Full wwPDB EM Validation Report ⓘ

May 26, 2022 – 04:34 pm BST

PDB ID	:	7QO4
EMDB ID	:	EMD-14083
Title	:	26S proteasome WT-Ubp6-UbVS complex in the si state (ATPases, Rpn1, Ubp6, and UbVS)
Authors	:	Hung, K.Y.S.; Klumpe, S.; Eisele, M.R.; Elsasser, S.; Geng, T.T.; Cheng, C.; Joshi, T.; Rudack, T.; Sakata, E.; Finley, D.
Deposited on	:	2021-12-23
Resolution	:	7.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

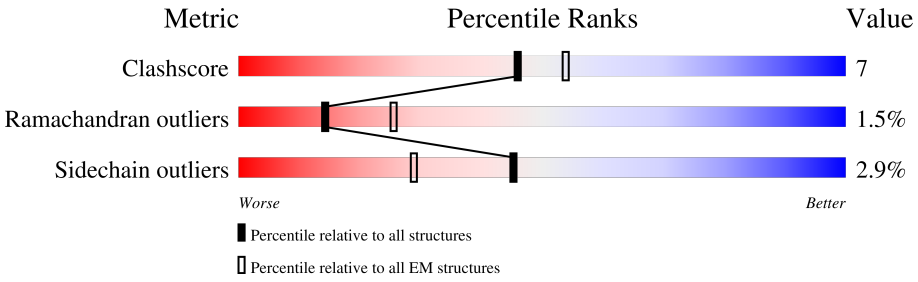
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 7.00 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 <=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	Z	993	41% 74% 13% • • 9%
2	H	467	24% 67% 14% • 16%
3	I	437	22% 73% 13% •• 12%
4	K	428	26% 74% 16% • 8%
5	L	437	22% 79% 8% • 11%
6	M	434	30% 80% 14% • • •
7	J	405	41% 84% 13% •
8	8	499	34% 65% 8% • 25%

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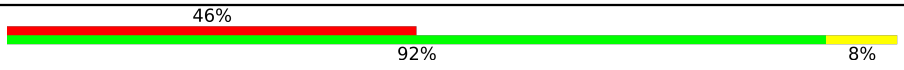
Mol	Chain	Length	Quality of chain
9	9	76	

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	GLZ	9	76	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 29551 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 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	Z	906	7005	4416	1150	1409	30	0	0

- Molecule 2 is a protein called RPT1 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	391	3057	1922	547	571	17	0	0

- Molecule 3 is a protein called RPT2 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	I	384	3015	1895	507	596	17	0	0

- Molecule 4 is a protein called RPT3 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	K	394	3113	1951	548	604	10	0	0

- Molecule 5 is a protein called RPT4 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	388	3082	1942	548	580	12	0	0

- Molecule 6 is a protein called RPT5 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	M	421	3285	2043	573	656	13	0	0

- Molecule 7 is a protein called RPT6 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	J	405	3171	1995	565	593	18	0	0

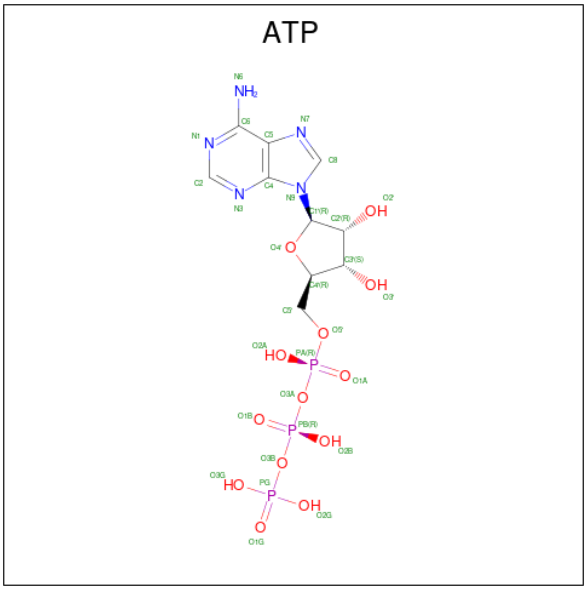
- Molecule 8 is a protein called Ubiquitin carboxyl-terminal hydrolase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	8	372	3034	1918	521	583	12	0	0

