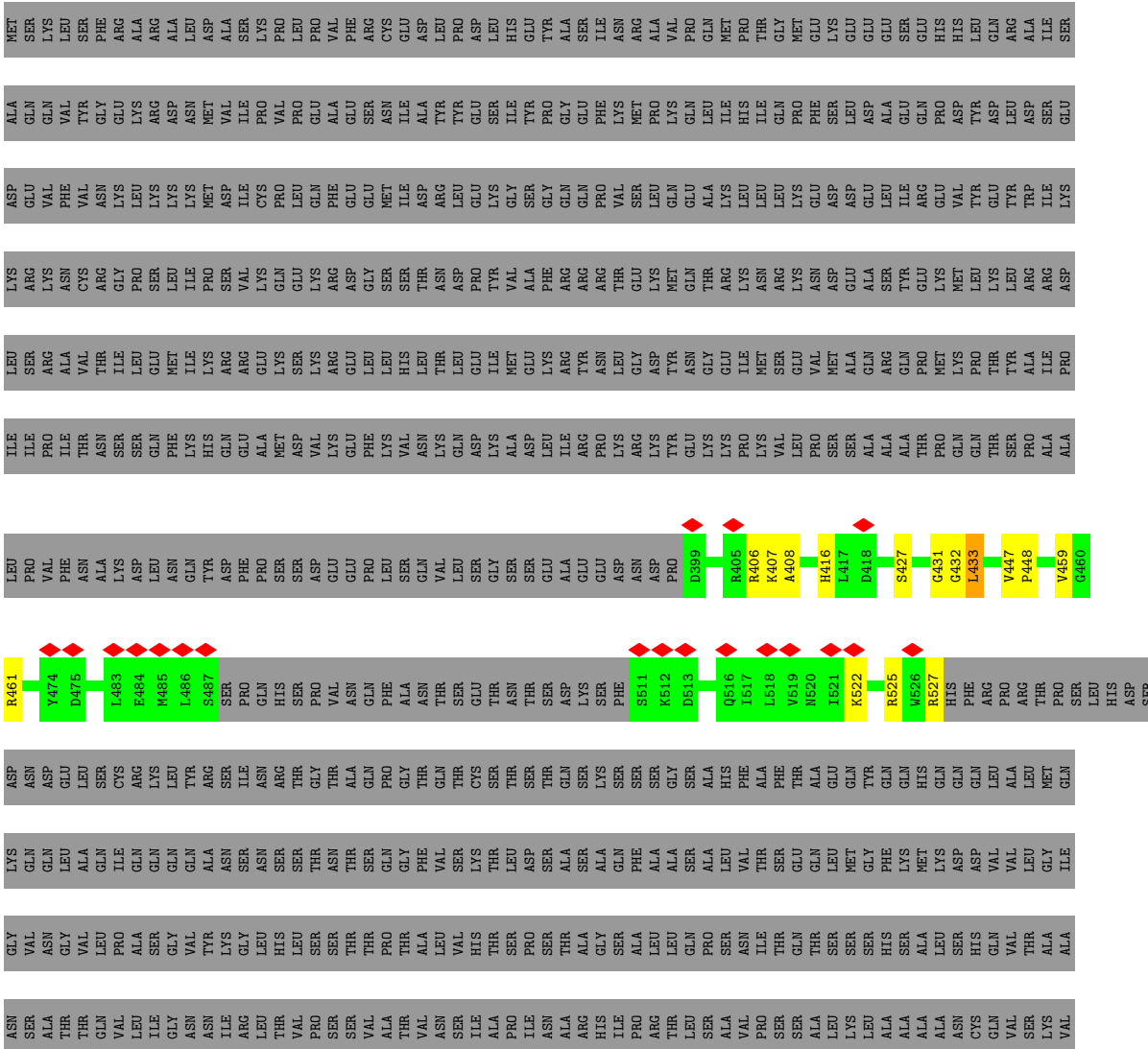




• Molecule 6: Actin, cytoplasmic 1



• Molecule 7: Isoform 2 of Enhancer of polycomb homolog 1





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	701594	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.252	Depositor
Minimum map value	-0.125	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.024	Depositor
Map size (Å)	400.2, 400.2, 400.2	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.334, 1.334, 1.334	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

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	0.24	0/3321	0.41	0/4476
1	C	0.23	0/3251	0.39	0/4380
1	E	0.24	0/3389	0.40	0/4569
2	B	0.23	0/3134	0.42	0/4219
2	D	0.24	0/3352	0.42	1/4510 (0.0%)
2	F	0.23	0/3276	0.41	0/4405
3	G	0.24	0/1759	0.38	0/2364
4	H	0.23	0/7045	0.38	0/9520
5	I	0.24	0/2771	0.41	0/3756
5	J	0.24	0/3209	0.41	0/4349
6	K	0.24	0/2792	0.39	0/3782
7	M	0.24	0/883	0.42	0/1191
8	N	0.24	0/1225	0.39	0/1669
All	All	0.24	0/39407	0.40	1/53190 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	400	ARG	NE-CZ-NH2	-5.23	117.69	120.30

There are no chirality outliers.

There are no planarity outliers.

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen



atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3279	0	3385	56	0
1	C	3210	0	3324	76	0
1	E	3344	0	3446	59	0
2	B	3101	0	3172	50	0
2	D	3315	0	3391	60	0
2	F	3242	0	3321	69	0
3	G	1717	0	1705	26	0
4	H	6900	0	7025	80	0
5	I	2715	0	2657	71	0
5	J	3139	0	3077	30	0
6	K	2733	0	2714	43	0
7	M	861	0	841	11	0
8	N	1188	0	1214	19	0
9	A	27	0	12	14	0
9	B	27	0	12	9	0
9	C	27	0	12	29	0
9	D	27	0	12	11	0
9	E	27	0	12	19	0
9	F	27	0	11	10	0
9	I	27	0	12	24	0
9	J	27	0	12	5	0
9	K	27	0	11	18	0
All	All	38987	0	39378	588	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 8.

All (588) 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:F:47:VAL:CG1	2:F:370:ILE:CG2	2.21	1.16
2:F:47:VAL:HG12	2:F:370:ILE:HG22	1.27	1.14
2:F:27:HIS:CE1	9:F:501:ADP:O2'	2.02	1.12
2:F:47:VAL:CG1	2:F:370:ILE:HG22	1.78	1.11
2:F:370:ILE:HD12	2:F:399:LEU:HD21	1.27	1.11
5:I:24:ARG:NH2	9:I:501:ADP:O2'	1.83	1.11
6:K:305:MET:HB2	9:K:401:ADP:C2	1.92	1.05
2:F:370:ILE:CD1	2:F:399:LEU:HD21	1.88	1.00
2:B:362:TYR:OH	9:B:501:ADP:N7	1.92	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:247:ILE:HG21	2:D:267:GLU:OE2	1.60	0.98
1:C:180:LEU:HG	1:C:181:GLN:H	1.29	0.97
1:C:411:THR:OG1	1:C:412:PRO:HD3	1.63	0.96
1:C:374:ILE:CD1	9:C:501:ADP:N3	2.28	0.96
1:A:366:TYR:OH	9:A:501:ADP:N7	1.98	0.95
2:F:47:VAL:HG11	2:F:370:ILE:HG23	1.49	0.95
1:C:374:ILE:HD11	9:C:501:ADP:C4	2.02	0.94
1:C:374:ILE:CD1	9:C:501:ADP:C4	2.51	0.93
1:C:374:ILE:HD11	9:C:501:ADP:N3	1.83	0.93
2:F:47:VAL:CG1	2:F:370:ILE:HG23	1.96	0.93
5:I:20:SER:HB2	9:I:501:ADP:N7	1.84	0.92
2:F:362:TYR:CZ	9:F:501:ADP:N7	2.40	0.89
2:F:362:TYR:OH	9:F:501:ADP:N7	2.04	0.89
1:E:404:ARG:NH2	9:E:501:ADP:O3B	2.05	0.89
2:F:47:VAL:HG11	2:F:370:ILE:CG2	2.00	0.89
2:F:400:ARG:NH2	9:F:501:ADP:O2A	2.06	0.89
2:B:362:TYR:CZ	9:B:501:ADP:N7	2.40	0.88
1:E:39:LEU:HD12	9:E:501:ADP:N6	1.89	0.88
6:K:305:MET:HB2	9:K:401:ADP:N1	1.88	0.88
2:F:27:HIS:HE1	9:F:501:ADP:O2'	1.56	0.85
1:C:374:ILE:HD11	9:C:501:ADP:H1'	1.58	0.85
2:D:247:ILE:CG2	2:D:267:GLU:OE2	2.25	0.85
5:I:70:ILE:CD1	5:I:102:ILE:HA	2.08	0.83
3:G:76:THR:HG21	4:H:2190:GLU:OE1	1.78	0.82
1:E:362:ARG:NH1	1:E:364:MET:SD	2.53	0.81
3:G:170:ARG:NH1	5:J:184:ASP:OD2	2.14	0.81
2:B:179:ILE:HD12	2:B:182:LEU:HD11	1.62	0.81
2:B:165:THR:OG1	2:B:168:MET:O	1.99	0.80
6:K:157:ASP:OD1	9:K:401:ADP:O5'	2.00	0.80
6:K:160:THR:OG1	6:K:178:LEU:HB3	1.81	0.80
2:F:32:GLY:O	2:F:53:ARG:NH2	2.14	0.80
4:H:1891:LEU:HD22	4:H:1934:ILE:CG2	2.12	0.79
4:H:2209:MET:SD	7:M:525:ARG:NH1	2.54	0.79
4:H:1880:ARG:O	4:H:1951:THR:OG1	1.99	0.79
1:C:20:HIS:CE1	9:C:501:ADP:O2'	2.35	0.79
1:C:180:LEU:HG	1:C:181:GLN:N	1.98	0.78
1:A:320:GLU:OE2	1:A:357:ARG:NH1	2.16	0.78
2:D:191:ASP:OD1	2:D:207:ARG:NH1	2.16	0.78
1:C:366:TYR:OH	9:C:501:ADP:N7	2.16	0.78
1:E:96:MET:SD	1:E:115:ASN:ND2	2.56	0.78
2:F:83:LYS:N	9:F:501:ADP:O1B	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:VAL:N	9:A:501:ADP:N1	2.31	0.77
1:E:374:ILE:HG12	9:E:501:ADP:C2	2.19	0.77
1:E:105:GLU:OE2	2:F:265:THR:OG1	2.02	0.77
4:H:829:ARG:NH1	8:N:271:ASP:OD2	2.17	0.76
1:C:75:GLY:HA2	9:C:501:ADP:PA	2.26	0.76
5:I:269:VAL:O	5:I:359:SER:OG	2.04	0.76
1:E:218:GLU:OE1	2:F:177:LYS:NZ	2.19	0.76
2:F:370:ILE:CD1	2:F:399:LEU:CD2	2.63	0.76
4:H:793:GLU:OE1	7:M:461:ARG:NH1	2.20	0.75
2:D:247:ILE:CG2	2:D:267:GLU:OE1	2.34	0.75
1:E:18:HIS:HB3	9:E:501:ADP:C3'	2.17	0.75
2:D:21:ARG:O	1:E:322:SER:OG	2.04	0.75
1:C:374:ILE:HD12	9:C:501:ADP:C4	2.20	0.74
1:C:55:LEU:O	1:C:58:SER:OG	2.05	0.74
4:H:1330:ARG:NH1	4:H:1958:ASP:OD1	2.19	0.74
2:B:83:LYS:HB3	9:B:501:ADP:O1B	1.87	0.73
1:E:332:ASN:ND2	2:F:349:ASP:OD2	2.22	0.73
2:B:407:THR:OG1	1:C:64:ARG:NH2	2.22	0.73
5:I:21:TYR:CD2	9:I:501:ADP:H3'	2.23	0.73
5:I:70:ILE:HD12	5:I:102:ILE:HD12	1.72	0.72
1:C:268:LYS:O	1:C:269:THR:OG1	2.04	0.72
1:A:432:GLU:OE2	2:B:54:ARG:NH1	2.22	0.72
5:I:202:ILE:HG22	5:I:304:ILE:HG21	1.72	0.71
1:E:39:LEU:HD12	9:E:501:ADP:C6	2.25	0.70
5:I:363:ARG:NH1	5:I:367:GLU:OE1	2.25	0.70
3:G:74:SER:O	4:H:2187:TYR:N	2.25	0.70
2:B:121:GLN:OE1	2:B:125:ARG:NH2	2.25	0.70
1:C:180:LEU:CG	1:C:181:GLN:H	2.01	0.70
5:I:353:GLY:HA3	9:I:501:ADP:H4'	1.74	0.70
1:E:39:LEU:CD1	9:E:501:ADP:N6	2.55	0.69
2:F:342:SER:OG	2:F:346:ILE:O	2.07	0.69
1:C:374:ILE:HD12	9:C:501:ADP:N3	2.07	0.69
2:D:247:ILE:CG2	2:D:267:GLU:CD	2.60	0.69
3:G:76:THR:HG22	4:H:2189:ARG:HG2	1.73	0.69
4:H:1190:GLY:O	4:H:1196:TRP:NE1	2.26	0.69
2:B:255:GLN:N	2:B:255:GLN:OE1	2.25	0.69
4:H:1907:ARG:NH1	4:H:1909:ASP:OD2	2.26	0.69
5:I:70:ILE:O	5:I:70:ILE:HG13	1.92	0.69
2:D:448:ASP:OD1	2:D:449:ALA:N	2.26	0.68
2:F:117:GLU:N	2:F:117:GLU:OE1	2.26	0.68
5:I:70:ILE:HD12	5:I:102:ILE:HA	1.72	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ARG:O	1:A:201:LYS:NZ	2.25	0.68
4:H:774:SER:OG	4:H:777:ASP:OD1	2.10	0.68
5:I:368:LEU:O	5:I:372:THR:OG1	2.10	0.68
1:A:263:LEU:HD12	1:A:263:LEU:O	1.93	0.68
5:I:117:LEU:O	5:I:118:HIS:ND1	2.27	0.68
1:A:270:GLU:HB2	1:A:275:LEU:HD23	1.77	0.67
4:H:1891:LEU:HD22	4:H:1934:ILE:HG22	1.75	0.67
1:C:49:CYS:SG	1:C:83:ILE:HD11	2.35	0.67
1:E:374:ILE:HG12	9:E:501:ADP:N1	2.08	0.67
6:K:213:LYS:HZ2	9:K:401:ADP:H1'	1.60	0.67
1:A:63:GLY:N	1:A:324:ALA:O	2.28	0.67
4:H:1734:ASP:OD1	4:H:1737:ARG:NH1	2.28	0.67
1:C:411:THR:HG1	1:C:412:PRO:HD3	1.60	0.67
5:I:388:GLU:OE1	5:I:388:GLU:N	2.28	0.67
3:G:76:THR:CG2	4:H:2190:GLU:OE1	2.42	0.66
4:H:1049:SER:OG	4:H:1099:CYS:SG	2.51	0.66
1:E:27:ASP:OD1	1:E:31:LEU:N	2.28	0.66
3:G:68:ALA:HB3	3:G:69:PRO:HD3	1.76	0.66
1:A:357:ARG:O	2:F:404:GLN:NE2	2.28	0.66
1:A:404:ARG:NH2	9:A:501:ADP:H4'	2.10	0.66
5:I:271:ASP:O	5:I:366:ARG:NH1	2.29	0.66
6:K:160:THR:HG23	6:K:180:LEU:O	1.95	0.66
2:D:390:LEU:HD21	2:D:406:ILE:HG13	1.78	0.66
1:E:117:ARG:NE	1:E:275:LEU:HD11	2.11	0.66
1:C:14:ARG:NH1	2:D:319:ASP:O	2.29	0.65
8:N:198:LYS:O	8:N:202:HIS:ND1	2.17	0.65
5:I:71:ASP:OD1	5:I:72:THR:N	2.29	0.65
5:J:21:TYR:HD2	9:J:502:ADP:H3'	1.61	0.65
2:F:47:VAL:HG13	2:F:370:ILE:CG2	2.26	0.65
2:D:390:LEU:HD21	2:D:406:ILE:CG1	2.27	0.65
1:C:33:LYS:O	1:C:46:ARG:NH2	2.30	0.65
4:H:1296:GLN:NE2	4:H:1333:ASN:O	2.30	0.65
5:I:21:TYR:HB3	9:I:501:ADP:H3'	1.78	0.65
3:G:95:TRP:O	6:K:121:GLN:NE2	2.30	0.65
5:J:353:GLY:HA3	9:J:502:ADP:H4'	1.78	0.65
3:G:176:ASP:O	5:J:190:GLN:NE2	2.30	0.64
1:A:374:ILE:HG12	9:A:501:ADP:C2	2.32	0.64
4:H:1936:SER:O	4:H:1937:THR:OG1	2.13	0.64
2:F:49:GLN:NE2	2:F:360:THR:O	2.30	0.64
6:K:283:MET:SD	6:K:290:ARG:NH2	2.72	0.63
1:E:113:MET:CG	1:E:275:LEU:HD21	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:21:TYR:HB3	9:I:501:ADP:H2'	1.81	0.63
1:E:374:ILE:HG23	9:E:501:ADP:N3	2.14	0.63
5:I:269:VAL:HG23	5:I:357:ILE:HG21	1.80	0.63
5:I:417:GLU:N	5:I:417:GLU:OE1	2.32	0.62
4:H:2021:GLN:OE1	4:H:2021:GLN:N	2.32	0.62
5:J:264:ALA:HB2	9:J:502:ADP:O2B	1.99	0.62
1:E:100:GLU:OE2	2:F:314:ARG:NH2	2.32	0.62
2:F:264:ASP:OD1	2:F:266:GLY:N	2.33	0.62
6:K:13:GLY:HA3	9:K:401:ADP:O2B	1.99	0.62
2:B:62:MET:SD	2:B:71:ARG:NE	2.73	0.62
4:H:2195:MET:SD	7:M:527:ARG:NE	2.72	0.62
1:C:374:ILE:HD11	9:C:501:ADP:C1'	2.29	0.62
5:I:170:LEU:HD21	5:I:325:VAL:CG1	2.29	0.61
2:D:247:ILE:HG23	2:D:267:GLU:OE1	1.99	0.61
4:H:2010:GLN:O	4:H:2010:GLN:NE2	2.33	0.61
5:J:43:MET:O	5:J:83:GLU:N	2.31	0.61
4:H:832:ARG:NH2	8:N:271:ASP:OD1	2.34	0.61
1:A:43:GLU:OE1	1:A:43:GLU:N	2.32	0.61
5:I:213:MET:SD	5:I:213:MET:N	2.74	0.61
1:E:209:TYR:CE1	8:N:286:VAL:HG22	2.36	0.61
2:D:136:GLU:OE1	2:D:235:ARG:NH2	2.34	0.60
2:D:253:ARG:NH2	4:H:1844:THR:OG1	2.34	0.60
1:A:162:LYS:O	1:A:205:ARG:NH2	2.34	0.60
5:I:70:ILE:HD12	5:I:102:ILE:CD1	2.31	0.60
2:B:362:TYR:OH	9:B:501:ADP:C5	2.55	0.60
1:A:233:GLU:N	1:A:233:GLU:OE1	2.34	0.60
1:E:14:ARG:NH2	2:F:321:ALA:O	2.35	0.60
4:H:738:GLN:N	4:H:738:GLN:OE1	2.34	0.60
4:H:1945:ASN:OD1	4:H:1946:LEU:N	2.35	0.60
1:A:201:LYS:O	4:H:1823:ARG:NH1	2.35	0.59
2:B:249:VAL:O	2:B:255:GLN:NE2	2.32	0.59
1:C:382:GLU:OE2	1:C:411:THR:CG2	2.50	0.59
2:F:286:GLU:OE1	2:F:286:GLU:N	2.35	0.59
5:I:21:TYR:CB	9:I:501:ADP:H3'	2.32	0.59
4:H:1784:CYS:SG	4:H:1794:ARG:NH1	2.76	0.58
2:D:240:HIS:ND1	4:H:1789:GLN:OE1	2.35	0.58
1:E:43:GLU:N	1:E:43:GLU:OE1	2.34	0.58
6:K:302:GLY:O	9:K:401:ADP:N3	2.35	0.58
1:A:111:VAL:O	1:A:115:ASN:ND2	2.36	0.58
1:C:39:LEU:HA	9:C:501:ADP:N1	2.19	0.58
2:D:305:ASP:OD1	2:D:306:ILE:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:HIS:HE1	9:C:501:ADP:O2'	1.86	0.58
3:G:72:LEU:H	3:G:72:LEU:HD23	1.67	0.58
2:F:213:ARG:NH1	2:F:214:ASP:OD1	2.37	0.58
1:A:75:GLY:HA2	9:A:501:ADP:O2A	2.04	0.58
1:A:134:GLU:N	1:A:160:GLY:O	2.34	0.57
1:C:42:GLN:NE2	1:C:364:MET:O	2.37	0.57
5:J:207:ARG:NH2	5:J:256:ASN:OD1	2.37	0.57
6:K:213:LYS:NZ	9:K:401:ADP:H1'	2.18	0.57
2:F:305:ASP:OD1	2:F:306:ILE:N	2.37	0.57
2:F:136:GLU:N	2:F:136:GLU:OE1	2.37	0.57
5:I:70:ILE:HD11	5:I:105:HIS:CB	2.34	0.57
4:H:1842:GLN:O	4:H:1843:THR:OG1	2.13	0.57
2:F:32:GLY:O	2:F:33:LEU:HD12	2.05	0.57
6:K:78:ASN:ND2	6:K:81:ASP:OD1	2.37	0.57
8:N:335:THR:OG1	8:N:347:GLU:O	2.11	0.57
2:B:237:GLU:OE1	2:B:237:GLU:N	2.38	0.57
1:C:43:GLU:N	1:C:43:GLU:OE1	2.36	0.57
2:F:27:HIS:NE2	9:F:501:ADP:N3	2.52	0.57
1:A:313:THR:HG21	2:F:303:MET:SD	2.45	0.56
2:F:416:ARG:NH1	2:F:425:ASP:OD1	2.37	0.56
8:N:306:THR:HG21	8:N:319:ILE:HG22	1.86	0.56
1:A:308:ASP:OD1	1:A:309:ILE:N	2.37	0.56
6:K:156:GLY:HA2	9:K:401:ADP:O1B	2.04	0.56
1:C:20:HIS:HE1	9:C:501:ADP:C2'	2.18	0.56
1:E:308:ASP:OD1	1:E:309:ILE:N	2.38	0.56
4:H:1086:LYS:NZ	4:H:1211:ILE:O	2.38	0.56
1:C:20:HIS:CE1	9:C:501:ADP:C2'	2.89	0.56
2:F:34:ASP:OD1	2:F:40:ARG:NE	2.31	0.56
1:E:18:HIS:HB3	9:E:501:ADP:H3'	1.87	0.56
1:C:76:LYS:HG2	9:C:501:ADP:O1B	2.06	0.56
4:H:1940:ARG:HD2	4:H:1942:THR:HG22	1.88	0.56
1:C:303:GLU:OE1	1:C:305:HIS:NE2	2.39	0.56
2:F:324:LEU:HD23	2:F:325:ILE:N	2.21	0.56
2:B:229:ASP:OD1	2:B:230:GLY:N	2.38	0.56
5:I:21:TYR:CD2	9:I:501:ADP:C3'	2.89	0.56
1:A:118:ARG:NE	2:B:270:SER:OG	2.39	0.56
2:D:188:GLN:N	2:D:191:ASP:OD2	2.39	0.55
5:J:81:ASN:O	5:J:245:GLN:NE2	2.39	0.55
1:A:302:ASP:OD1	1:A:303:GLU:N	2.39	0.55
2:F:246:GLU:OE1	4:H:1756:ARG:NH1	2.40	0.55
5:I:70:ILE:HD11	5:I:105:HIS:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:300:GLU:OE1	5:I:300:GLU:N	2.38	0.55
2:F:430:TYR:O	2:F:438:ARG:NH2	2.40	0.55
6:K:67:LEU:HD12	6:K:67:LEU:O	2.06	0.55
2:D:82:GLY:HA2	9:D:501:ADP:O1A	2.06	0.55
5:J:38:PRO:O	5:J:70:ILE:HD11	2.07	0.55
1:C:207:ASP:OD1	1:C:208:THR:N	2.39	0.55
1:E:209:TYR:HE1	8:N:286:VAL:HG22	1.71	0.55
5:I:174:ALA:HB3	9:I:501:ADP:C8	2.42	0.54
1:C:302:ASP:OD1	1:C:303:GLU:N	2.39	0.54
1:A:75:GLY:N	9:A:501:ADP:O3B	2.39	0.54
5:I:202:ILE:HD11	5:I:263:GLN:HB2	1.89	0.54
1:E:113:MET:CG	1:E:275:LEU:CD2	2.86	0.54
3:G:81:ARG:O	8:N:288:VAL:HG22	2.07	0.54
5:I:407:GLN:N	5:I:407:GLN:OE1	2.40	0.54
2:B:435:ASP:OD1	2:B:436:GLU:N	2.40	0.54
1:E:18:HIS:HB3	9:E:501:ADP:O3'	2.08	0.54
2:F:400:ARG:HH21	9:F:501:ADP:PA	2.28	0.54
1:C:411:THR:OG1	1:C:412:PRO:CD	2.46	0.54
3:G:240:GLN:NE2	4:H:2233:MET:SD	2.81	0.54
2:D:274:GLU:OE1	2:D:274:GLU:N	2.39	0.54
1:A:20:HIS:NE2	9:A:501:ADP:O2'	2.36	0.53
1:A:302:ASP:OD2	2:B:314:ARG:NE	2.41	0.53
1:E:18:HIS:CD2	9:E:501:ADP:H3'	2.43	0.53
6:K:196:ARG:NH1	6:K:253:GLU:OE2	2.40	0.53
2:B:133:GLU:N	2:B:133:GLU:OE1	2.42	0.53
2:B:268:ILE:HG22	2:B:271:GLU:HB2	1.89	0.53
1:E:68:LEU:HD13	1:E:79:LEU:HD11	1.89	0.53
3:G:149:ASP:OD1	3:G:150:ASP:N	2.41	0.53
2:D:82:GLY:N	9:D:501:ADP:O3A	2.41	0.53
5:I:21:TYR:CG	9:I:501:ADP:H3'	2.44	0.53
1:E:20:HIS:NE2	9:E:501:ADP:C2	2.76	0.53
1:E:28:GLU:OE1	1:E:28:GLU:N	2.40	0.53
1:E:33:LYS:O	1:E:46:ARG:NH2	2.41	0.53
5:I:390:ARG:NH1	9:I:501:ADP:O3'	2.42	0.53
1:C:75:GLY:HA2	9:C:501:ADP:O1A	2.08	0.53
6:K:302:GLY:HA3	9:K:401:ADP:H5'2	1.90	0.53
1:A:262:GLN:H	2:B:258:LEU:HD11	1.74	0.53
2:D:85:ALA:HB2	9:D:501:ADP:O1A	2.09	0.53
2:F:64:ARG:NH2	2:F:93:ALA:O	2.42	0.53
1:A:40:VAL:O	9:A:501:ADP:N6	2.42	0.53
2:D:32:GLY:O	2:D:53:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:ASP:OD1	1:E:228:VAL:N	2.42	0.53
2:F:362:TYR:HE2	9:F:501:ADP:HN61	1.57	0.53
1:C:40:VAL:N	9:C:501:ADP:N1	2.57	0.52
1:C:180:LEU:HD23	1:C:182:LYS:HZ2	1.74	0.52
2:D:400:ARG:CZ	9:D:501:ADP:H5'1	2.40	0.52
2:F:401:TYR:CE2	2:F:405:LEU:HD11	2.44	0.52
2:B:19:ILE:HG22	1:C:323:ILE:HG22	1.92	0.52
2:B:253:ARG:O	2:B:254:THR:OG1	2.22	0.52
4:H:1090:ILE:CD1	4:H:1210:LEU:HD11	2.39	0.52
1:E:113:MET:HG2	1:E:275:LEU:CD2	2.40	0.52
2:D:82:GLY:CA	9:D:501:ADP:O3A	2.57	0.52
4:H:1910:GLU:OE1	4:H:1910:GLU:N	2.42	0.52
6:K:213:LYS:NZ	9:K:401:ADP:C1'	2.72	0.52
4:H:2190:GLU:OE1	4:H:2190:GLU:N	2.41	0.52
1:A:389:GLU:OE1	1:A:389:GLU:N	2.38	0.52
5:I:20:SER:HG	9:I:501:ADP:HN61	1.56	0.52
5:J:99:PHE:CE2	5:J:103:LEU:HD11	2.45	0.52
1:C:423:ASP:OD1	1:C:424:SER:N	2.43	0.52
2:D:27:HIS:NE2	9:D:501:ADP:C2	2.78	0.52
2:F:247:ILE:HG22	2:F:276:ILE:HG13	1.90	0.52
2:F:424:ASP:OD1	2:F:425:ASP:N	2.42	0.52
3:G:260:GLU:OE1	4:H:748:ARG:NH2	2.43	0.52
4:H:1874:LEU:HD13	4:H:1881:VAL:HG22	1.90	0.52
2:D:399:LEU:HD23	9:D:501:ADP:C1'	2.40	0.52
2:F:370:ILE:HD11	2:F:399:LEU:CD2	2.39	0.52
2:B:119:LEU:HD21	2:B:312:LEU:HD21	1.92	0.51
2:B:134:GLU:OE1	2:B:134:GLU:N	2.43	0.51
5:I:390:ARG:HD2	9:I:501:ADP:O3'	2.10	0.51
5:J:71:ASP:OD1	5:J:72:THR:N	2.43	0.51
6:K:286:ASP:OD1	6:K:287:VAL:N	2.43	0.51
1:A:405:TYR:CE2	1:A:409:LEU:HD11	2.46	0.51
1:C:102:TYR:OH	1:C:308:ASP:OD1	2.25	0.51
6:K:13:GLY:CA	9:K:401:ADP:O2B	2.58	0.51
1:E:132:GLU:N	1:E:132:GLU:OE1	2.44	0.51
1:A:356:ASP:OD1	1:A:357:ARG:N	2.43	0.51
1:C:401:THR:O	1:C:402:THR:OG1	2.22	0.51
1:C:405:TYR:OH	1:C:437:PHE:O	2.28	0.51
1:C:123:ARG:NE	1:C:237:ASP:OD2	2.44	0.51
2:D:56:ALA:HB2	2:D:86:ILE:HD11	1.93	0.51
4:H:1091:ILE:HD11	4:H:1123:LEU:HD22	1.93	0.51
1:C:40:VAL:HG12	9:C:501:ADP:C2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:251:ASN:HB3	2:D:267:GLU:OE1	2.11	0.51
1:E:366:TYR:CE2	9:E:501:ADP:N7	2.79	0.51
1:A:404:ARG:NH2	9:A:501:ADP:O3'	2.38	0.51
1:C:353:ASP:OD1	1:C:354:LEU:N	2.43	0.50
4:H:1104:TRP:O	4:H:1107:HIS:NE2	2.44	0.50
1:C:40:VAL:HG12	9:C:501:ADP:N1	2.26	0.50
5:J:343:GLY:O	5:J:347:SER:OG	2.29	0.50
6:K:302:GLY:O	9:K:401:ADP:C2	2.65	0.50
1:A:105:GLU:OE1	1:A:105:GLU:N	2.41	0.50
2:B:250:ILE:HG22	4:H:1364:LEU:HD12	1.93	0.50
6:K:36:GLY:O	6:K:58:ALA:N	2.44	0.50
2:F:250:ILE:O	2:F:250:ILE:HG22	2.12	0.50
5:J:169:ILE:N	5:J:169:ILE:HD12	2.27	0.50
4:H:1960:ASN:N	4:H:1964:ASP:OD1	2.39	0.50
5:J:70:ILE:HG23	5:J:70:ILE:O	2.11	0.50
1:C:374:ILE:HD11	9:C:501:ADP:N9	2.26	0.50
2:D:331:GLY:O	2:D:344:HIS:N	2.40	0.50
4:H:1975:GLY:O	4:H:1980:ILE:HG21	2.12	0.50
6:K:178:LEU:HD21	6:K:180:LEU:HD11	1.93	0.50
5:I:275:ASP:OD1	5:I:276:GLU:N	2.44	0.50
6:K:180:LEU:O	6:K:180:LEU:HD12	2.12	0.50
5:I:333:VAL:HG11	5:I:345:TYR:CZ	2.46	0.49
2:D:49:GLN:NE2	2:D:360:THR:O	2.43	0.49
2:F:170:THR:HG23	8:N:302:ARG:H	1.77	0.49
2:F:250:ILE:HD11	4:H:1756:ARG:HG3	1.94	0.49
5:J:329:VAL:O	5:J:333:VAL:HG23	2.11	0.49
1:E:56:ILE:HD13	1:E:298:VAL:HG21	1.94	0.49
1:E:113:MET:SD	1:E:275:LEU:HD21	2.53	0.49
2:B:29:ARG:NH2	2:B:377:GLU:OE1	2.44	0.49
2:B:45:GLY:O	9:B:501:ADP:C2	2.65	0.49
5:I:21:TYR:HD2	9:I:501:ADP:O3'	1.95	0.49
5:I:174:ALA:HB2	9:I:501:ADP:H5'1	1.94	0.49
2:B:145:ILE:HG22	2:B:146:GLN:N	2.26	0.49
1:E:79:LEU:HD12	1:E:80:ALA:N	2.27	0.49
8:N:282:ARG:NH1	8:N:283:PRO:O	2.46	0.49
1:E:117:ARG:HG3	1:E:275:LEU:HD11	1.95	0.49
2:F:408:ALA:HB3	2:F:429:VAL:HG11	1.93	0.49
3:G:69:PRO:N	3:G:70:PRO:CD	2.76	0.49
6:K:302:GLY:HA3	9:K:401:ADP:C5'	2.42	0.49
1:C:374:ILE:CD1	9:C:501:ADP:H1'	2.36	0.49
4:H:1162:TYR:OH	4:H:1183:ASP:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:24:ARG:NH2	9:I:501:ADP:HO2'	2.06	0.49
1:E:173:ASP:O	1:E:176:ILE:HG22	2.13	0.49
4:H:841:ILE:HD13	5:I:403:LEU:HD11	1.94	0.49
6:K:282:ILE:HG21	6:K:294:TYR:CZ	2.48	0.49
2:B:45:GLY:O	9:B:501:ADP:H2	1.96	0.48
1:C:255:ASP:OD1	1:C:258:SER:N	2.42	0.48
2:D:260:LEU:O	1:E:271:ILE:HG22	2.12	0.48
1:E:142:GLU:OE2	4:H:2160:TRP:NE1	2.45	0.48
2:D:117:GLU:OE1	2:D:121:GLN:NE2	2.47	0.48
1:A:131:TYR:N	1:A:193:ILE:O	2.44	0.48
2:D:21:ARG:HB2	1:E:62:ALA:HB2	1.94	0.48
1:A:66:VAL:O	1:A:329:PHE:N	2.43	0.48
5:J:182:VAL:HG12	5:J:187:VAL:HG22	1.95	0.48
1:A:426:GLU:N	1:A:426:GLU:OE1	2.47	0.48
4:H:1898:LEU:O	4:H:1902:TYR:N	2.46	0.48
5:I:169:ILE:HD12	5:I:169:ILE:N	2.28	0.48
2:B:129:VAL:HG22	2:B:291:ILE:HG22	1.96	0.48
2:F:178:MET:O	2:F:182:LEU:HD23	2.14	0.48
1:C:176:ILE:O	1:C:176:ILE:HG22	2.14	0.48
1:C:315:LEU:HD21	1:C:329:PHE:CZ	2.48	0.48
3:G:164:SER:HA	3:G:174:ILE:HD11	1.96	0.48
5:I:353:GLY:HA3	9:I:501:ADP:C4'	2.42	0.48
2:F:264:ASP:OD1	2:F:265:THR:N	2.46	0.47
5:I:21:TYR:HD2	9:I:501:ADP:C3'	2.26	0.47
2:B:145:ILE:HG22	2:B:146:GLN:H	1.79	0.47
1:E:374:ILE:HG23	9:E:501:ADP:C2	2.50	0.47
1:C:105:GLU:N	1:C:105:GLU:OE1	2.47	0.47
1:A:273:ASP:OD1	1:A:274:LYS:N	2.47	0.47
2:B:362:TYR:CE2	9:B:501:ADP:N7	2.82	0.47
5:I:170:LEU:HD21	5:I:325:VAL:HG13	1.94	0.47
1:E:18:HIS:HD2	9:E:501:ADP:H5'2	1.80	0.47
3:G:123:ASP:OD1	3:G:124:TYR:N	2.46	0.47
2:B:424:ASP:OD1	2:B:425:ASP:N	2.48	0.47
1:E:39:LEU:CD1	9:E:501:ADP:C6	2.96	0.47
4:H:1799:ILE:O	4:H:1799:ILE:HG22	2.15	0.47
2:D:370:ILE:HG23	9:D:501:ADP:C2	2.50	0.47
2:D:381:GLU:N	2:D:381:GLU:OE1	2.48	0.47
2:B:161:LEU:HD13	2:B:182:LEU:HD13	1.97	0.47
2:B:301:VAL:HG21	2:B:326:MET:SD	2.55	0.47
1:C:76:LYS:HG2	9:C:501:ADP:PB	2.54	0.47
1:C:122:LEU:N	1:C:238:VAL:O	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:1273:LYS:O	4:H:1276:VAL:HG22	2.14	0.47
1:C:76:LYS:CG	9:C:501:ADP:O1B	2.63	0.47
1:E:18:HIS:O	1:E:18:HIS:ND1	2.46	0.47
1:E:186:GLU:OE1	1:E:186:GLU:N	2.41	0.47
4:H:2237:THR:HG23	4:H:2237:THR:O	2.15	0.47
6:K:37:ARG:O	6:K:66:THR:OG1	2.30	0.47
1:A:190:VAL:C	1:A:191:ILE:HD12	2.35	0.47
1:C:204:GLY:O	1:C:205:ARG:NE	2.43	0.47
5:I:174:ALA:CB	9:I:501:ADP:C8	2.97	0.47
1:A:404:ARG:HH21	9:A:501:ADP:H4'	1.80	0.46
2:B:34:ASP:OD1	2:B:40:ARG:NE	2.47	0.46
5:J:337:ASP:OD1	5:J:338:ILE:N	2.48	0.46
1:A:159:ILE:HB	1:A:170:LEU:HD11	1.97	0.46
2:B:119:LEU:HD21	2:B:312:LEU:CD2	2.45	0.46
8:N:349:LEU:N	8:N:350:PRO:HD2	2.30	0.46
2:F:26:SER:O	2:F:29:ARG:NH1	2.47	0.46
2:F:309:PHE:CZ	2:F:346:ILE:HG22	2.50	0.46
4:H:1781:LEU:O	4:H:1783:ARG:NH1	2.45	0.46
5:I:21:TYR:CD2	9:I:501:ADP:O3'	2.68	0.46
5:J:178:THR:HG22	5:J:180:ILE:HG13	1.97	0.46
5:J:354:ASN:O	5:J:357:ILE:HG12	2.14	0.46
2:F:317:GLU:OE2	2:F:353:ARG:NH1	2.48	0.46
1:C:271:ILE:HG23	1:C:274:LYS:H	1.80	0.46
4:H:1090:ILE:HD12	4:H:1210:LEU:HD11	1.97	0.46
6:K:270:GLU:N	6:K:270:GLU:OE1	2.48	0.46
2:D:61:GLU:OE1	2:D:64:ARG:NH2	2.45	0.46
2:D:400:ARG:NH2	9:D:501:ADP:H5'1	2.31	0.46
6:K:205:GLU:O	6:K:209:VAL:HG23	2.16	0.46
1:C:257:LEU:HD13	4:H:1829:LEU:HD23	1.96	0.46
5:I:269:VAL:HG23	5:I:357:ILE:CG2	2.44	0.46
5:J:200:ASP:OD1	5:J:201:PHE:N	2.49	0.46
6:K:287:VAL:HG12	6:K:288:ASP:N	2.31	0.46
1:A:246:ALA:O	1:A:251:GLN:NE2	2.49	0.46
1:C:343:ASP:OD1	1:C:344:ILE:N	2.49	0.46
4:H:2200:GLU:O	7:M:522:LYS:NZ	2.49	0.46
5:I:180:ILE:HG23	5:I:187:VAL:HG13	1.98	0.46
6:K:305:MET:CB	9:K:401:ADP:N1	2.71	0.46
1:A:405:TYR:CZ	1:A:409:LEU:HD11	2.50	0.45
2:B:370:ILE:HG21	2:B:399:LEU:HD21	1.98	0.45
4:H:1889:LEU:HD22	4:H:1889:LEU:H	1.81	0.45
5:J:387:VAL:HG12	5:J:387:VAL:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:357:LEU:HD23	8:N:359:GLN:N	2.31	0.45
3:G:232:ARG:NH2	7:M:406:ARG:O	2.49	0.45
4:H:785:TRP:NE1	7:M:459:VAL:O	2.49	0.45
4:H:1940:ARG:O	4:H:1941:THR:OG1	2.30	0.45
2:B:47:VAL:H	9:B:501:ADP:HN62	1.65	0.45
1:E:408:GLN:O	2:F:71:ARG:NH2	2.50	0.45
1:E:265:LYS:N	1:E:266:PRO:CD	2.80	0.45
5:I:350:VAL:O	5:I:389:ARG:NH1	2.45	0.45
6:K:156:GLY:CA	9:K:401:ADP:O1B	2.65	0.45
2:B:274:GLU:OE1	2:B:274:GLU:N	2.38	0.44
5:J:176:HIS:HE1	9:J:502:ADP:N6	2.14	0.44
1:A:39:LEU:HA	9:A:501:ADP:N1	2.32	0.44
2:B:430:TYR:O	2:B:438:ARG:NH1	2.51	0.44
1:E:401:THR:OG1	1:E:402:THR:N	2.50	0.44
4:H:1950:ASP:HB3	4:H:1980:ILE:HG22	1.99	0.44
5:I:128:ASN:ND2	5:I:129:THR:O	2.51	0.44
5:I:170:LEU:N	5:I:349:ILE:O	2.46	0.44
1:C:310:GLU:OE1	1:C:310:GLU:N	2.44	0.44
2:F:405:LEU:CD2	2:F:429:VAL:HG12	2.48	0.44
4:H:2007:VAL:HG12	4:H:2008:ALA:N	2.32	0.44
5:I:269:VAL:HG22	5:I:305:PRO:HB3	1.98	0.44
8:N:349:LEU:N	8:N:350:PRO:CD	2.80	0.44
5:I:202:ILE:HG22	5:I:304:ILE:CG2	2.45	0.44
5:J:226:LYS:NZ	6:K:319:ALA:O	2.49	0.44
6:K:23:GLY:N	6:K:344:SER:OG	2.50	0.44
7:M:447:VAL:HB	7:M:448:PRO:HD3	1.99	0.44
1:E:18:HIS:HD2	9:E:501:ADP:H3'	1.83	0.44
4:H:1217:ASN:O	4:H:1218:THR:OG1	2.30	0.44
5:J:41:ILE:HG22	5:J:70:ILE:HB	1.99	0.44
7:M:407:LYS:NZ	7:M:408:ALA:O	2.51	0.44
2:B:22:ILE:HD12	2:B:22:ILE:N	2.32	0.44
2:B:250:ILE:HD11	4:H:1360:ILE:O	2.18	0.44
2:D:107:GLU:OE2	1:E:317:ARG:NH2	2.49	0.44
1:E:396:GLU:O	1:E:399:THR:OG1	2.28	0.44
2:F:348:ILE:HD13	2:F:351:LEU:HD12	2.00	0.44
2:B:108:ILE:HD13	2:B:304:LEU:HD22	1.99	0.44
1:C:205:ARG:HB3	1:C:221:VAL:HG22	1.99	0.44
2:D:251:ASN:OD1	2:D:252:SER:N	2.50	0.44
5:J:223:ILE:N	5:J:223:ILE:HD12	2.33	0.44
1:A:76:LYS:HG2	9:A:501:ADP:PB	2.58	0.44
1:A:326:ILE:HD12	1:A:326:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:358:GLN:O	5:I:359:SER:OG	2.35	0.44
2:D:313:ASN:ND2	2:D:349:ASP:OD2	2.51	0.43
6:K:157:ASP:OD1	9:K:401:ADP:C5'	2.33	0.43
7:M:432:GLY:C	7:M:433:LEU:HD23	2.39	0.43
1:A:24:LEU:HD21	1:A:49:CYS:CB	2.48	0.43
2:B:249:VAL:O	2:B:249:VAL:HG12	2.17	0.43
1:C:75:GLY:HA2	9:C:501:ADP:O3A	2.18	0.43
2:D:83:LYS:H	9:D:501:ADP:PB	2.41	0.43
4:H:1265:GLN:N	4:H:1266:PRO:HD2	2.33	0.43
4:H:1799:ILE:N	4:H:1800:PRO:HD3	2.33	0.43
7:M:416:HIS:O	7:M:416:HIS:ND1	2.50	0.43
1:C:172:LEU:HD21	1:C:176:ILE:HG21	2.00	0.43
1:E:20:HIS:HE1	9:E:501:ADP:O2'	2.01	0.43
5:I:77:VAL:HG23	5:I:77:VAL:O	2.18	0.43
1:C:20:HIS:CE1	9:C:501:ADP:H2'	2.53	0.43
1:C:138:LEU:HD12	1:C:159:ILE:HG22	2.00	0.43
2:D:63:ILE:HD13	2:D:295:VAL:HG21	2.00	0.43
4:H:1789:GLN:O	4:H:1794:ARG:NH2	2.52	0.43
6:K:282:ILE:HG21	6:K:294:TYR:CE2	2.54	0.43
8:N:306:THR:HG22	8:N:323:TYR:HB2	2.01	0.43
1:A:404:ARG:NH2	9:A:501:ADP:C4'	2.79	0.43
2:B:180:GLU:OE1	2:B:180:GLU:N	2.41	0.43
2:D:127:ILE:CG2	2:D:291:ILE:HD11	2.48	0.43
2:D:247:ILE:HG21	2:D:267:GLU:CD	2.27	0.43
4:H:1046:ASN:ND2	4:H:1064:ASP:OD1	2.51	0.43
6:K:214:GLU:HB2	9:K:401:ADP:N6	2.34	0.43
8:N:357:LEU:HD23	8:N:359:GLN:H	1.83	0.43
1:A:26:LEU:HD12	1:A:30:GLY:O	2.18	0.43
3:G:153:THR:HG23	3:G:156:GLU:H	1.84	0.43
6:K:374:CYS:SG	6:K:375:PHE:N	2.91	0.43
1:C:326:ILE:HD12	1:C:326:ILE:N	2.34	0.43
4:H:1731:TYR:CE2	4:H:1735:LEU:HD11	2.54	0.43
5:I:41:ILE:N	5:I:85:ILE:O	2.45	0.43
5:J:334:GLY:O	5:J:341:ARG:NH2	2.52	0.43
1:A:323:ILE:HG22	2:F:19:ILE:HG22	2.01	0.43
2:F:141:GLU:N	2:F:164:LYS:O	2.51	0.43
2:F:306:ILE:HD13	2:F:338:THR:CG2	2.49	0.43
4:H:1947:VAL:HG11	4:H:1950:ASP:OD1	2.18	0.43
5:I:151:LEU:N	5:I:151:LEU:HD23	2.33	0.43
5:J:156:VAL:HG23	5:J:187:VAL:HG23	2.00	0.43
2:F:205:LEU:HD12	2:F:225:VAL:HB	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:1199:VAL:HG12	4:H:1199:VAL:O	2.19	0.43
5:I:73:ASN:O	5:I:77:VAL:HG22	2.19	0.43
1:A:40:VAL:H	9:A:501:ADP:N6	2.16	0.42
1:C:315:LEU:HD23	1:C:354:LEU:HD11	2.00	0.42
5:I:20:SER:CB	9:I:501:ADP:N7	2.71	0.42
1:A:42:GLN:HG3	1:A:45:ALA:HB3	2.00	0.42
1:A:135:VAL:CG2	1:A:191:ILE:HD13	2.48	0.42
1:A:170:LEU:C	1:A:170:LEU:HD12	2.39	0.42
2:D:174:LEU:HD13	2:D:182:LEU:HD12	2.01	0.42
2:D:355:LEU:HD12	2:D:355:LEU:O	2.18	0.42
1:E:144:GLU:OE1	1:E:145:ASN:N	2.52	0.42
1:C:189:ASP:OD1	1:C:190:VAL:N	2.53	0.42
5:I:21:TYR:HB3	9:I:501:ADP:C2'	2.47	0.42
5:I:21:TYR:HB3	9:I:501:ADP:C3'	2.46	0.42
6:K:213:LYS:HZ2	9:K:401:ADP:C1'	2.26	0.42
1:C:40:VAL:H	9:C:501:ADP:HN62	1.67	0.42
1:E:40:VAL:H	9:E:501:ADP:HN62	1.67	0.42
2:F:137:ILE:HD13	2:F:196:ASP:HB3	2.00	0.42
7:M:427:SER:O	7:M:431:GLY:N	2.46	0.42
2:B:33:LEU:O	2:B:40:ARG:NH2	2.53	0.42
1:E:256:ILE:O	1:E:256:ILE:HG22	2.19	0.42
5:I:175:THR:OG1	9:I:501:ADP:N6	2.52	0.42
1:C:28:GLU:OE1	1:C:28:GLU:N	2.45	0.42
2:D:209:PHE:HZ	8:N:218:THR:HG1	1.67	0.42
2:F:400:ARG:NH2	9:F:501:ADP:PA	2.91	0.42
3:G:78:GLN:OE1	3:G:79:GLY:N	2.52	0.42
2:B:303:MET:HG3	1:C:313:THR:HG21	2.01	0.42
1:C:180:LEU:CG	1:C:181:GLN:N	2.67	0.42
3:G:76:THR:HG21	4:H:2190:GLU:CD	2.39	0.42
4:H:1107:HIS:N	4:H:1156:HIS:O	2.50	0.42
4:H:2226:LEU:HD13	4:H:2226:LEU:O	2.20	0.42
5:I:317:LEU:N	5:I:317:LEU:HD23	2.35	0.42
6:K:219:VAL:HG23	6:K:306:TYR:HB3	2.02	0.42
1:A:24:LEU:HD21	1:A:49:CYS:HB2	2.00	0.42
3:G:114:TRP:NE1	6:K:117:GLU:OE1	2.48	0.42
5:I:103:LEU:HD23	5:I:144:TYR:CE1	2.54	0.42
1:A:33:LYS:O	1:A:46:ARG:NH1	2.53	0.42
2:D:409:ALA:HB1	2:D:421:VAL:HG11	2.02	0.42
6:K:303:THR:HG22	6:K:303:THR:O	2.19	0.42
2:F:23:GLY:O	2:F:374:ARG:NH2	2.52	0.42
3:G:80:TYR:O	3:G:84:LYS:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:247:ILE:HG23	2:D:272:VAL:HG11	2.02	0.41
3:G:174:ILE:O	3:G:178:TYR:N	2.52	0.41
5:I:158:THR:O	5:I:162:ASN:ND2	2.43	0.41
5:J:24:ARG:NH1	9:J:502:ADP:O2'	2.53	0.41
2:D:253:ARG:NH2	4:H:1843:THR:O	2.53	0.41
2:F:210:THR:O	2:F:210:THR:HG22	2.20	0.41
1:C:333:ARG:HH22	2:D:306:ILE:HD11	1.85	0.41
2:D:49:GLN:HG3	2:D:52:ALA:HB3	2.02	0.41
2:D:329:ASN:O	2:D:329:ASN:ND2	2.54	0.41
1:A:27:ASP:OD1	1:A:31:LEU:N	2.54	0.41
2:D:82:GLY:HA2	9:D:501:ADP:PA	2.60	0.41
2:D:416:ARG:NH2	2:D:422:GLN:OE1	2.53	0.41
5:I:70:ILE:HD11	5:I:105:HIS:HB2	2.02	0.41
5:I:171:ASP:OD1	5:I:172:SER:N	2.54	0.41
1:A:109:THR:HG1	2:F:106:SER:HG	1.59	0.41
2:B:249:VAL:O	2:B:250:ILE:HD13	2.21	0.41
2:D:121:GLN:NE2	2:D:265:THR:OG1	2.54	0.41
2:D:338:THR:OG1	2:D:339:SER:N	2.52	0.41
4:H:846:SER:OG	8:N:205:ARG:NH2	2.53	0.41
5:I:151:LEU:HD23	5:I:151:LEU:H	1.84	0.41
1:C:75:GLY:HA3	9:C:501:ADP:C8	2.56	0.41
1:C:76:LYS:N	9:C:501:ADP:O1B	2.54	0.41
2:D:247:ILE:HG23	2:D:272:VAL:CG1	2.51	0.41
1:E:265:LYS:O	1:E:267:LYS:N	2.49	0.41
3:G:72:LEU:HD21	4:H:796:TRP:HB2	2.02	0.41
4:H:1090:ILE:HD11	4:H:1210:LEU:HD11	2.02	0.41
5:I:387:VAL:HG22	5:I:387:VAL:O	2.21	0.41
2:F:83:LYS:NZ	2:F:329:ASN:OD1	2.44	0.41
4:H:1077:ILE:HG13	4:H:1229:LEU:HD11	2.03	0.41
4:H:1777:LEU:N	4:H:1777:LEU:HD22	2.36	0.41
4:H:2008:ALA:O	4:H:2012:ASN:OD1	2.38	0.41
8:N:303:ASP:HB3	8:N:306:THR:HG1	1.86	0.41
2:B:27:HIS:HE1	9:B:501:ADP:O2'	2.04	0.41
2:D:180:GLU:O	2:D:183:THR:OG1	2.32	0.41
6:K:178:LEU:CD2	6:K:180:LEU:HD11	2.51	0.41
2:D:390:LEU:HD21	2:D:406:ILE:HG12	2.02	0.41
2:F:63:ILE:HD13	2:F:295:VAL:CG2	2.51	0.40
3:G:237:THR:OG1	3:G:238:PRO:HD3	2.21	0.40
1:C:411:THR:HG21	2:D:71:ARG:HH21	1.86	0.40
5:J:108:LYS:HG2	5:J:109:MET:CE	2.52	0.40
5:J:269:VAL:HG22	5:J:305:PRO:CB	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:237:THR:O	3:G:241:VAL:HG23	2.22	0.40
4:H:1912:ALA:O	4:H:1917:ARG:NE	2.54	0.40
5:I:414:GLN:OE1	5:I:414:GLN:N	2.54	0.40
6:K:190:MET:HG3	6:K:209:VAL:HG11	2.04	0.40
8:N:305:VAL:HG11	8:N:358:ARG:HG2	2.03	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	422/456 (92%)	410 (97%)	12 (3%)	0	100	100
1	C	410/456 (90%)	394 (96%)	16 (4%)	0	100	100
1	E	433/456 (95%)	419 (97%)	14 (3%)	0	100	100
2	B	391/463 (84%)	374 (96%)	17 (4%)	0	100	100
2	D	423/463 (91%)	406 (96%)	17 (4%)	0	100	100
2	F	411/463 (89%)	398 (97%)	13 (3%)	0	100	100
3	G	197/467 (42%)	187 (95%)	10 (5%)	0	100	100
4	H	829/3123 (26%)	792 (96%)	37 (4%)	0	100	100
5	I	341/429 (80%)	326 (96%)	15 (4%)	0	100	100
5	J	399/429 (93%)	377 (94%)	22 (6%)	0	100	100
6	K	346/375 (92%)	335 (97%)	11 (3%)	0	100	100
7	M	102/813 (12%)	97 (95%)	5 (5%)	0	100	100
8	N	144/364 (40%)	129 (90%)	15 (10%)	0	100	100
All	All	4848/8757 (55%)	4644 (96%)	204 (4%)	0	100	100

There are no Ramachandran outliers to report.



### 5.3.2 Protein sidechains [i](#)

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	360/387 (93%)	359 (100%)	1 (0%)	92	96
1	C	353/387 (91%)	348 (99%)	5 (1%)	67	86
1	E	367/387 (95%)	363 (99%)	4 (1%)	73	88
2	B	338/390 (87%)	338 (100%)	0	100	100
2	D	359/390 (92%)	352 (98%)	7 (2%)	57	81
2	F	352/390 (90%)	351 (100%)	1 (0%)	92	96
3	G	179/400 (45%)	177 (99%)	2 (1%)	73	88
4	H	751/2634 (28%)	745 (99%)	6 (1%)	81	93
5	I	299/364 (82%)	295 (99%)	4 (1%)	69	87
5	J	343/364 (94%)	339 (99%)	4 (1%)	71	88
6	K	297/318 (93%)	297 (100%)	0	100	100
7	M	91/718 (13%)	90 (99%)	1 (1%)	73	88
8	N	130/312 (42%)	127 (98%)	3 (2%)	50	78
All	All	4219/7441 (57%)	4181 (99%)	38 (1%)	79	91

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	LEU
1	C	201	LYS
1	C	205	ARG
1	C	264	MET
1	C	274	LYS
1	C	378	ARG
2	D	21	ARG
2	D	88	MET
2	D	269	LYS
2	D	355	LEU
2	D	400	ARG
2	D	428	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	D	444	LYS
1	E	18	HIS
1	E	184	ARG
1	E	249	ARG
1	E	316	HIS
2	F	257	PHE
3	G	66	LYS
3	G	226	ARG
4	H	776	TRP
4	H	1200	PHE
4	H	1749	TRP
4	H	1928	ARG
4	H	1976	ARG
4	H	2010	GLN
5	I	130	ARG
5	I	204	MET
5	I	210	PHE
5	I	213	MET
5	J	22	THR
5	J	230	ARG
5	J	302	LEU
5	J	363	ARG
7	M	433	LEU
8	N	181	GLU
8	N	282	ARG
8	N	314	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	18	HIS
2	B	49	GLN
2	B	302	HIS
1	C	20	HIS
2	D	121	GLN
2	D	302	HIS
1	E	42	GLN
1	E	115	ASN
1	E	241	HIS
1	E	254	GLN
1	E	373	GLN
2	F	27	HIS

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Mol	Chain	Res	Type
2	F	226	GLN
4	H	738	GLN
4	H	792	GLN
4	H	1206	GLN
4	H	1261	HIS
4	H	1858	GLN
4	H	2010	GLN
4	H	2179	GLN
5	I	128	ASN
5	I	205	GLN
5	I	383	ASN
5	J	190	GLN
5	J	251	HIS
6	K	12	ASN
6	K	88	HIS
6	K	92	ASN

### 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](#)

9 ligands are modelled in this entry.

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
9	ADP	B	501	-	24,29,29	1.03	2 (8%)	29,45,45	1.47	3 (10%)
9	ADP	C	501	-	24,29,29	0.93	1 (4%)	29,45,45	1.61	4 (13%)
9	ADP	J	502	-	24,29,29	0.95	1 (4%)	29,45,45	1.40	5 (17%)
9	ADP	E	501	-	24,29,29	1.01	1 (4%)	29,45,45	1.56	6 (20%)
9	ADP	D	501	-	24,29,29	0.98	1 (4%)	29,45,45	1.55	4 (13%)
9	ADP	A	501	-	24,29,29	0.93	1 (4%)	29,45,45	1.59	5 (17%)
9	ADP	I	501	-	24,29,29	1.08	2 (8%)	29,45,45	1.52	4 (13%)
9	ADP	K	401	-	24,29,29	0.96	1 (4%)	29,45,45	1.64	5 (17%)
9	ADP	F	501	-	24,29,29	1.08	2 (8%)	29,45,45	1.70	5 (17%)

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
9	ADP	B	501	-	-	5/12/32/32	0/3/3/3
9	ADP	C	501	-	-	3/12/32/32	0/3/3/3
9	ADP	J	502	-	-	4/12/32/32	0/3/3/3
9	ADP	E	501	-	-	6/12/32/32	0/3/3/3
9	ADP	D	501	-	-	5/12/32/32	0/3/3/3
9	ADP	A	501	-	-	5/12/32/32	0/3/3/3
9	ADP	I	501	-	-	4/12/32/32	0/3/3/3
9	ADP	K	401	-	-	4/12/32/32	0/3/3/3
9	ADP	F	501	-	-	4/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	501	ADP	C5-C4	3.03	1.49	1.40
9	B	501	ADP	C5-C4	2.74	1.48	1.40
9	I	501	ADP	C5-C4	2.74	1.48	1.40
9	C	501	ADP	C5-C4	2.58	1.47	1.40
9	D	501	ADP	C5-C4	2.50	1.47	1.40
9	A	501	ADP	C5-C4	2.46	1.47	1.40
9	J	502	ADP	C5-C4	2.45	1.47	1.40
9	K	401	ADP	C5-C4	2.45	1.47	1.40
9	E	501	ADP	C5-C4	2.39	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	501	ADP	C2-N3	2.06	1.35	1.32
9	F	501	ADP	O4'-C1'	2.01	1.43	1.41
9	B	501	ADP	O4'-C1'	2.00	1.43	1.41

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	501	ADP	C4-C5-N7	-4.58	104.62	109.40
9	D	501	ADP	PA-O3A-PB	-4.47	117.50	132.83
9	C	501	ADP	PA-O3A-PB	-4.17	118.51	132.83
9	K	401	ADP	PA-O3A-PB	-4.00	119.10	132.83
9	B	501	ADP	C4-C5-N7	-3.97	105.26	109.40
9	A	501	ADP	PA-O3A-PB	-3.92	119.39	132.83
9	E	501	ADP	PA-O3A-PB	-3.91	119.40	132.83
9	F	501	ADP	PA-O3A-PB	-3.86	119.57	132.83
9	I	501	ADP	C3'-C2'-C1'	3.58	106.36	100.98
9	B	501	ADP	PA-O3A-PB	-3.52	120.76	132.83
9	I	501	ADP	PA-O3A-PB	-3.37	121.28	132.83
9	K	401	ADP	C4-C5-N7	-3.36	105.90	109.40
9	E	501	ADP	N3-C2-N1	-3.28	123.55	128.68
9	A	501	ADP	N3-C2-N1	-3.18	123.71	128.68
9	A	501	ADP	C3'-C2'-C1'	3.17	105.74	100.98
9	C	501	ADP	N3-C2-N1	-3.10	123.83	128.68
9	J	502	ADP	N3-C2-N1	-3.08	123.87	128.68
9	J	502	ADP	PA-O3A-PB	-3.06	122.31	132.83
9	F	501	ADP	C3'-C2'-C1'	3.04	105.56	100.98
9	D	501	ADP	C4-C5-N7	-2.94	106.33	109.40
9	D	501	ADP	N3-C2-N1	-2.94	124.08	128.68
9	I	501	ADP	N3-C2-N1	-2.85	124.23	128.68
9	B	501	ADP	N3-C2-N1	-2.81	124.28	128.68
9	K	401	ADP	O3'-C3'-C4'	-2.81	102.93	111.05
9	C	501	ADP	C3'-C2'-C1'	2.74	105.11	100.98
9	K	401	ADP	N3-C2-N1	-2.72	124.42	128.68
9	I	501	ADP	C4-C5-N7	-2.69	106.59	109.40
9	E	501	ADP	C5'-C4'-C3'	-2.69	105.10	115.18
9	J	502	ADP	C3'-C2'-C1'	2.69	105.02	100.98
9	D	501	ADP	C3'-C2'-C1'	2.60	104.89	100.98
9	J	502	ADP	C4-C5-N7	-2.53	106.77	109.40
9	A	501	ADP	C4-C5-N7	-2.44	106.85	109.40
9	F	501	ADP	N3-C2-N1	-2.44	124.87	128.68
9	J	502	ADP	C2'-C3'-C4'	2.38	107.28	102.64
9	C	501	ADP	C4-C5-N7	-2.31	106.99	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	501	ADP	C4-C5-N7	-2.31	106.99	109.40
9	E	501	ADP	C2'-C3'-C4'	2.30	107.11	102.64
9	F	501	ADP	C5-C6-N6	2.18	123.66	120.35
9	E	501	ADP	C3'-C2'-C1'	2.17	104.24	100.98
9	K	401	ADP	O3B-PB-O2B	2.03	115.39	107.64
9	A	501	ADP	C2-N1-C6	2.01	122.20	118.75

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	501	ADP	O4'-C4'-C5'-O5'
9	B	501	ADP	C5'-O5'-PA-O1A
9	B	501	ADP	C5'-O5'-PA-O2A
9	C	501	ADP	C5'-O5'-PA-O1A
9	C	501	ADP	C5'-O5'-PA-O2A
9	D	501	ADP	C5'-O5'-PA-O3A
9	E	501	ADP	C5'-O5'-PA-O1A
9	E	501	ADP	C5'-O5'-PA-O2A
9	E	501	ADP	O4'-C4'-C5'-O5'
9	F	501	ADP	C5'-O5'-PA-O3A
9	I	501	ADP	C5'-O5'-PA-O2A
9	I	501	ADP	C5'-O5'-PA-O3A
9	J	502	ADP	C5'-O5'-PA-O3A
9	K	401	ADP	C5'-O5'-PA-O1A
9	K	401	ADP	C5'-O5'-PA-O2A
9	D	501	ADP	O4'-C4'-C5'-O5'
9	D	501	ADP	C3'-C4'-C5'-O5'
9	E	501	ADP	C3'-C4'-C5'-O5'
9	F	501	ADP	O4'-C4'-C5'-O5'
9	F	501	ADP	C3'-C4'-C5'-O5'
9	I	501	ADP	PA-O3A-PB-O3B
9	J	502	ADP	PA-O3A-PB-O3B
9	A	501	ADP	C5'-O5'-PA-O3A
9	D	501	ADP	C5'-O5'-PA-O1A
9	F	501	ADP	C5'-O5'-PA-O1A
9	J	502	ADP	C5'-O5'-PA-O2A
9	D	501	ADP	C4'-C5'-O5'-PA
9	B	501	ADP	O4'-C4'-C5'-O5'
9	E	501	ADP	PB-O3A-PA-O2A
9	A	501	ADP	C3'-C4'-C5'-O5'
9	K	401	ADP	O4'-C4'-C5'-O5'

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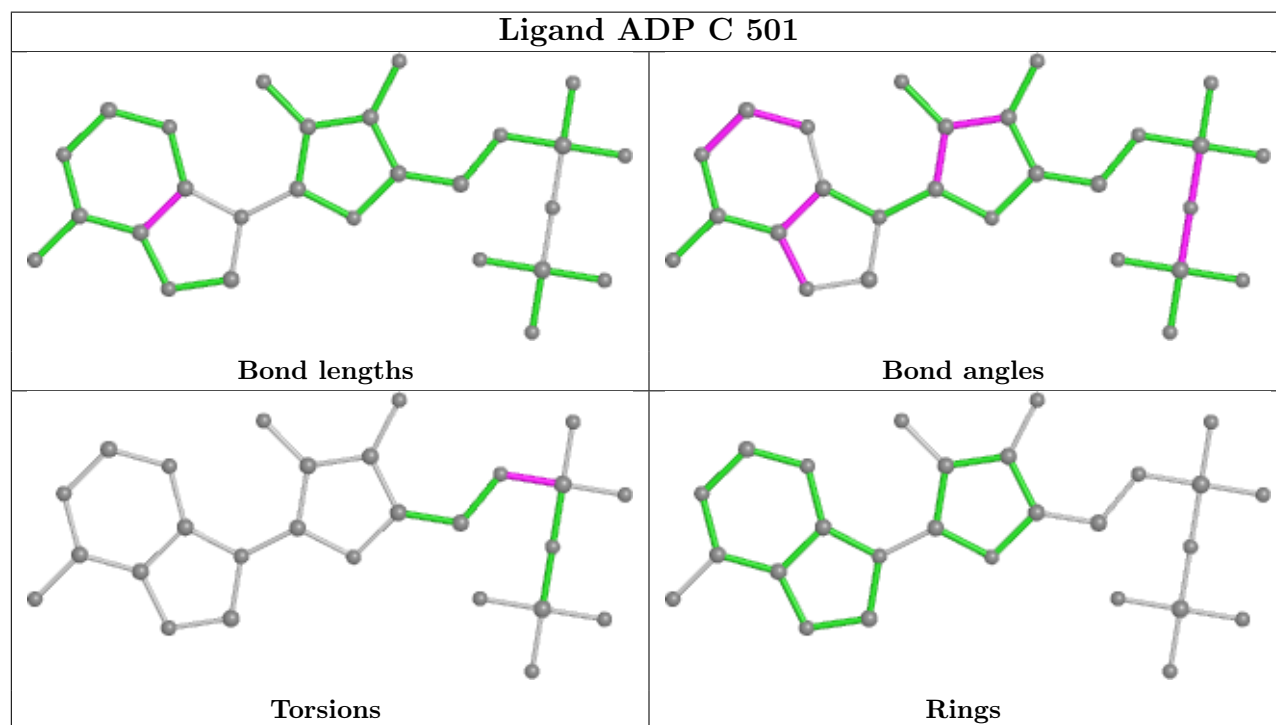
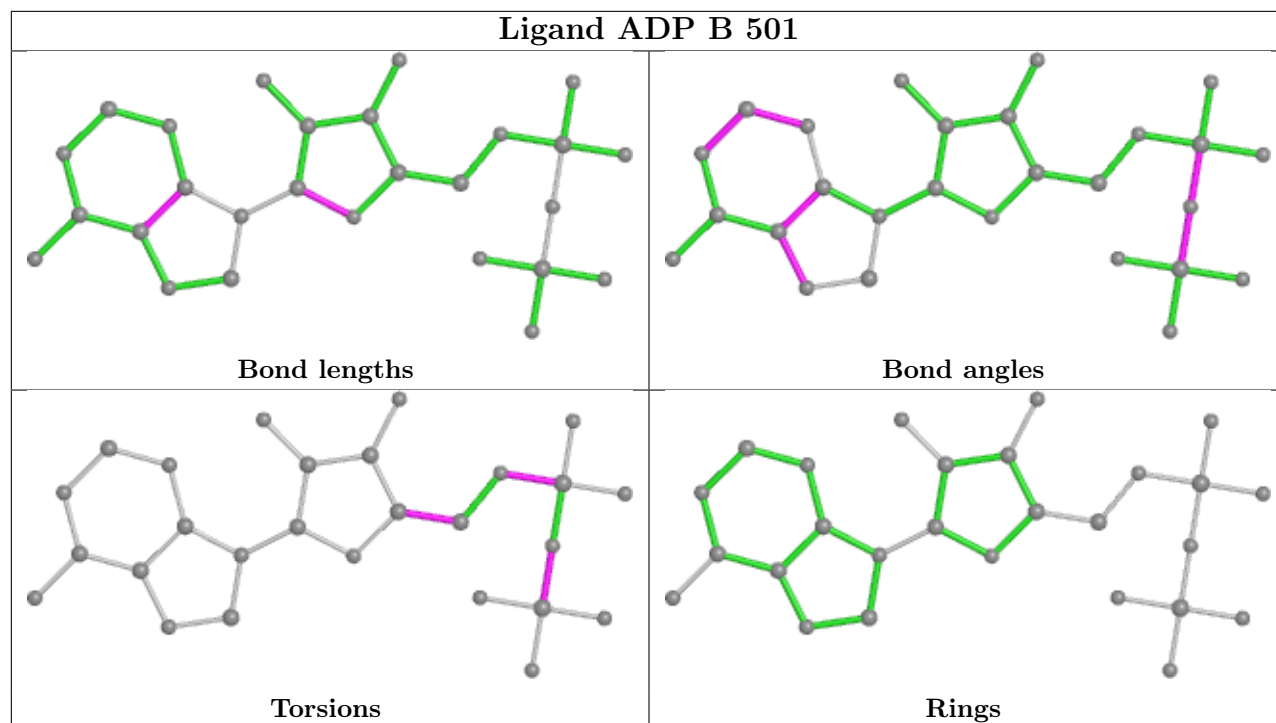
Mol	Chain	Res	Type	Atoms
9	A	501	ADP	PA-O3A-PB-O2B
9	B	501	ADP	PA-O3A-PB-O2B
9	B	501	ADP	C5'-O5'-PA-O3A
9	C	501	ADP	C5'-O5'-PA-O3A
9	E	501	ADP	C5'-O5'-PA-O3A
9	K	401	ADP	C5'-O5'-PA-O3A
9	A	501	ADP	C5'-O5'-PA-O1A
9	I	501	ADP	O4'-C4'-C5'-O5'
9	J	502	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

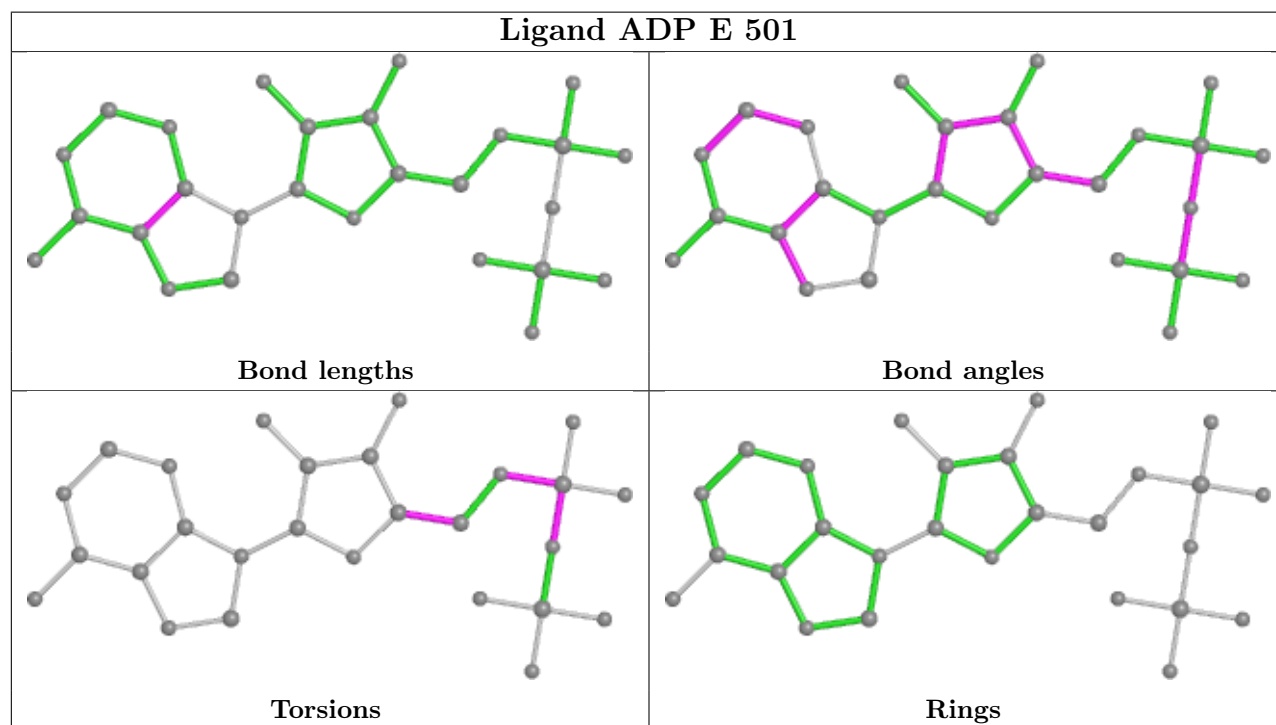
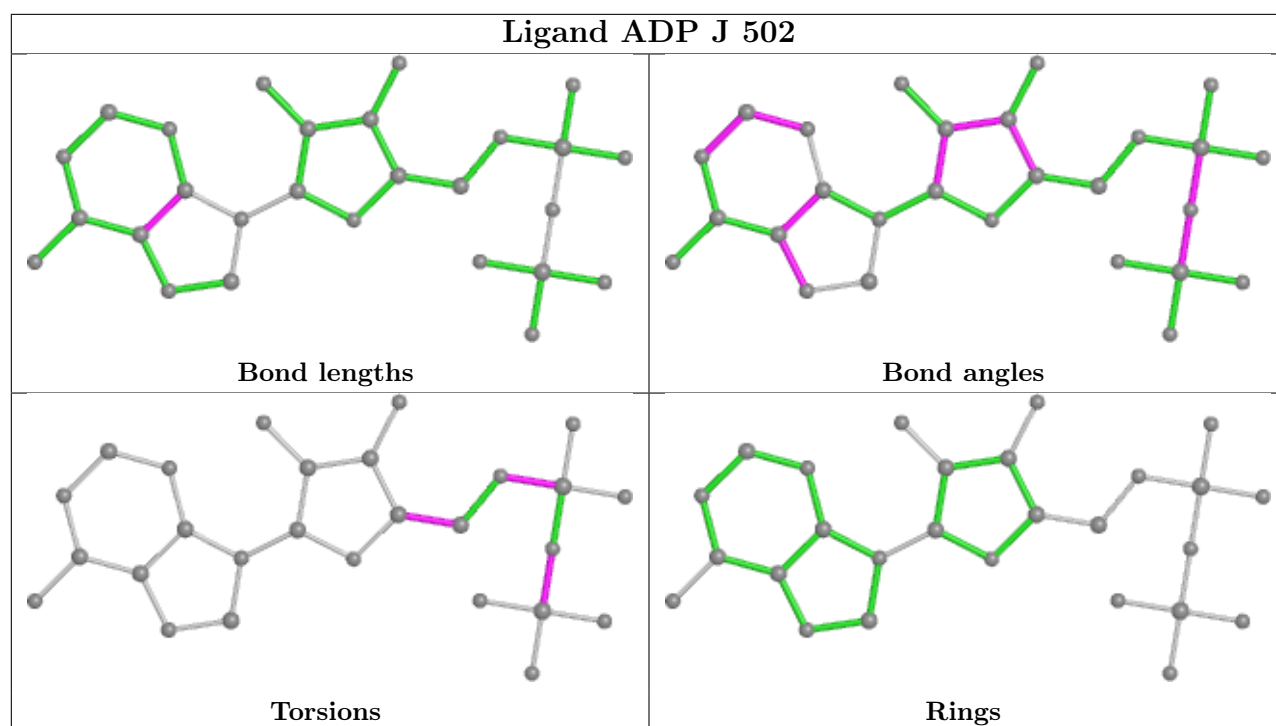
9 monomers are involved in 139 short contacts:

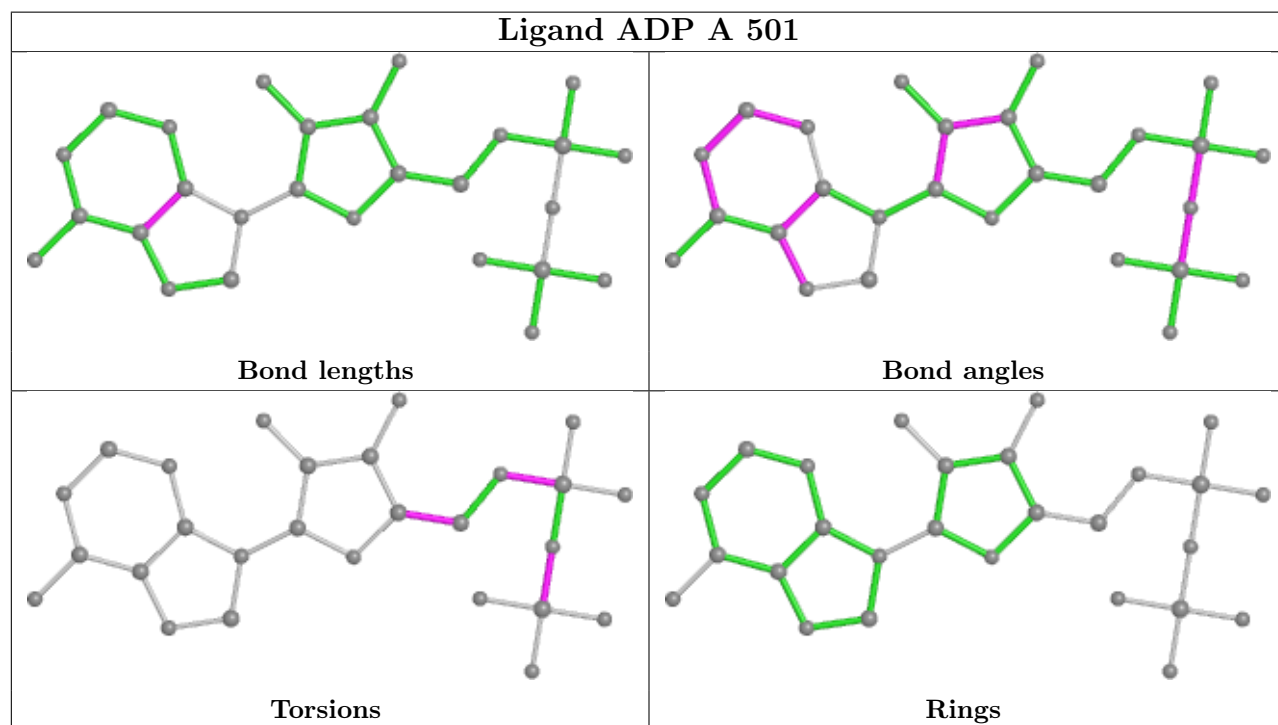
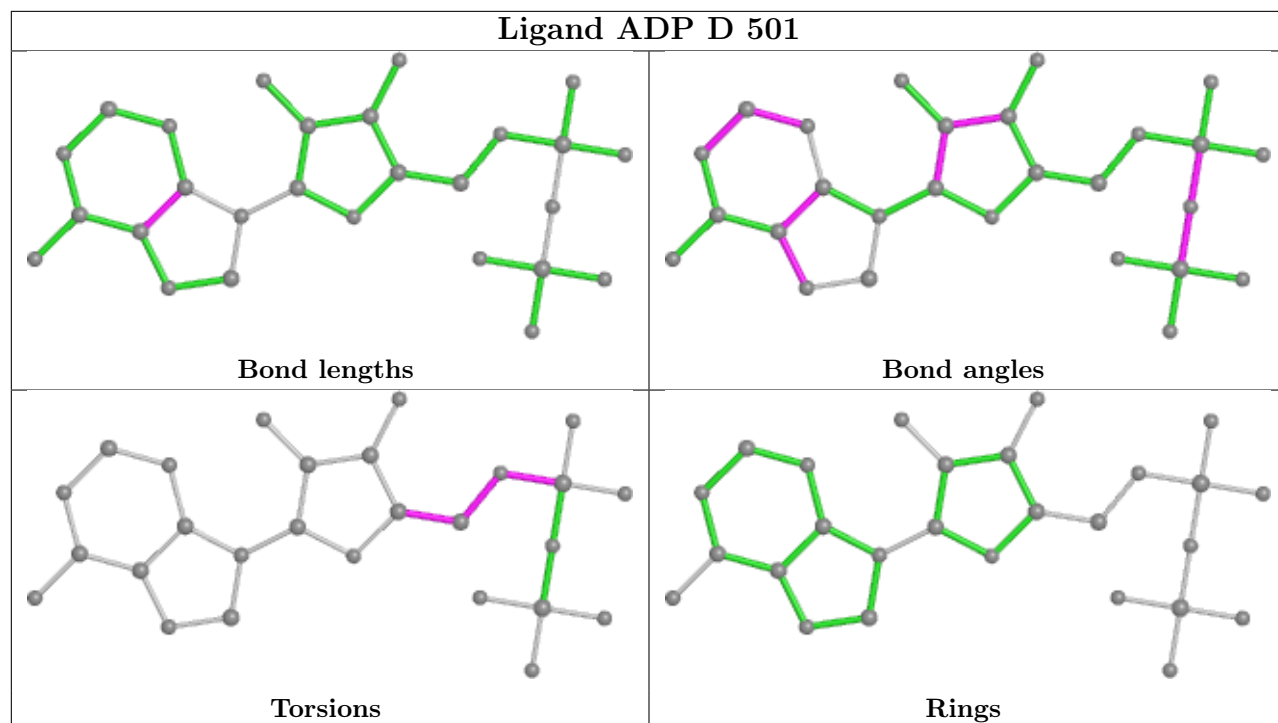
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	501	ADP	9	0
9	C	501	ADP	29	0
9	J	502	ADP	5	0
9	E	501	ADP	19	0
9	D	501	ADP	11	0
9	A	501	ADP	14	0
9	I	501	ADP	24	0
9	K	401	ADP	18	0
9	F	501	ADP	10	0

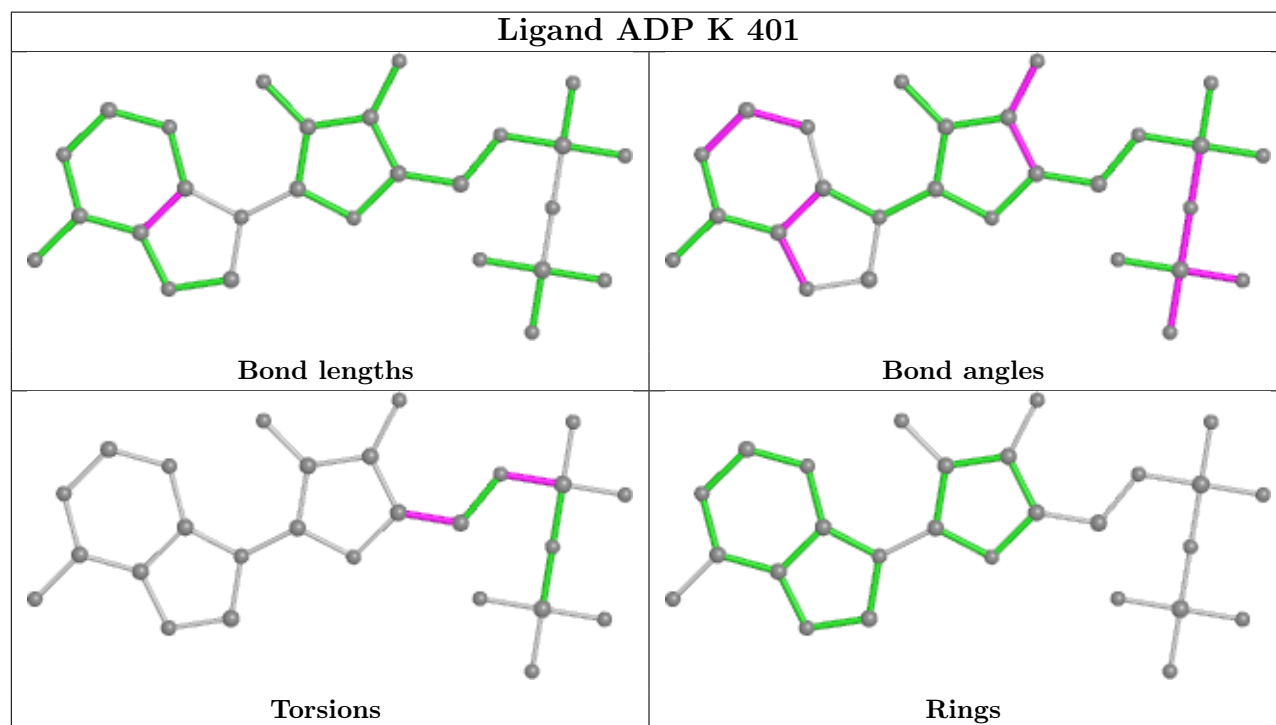
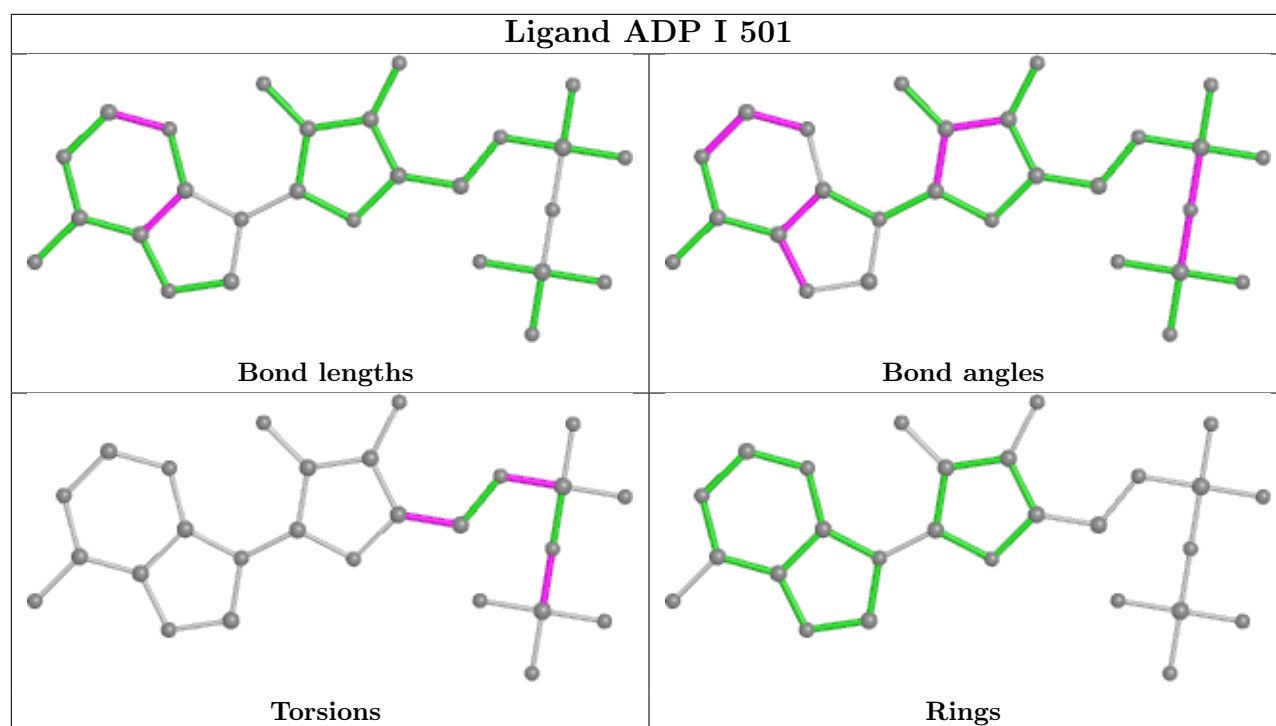
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

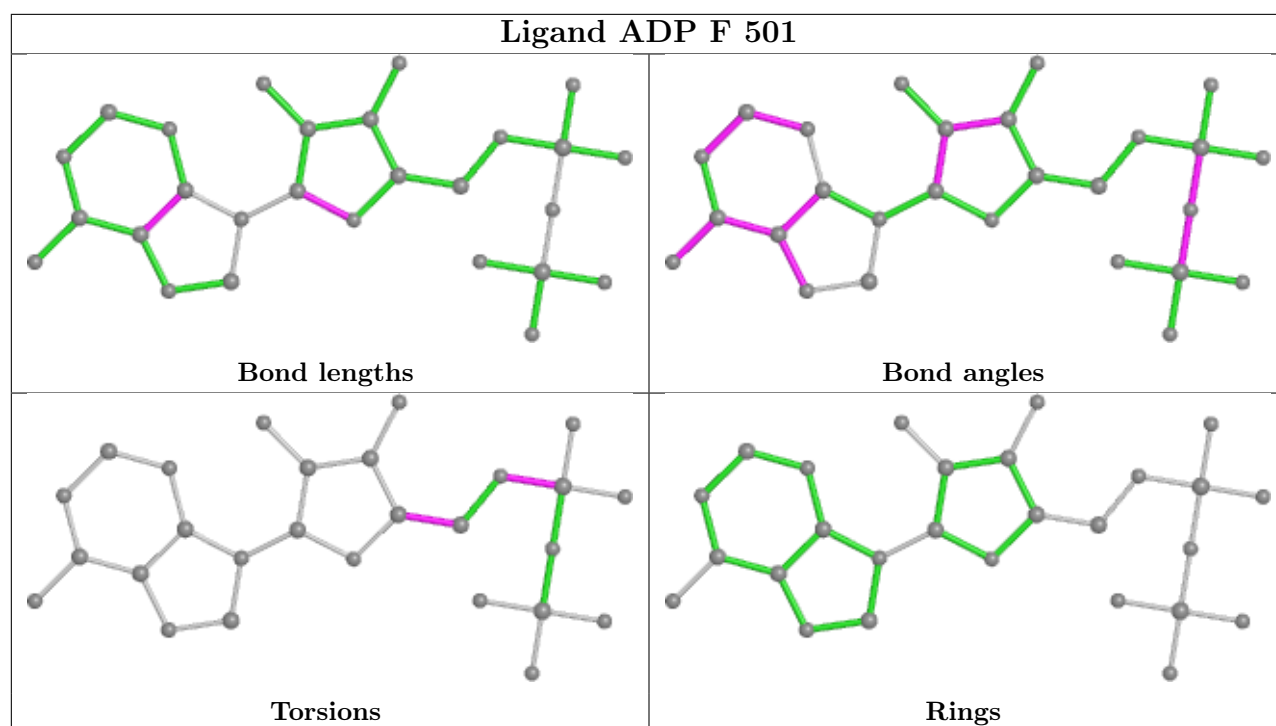












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

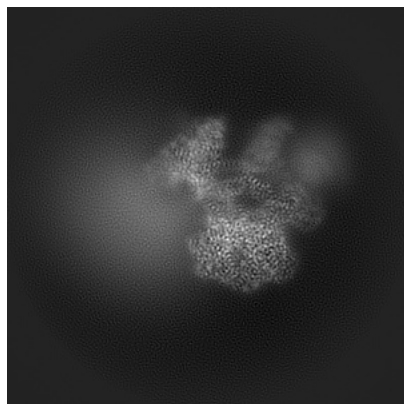
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38718. These allow visual inspection of the internal detail of the map and identification of artifacts.

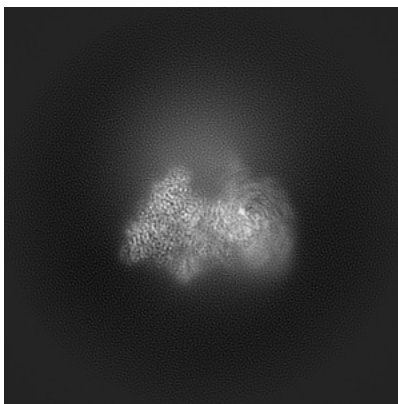
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

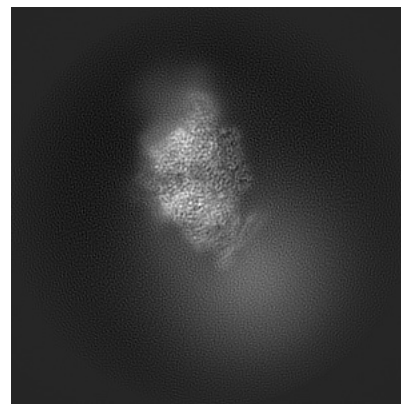
#### 6.1.1 Primary map



X

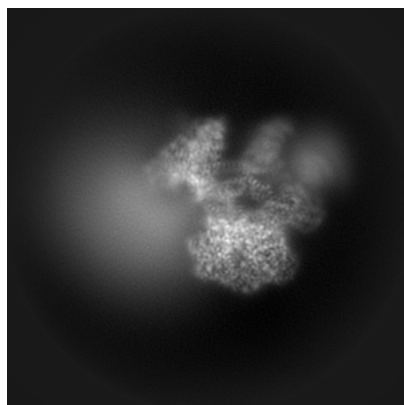


Y

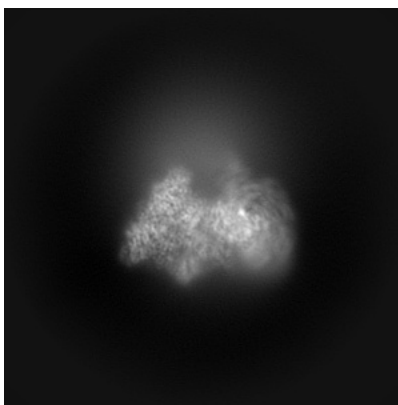


Z

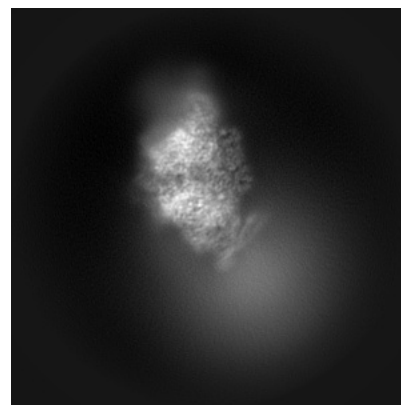
#### 6.1.2 Raw map



X



Y

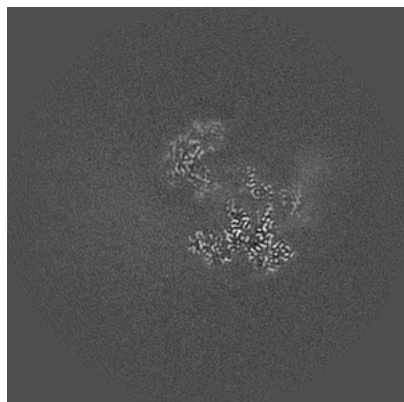


Z

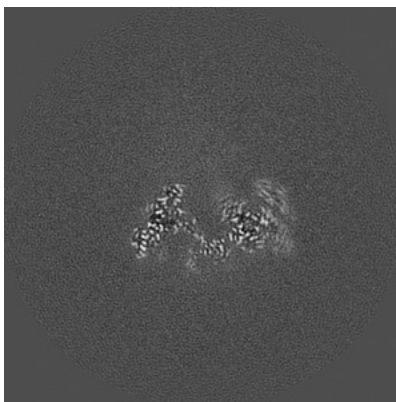
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

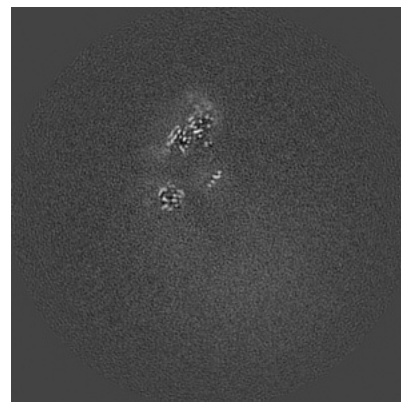
### 6.2.1 Primary map



X Index: 150

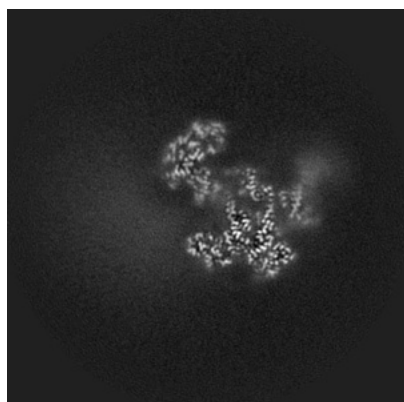


Y Index: 150

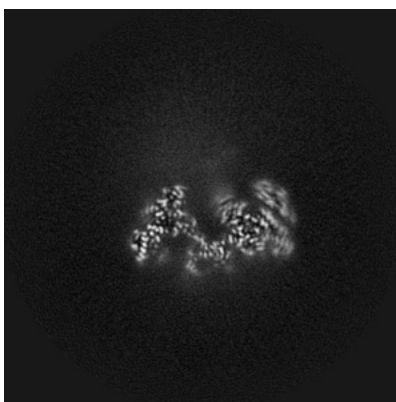


Z Index: 150

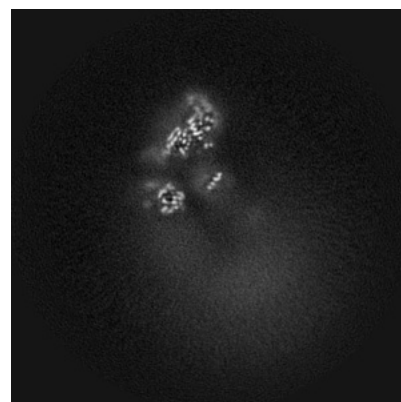
### 6.2.2 Raw map



X Index: 150



Y Index: 150

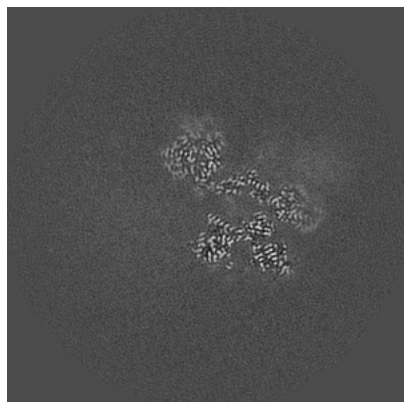


Z Index: 150

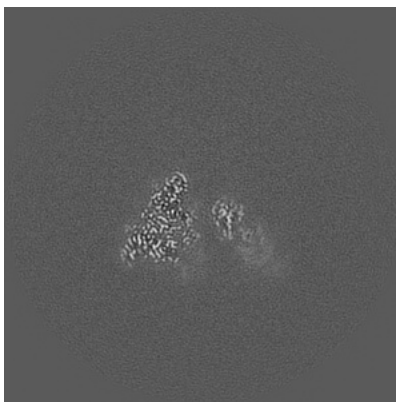
The images above show central slices of the map in three orthogonal directions.

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

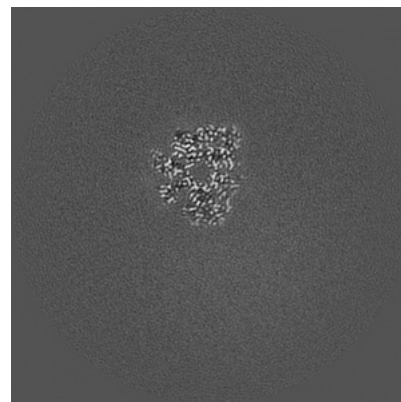
### 6.3.1 Primary map



X Index: 141

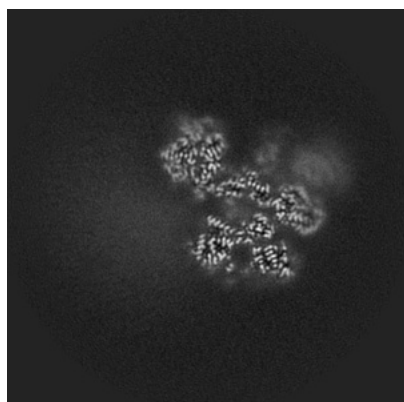


Y Index: 185

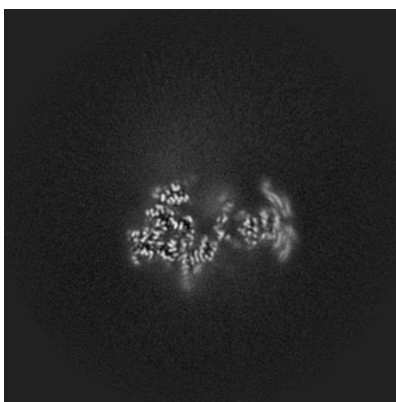


Z Index: 120

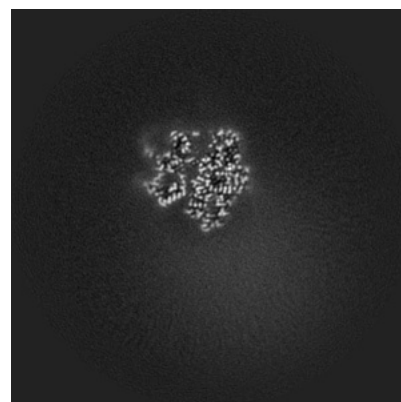
### 6.3.2 Raw map



X Index: 141



Y Index: 158

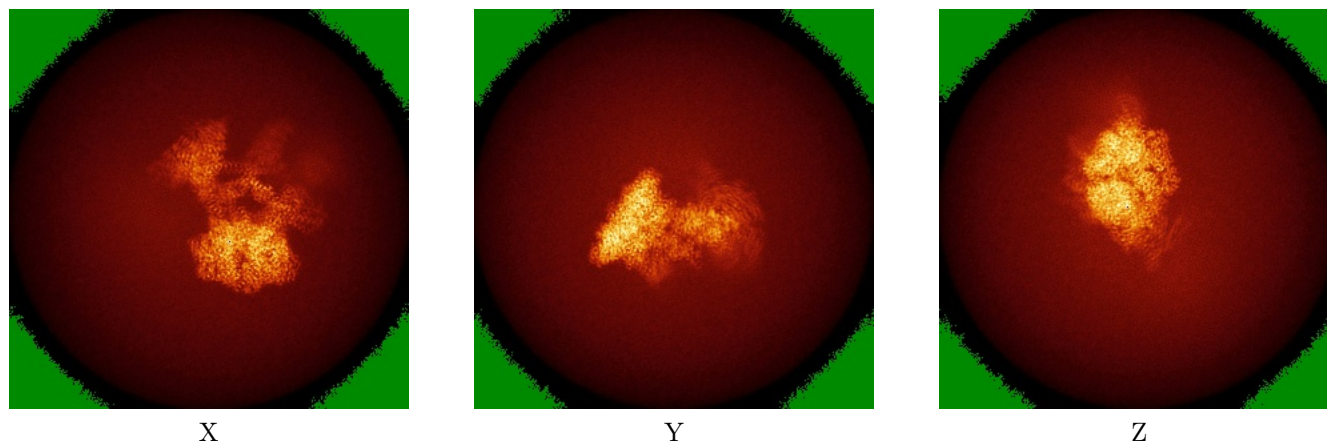


Z Index: 125

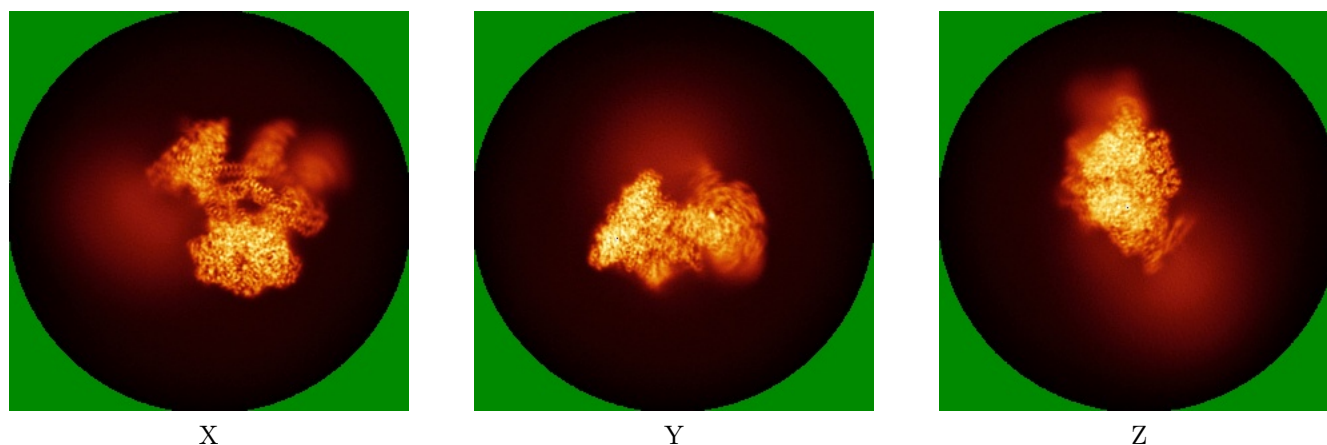
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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



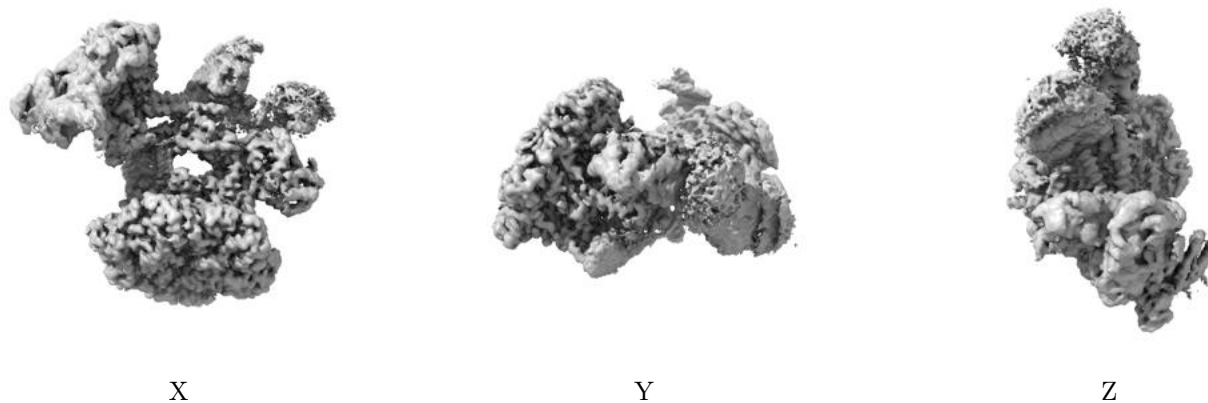
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.024. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

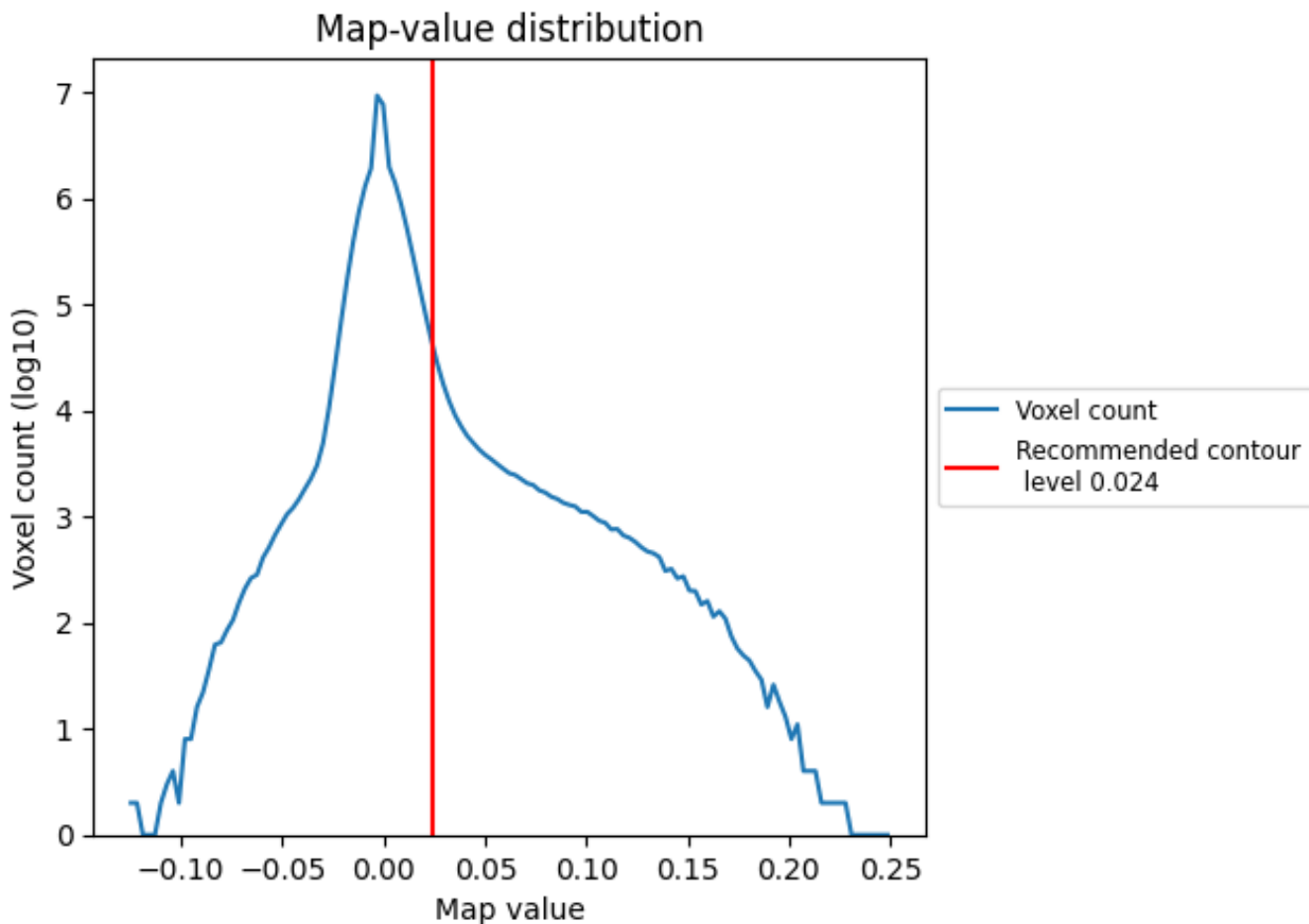
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

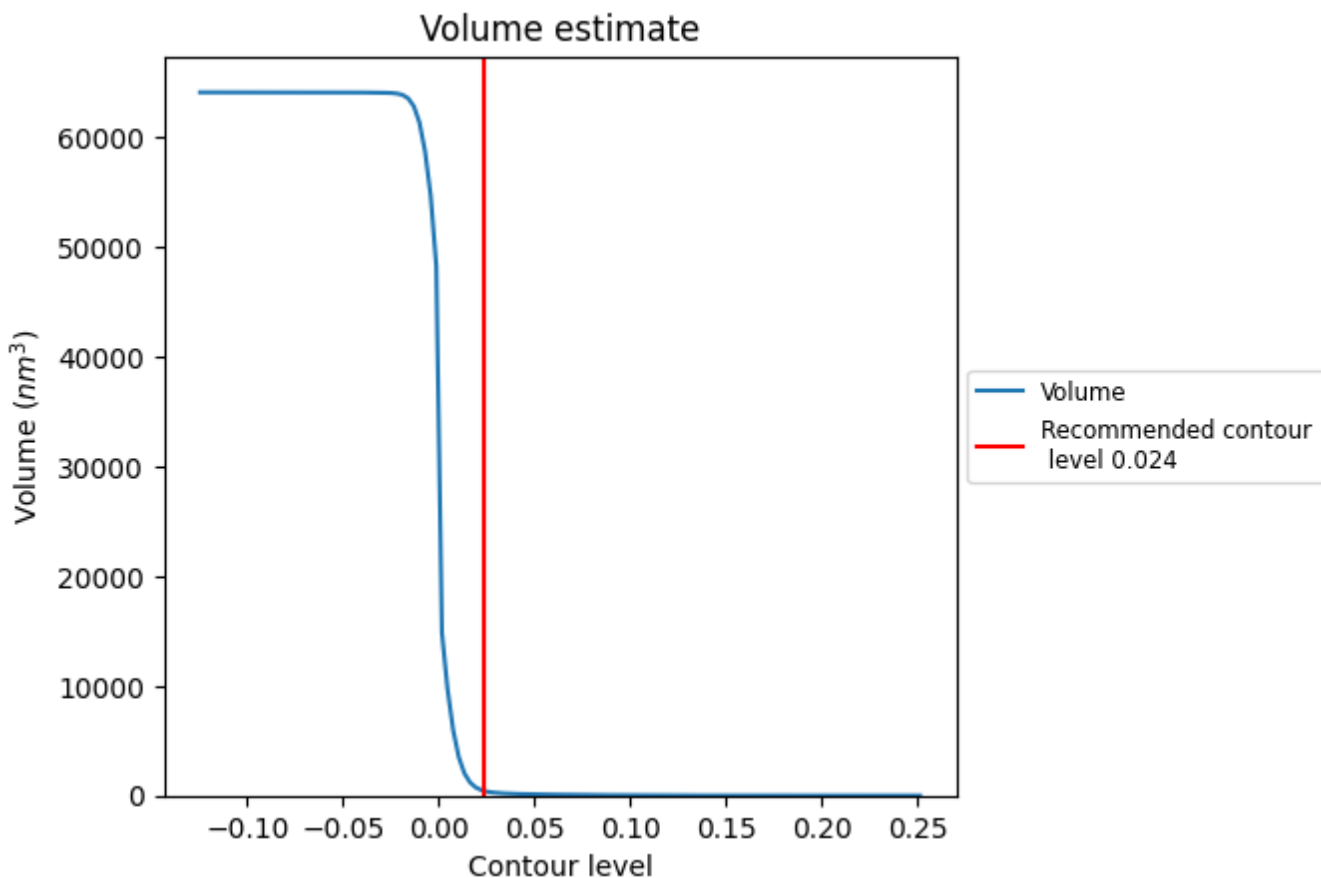
This section contains the results of statistical analysis of the map.

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



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

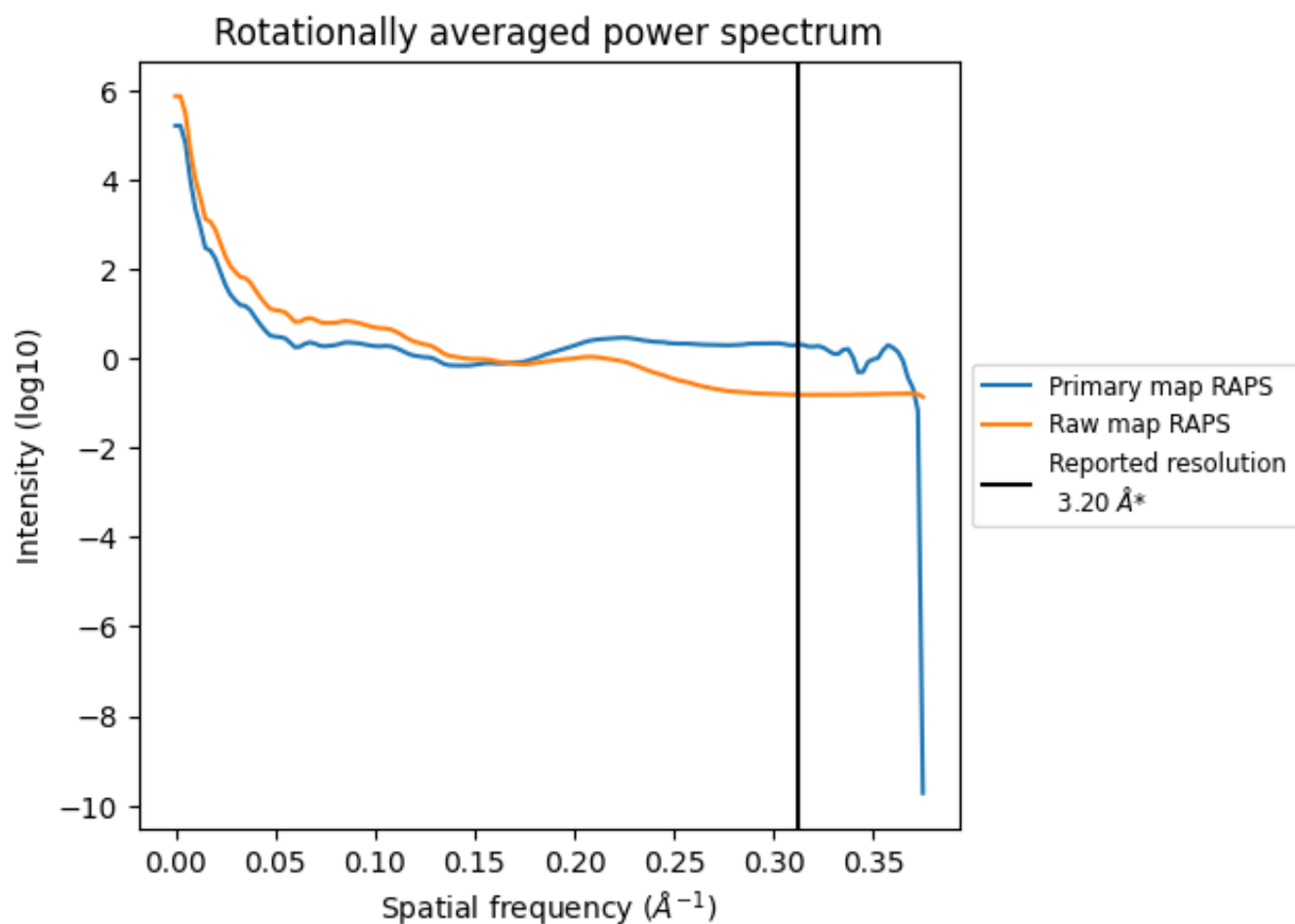
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 420  $\text{nm}^3$ ; this corresponds to an approximate mass of 379 kDa.

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

### 7.3 Rotationally averaged power spectrum i

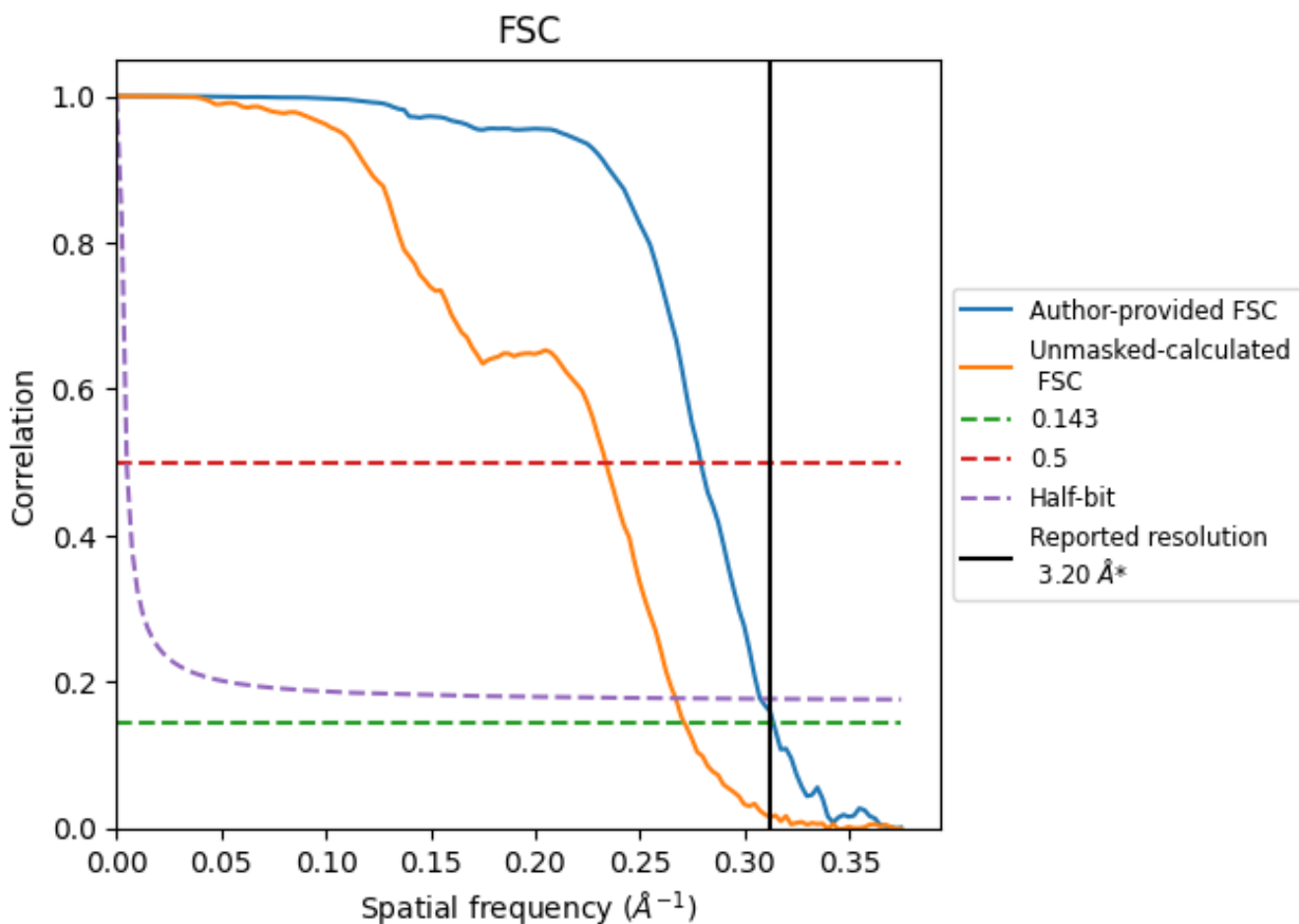


\*Reported resolution corresponds to spatial frequency of 0.312 Å<sup>-1</sup>

## 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 0.312 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

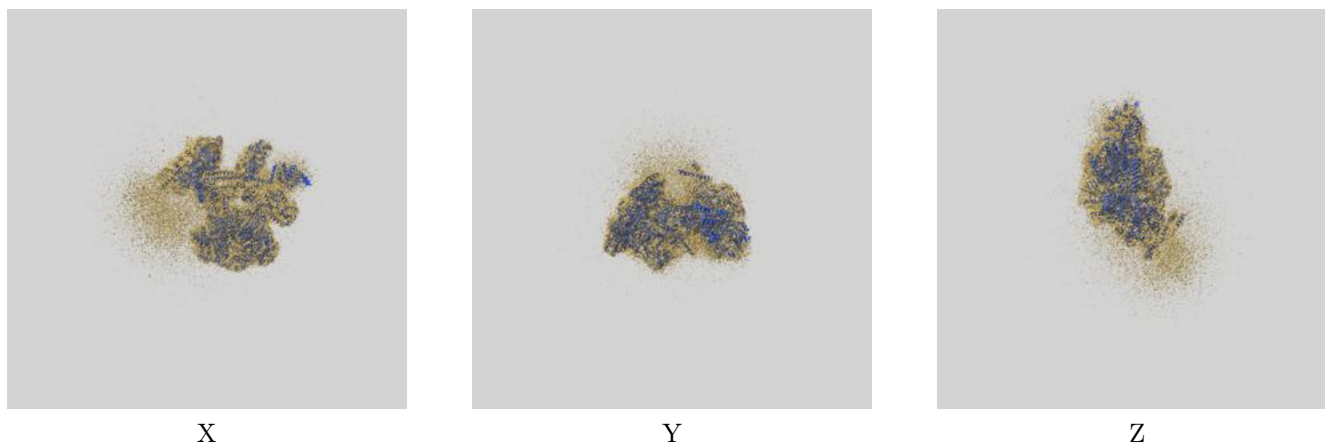
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.19	3.58	3.25
Unmasked-calculated*	3.69	4.28	3.75

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.69 differs from the reported value 3.2 by more than 10 %

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

This section contains information regarding the fit between EMDB map EMD-38718 and PDB model 8XVT. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



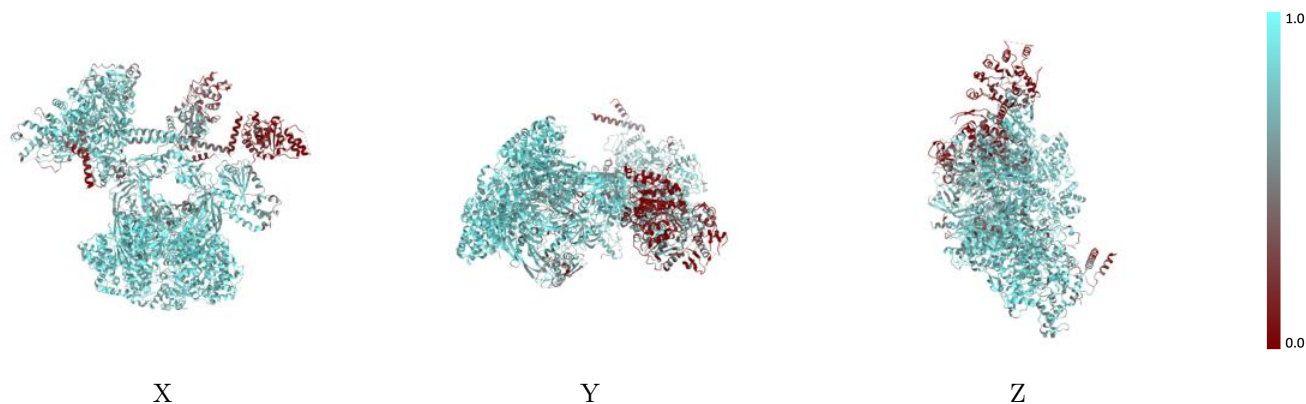
The images above show the 3D surface view of the map at the recommended contour level 0.024 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

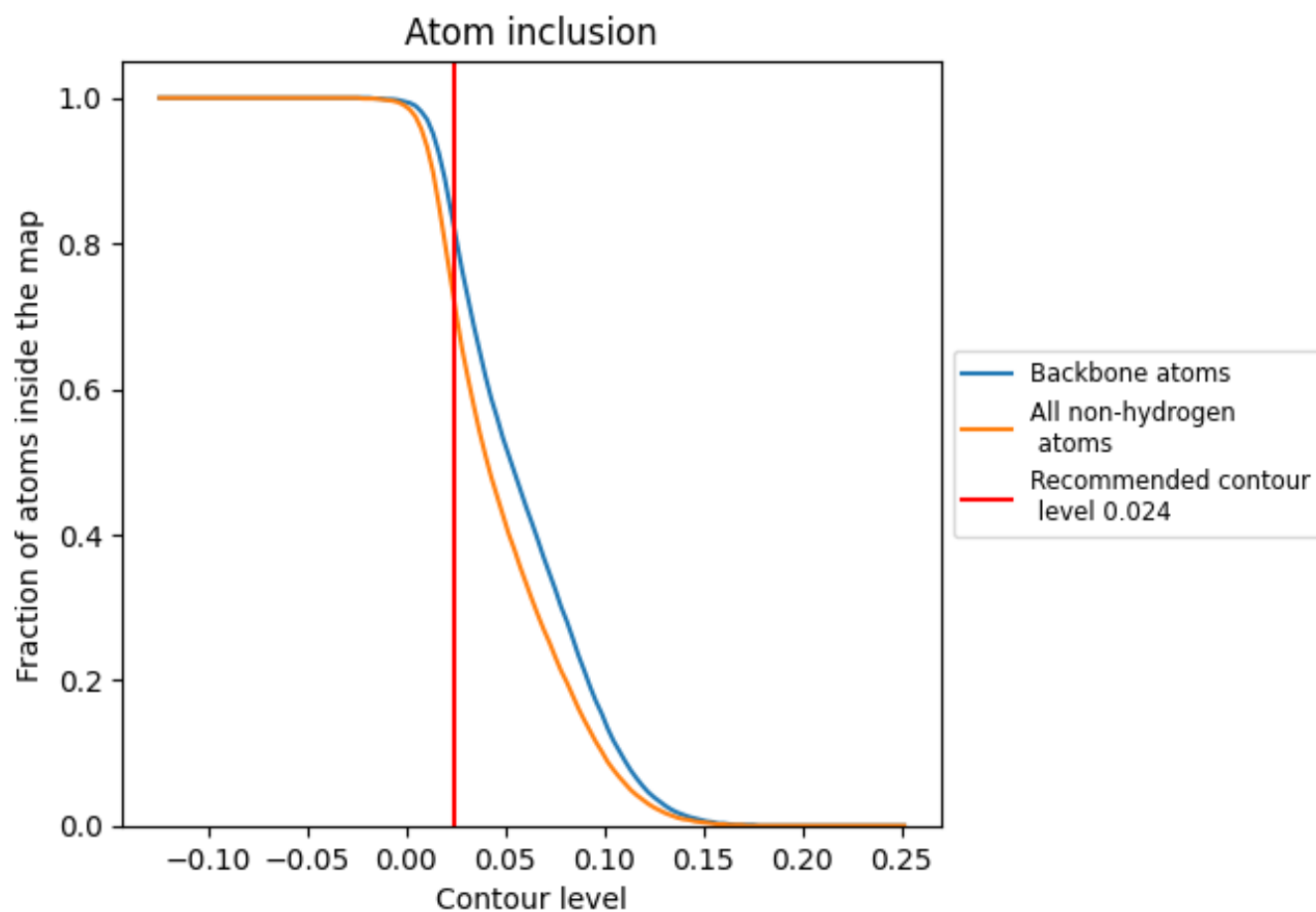
## 9.3 Atom inclusion mapped to coordinate model [\(i\)](#)



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 (0.024).































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 72% 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 (0.024) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7220	 0.3690
A	 0.8050	 0.4340
B	 0.7870	 0.4110
C	 0.8410	 0.4600
D	 0.8380	 0.4590
E	 0.8180	 0.4450
F	 0.8290	 0.4580
G	 0.6800	 0.2960
H	 0.5510	 0.2550
I	 0.3870	 0.1120
J	 0.7620	 0.3770
K	 0.7980	 0.4240
M	 0.7030	 0.3350
N	 0.6480	 0.3340