- Molecule 9 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	9	76	601	378	105	117	1	0	0

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



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	H	1	31	10	5	13	3	0
10	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	K	1	Total	C	N	O	P	0
			31	10	5	13	3	

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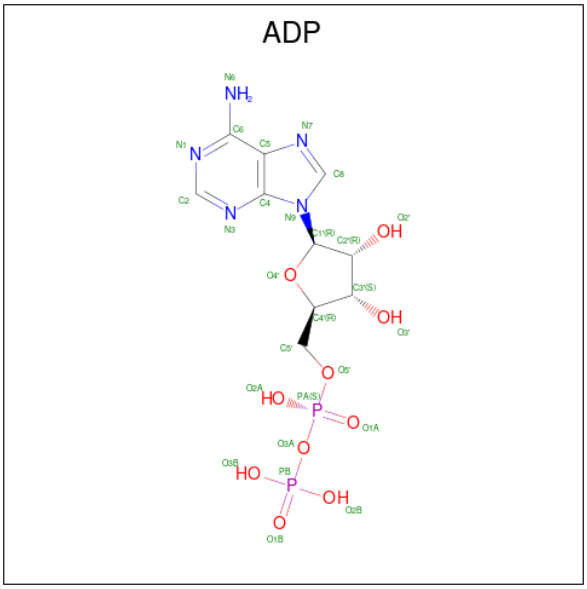
Mol	Chain	Residues	Atoms					AltConf
10	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	M	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
11	H	1	Total	Mg	0
			1	1	
11	I	1	Total	Mg	0
			1	1	
11	K	1	Total	Mg	0
			1	1	
11	L	1	Total	Mg	0
			1	1	
11	M	1	Total	Mg	0
			1	1	
11	J	1	Total	Mg	0
			1	1	

- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



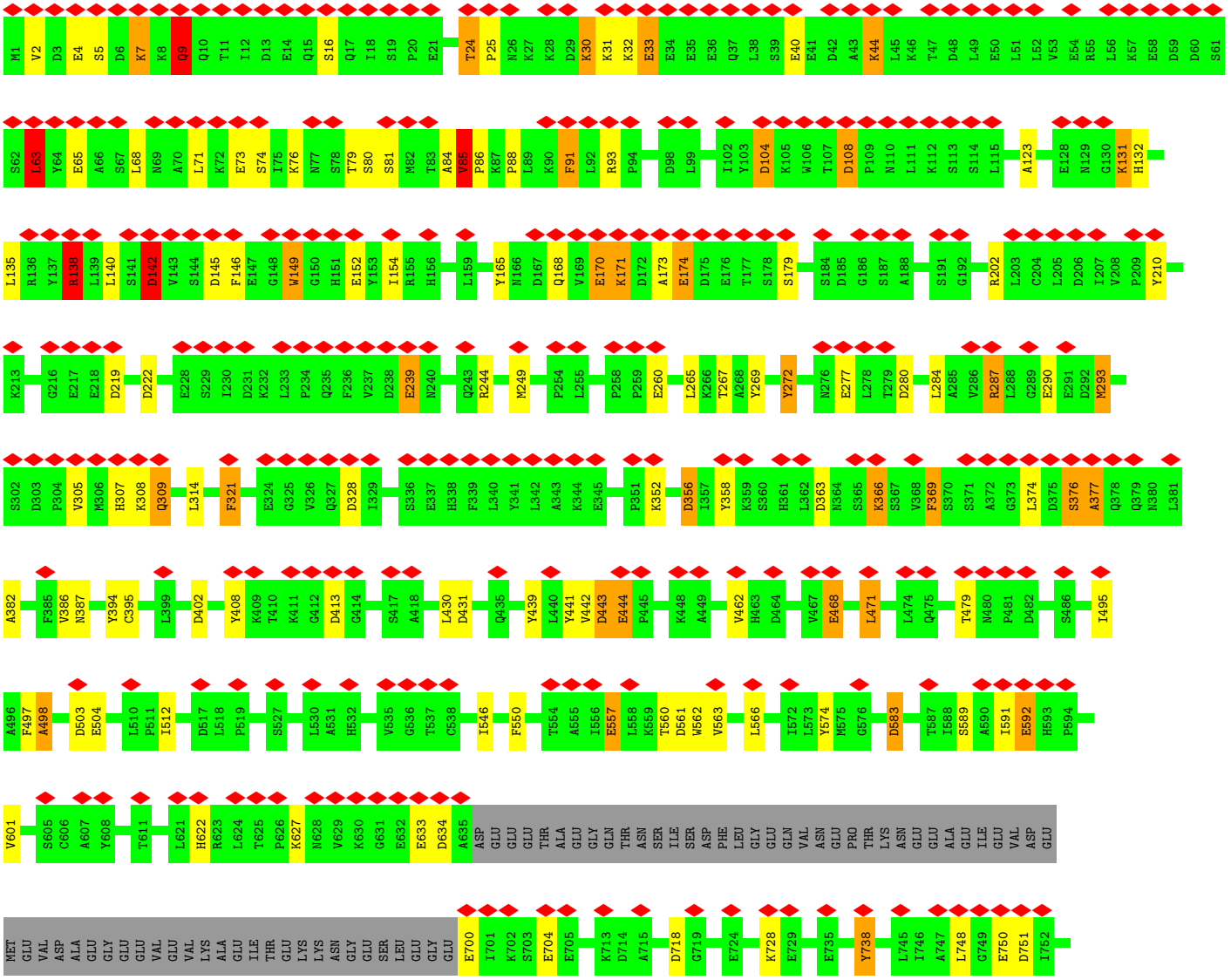
Mol	Chain	Residues	Atoms					AltConf
12	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

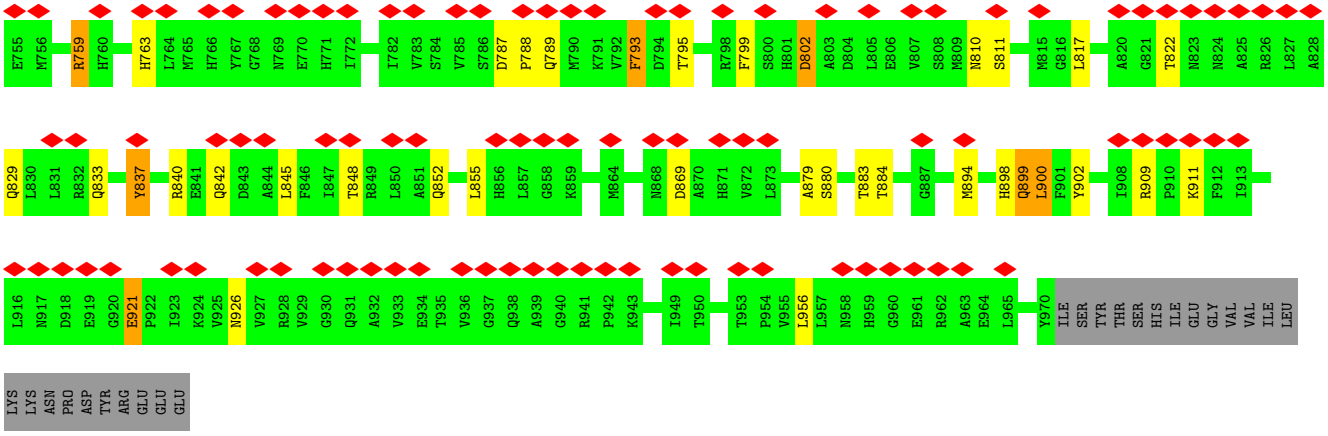
3 Residue-property plots (i)

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: 26S proteasome regulatory subunit RPN1

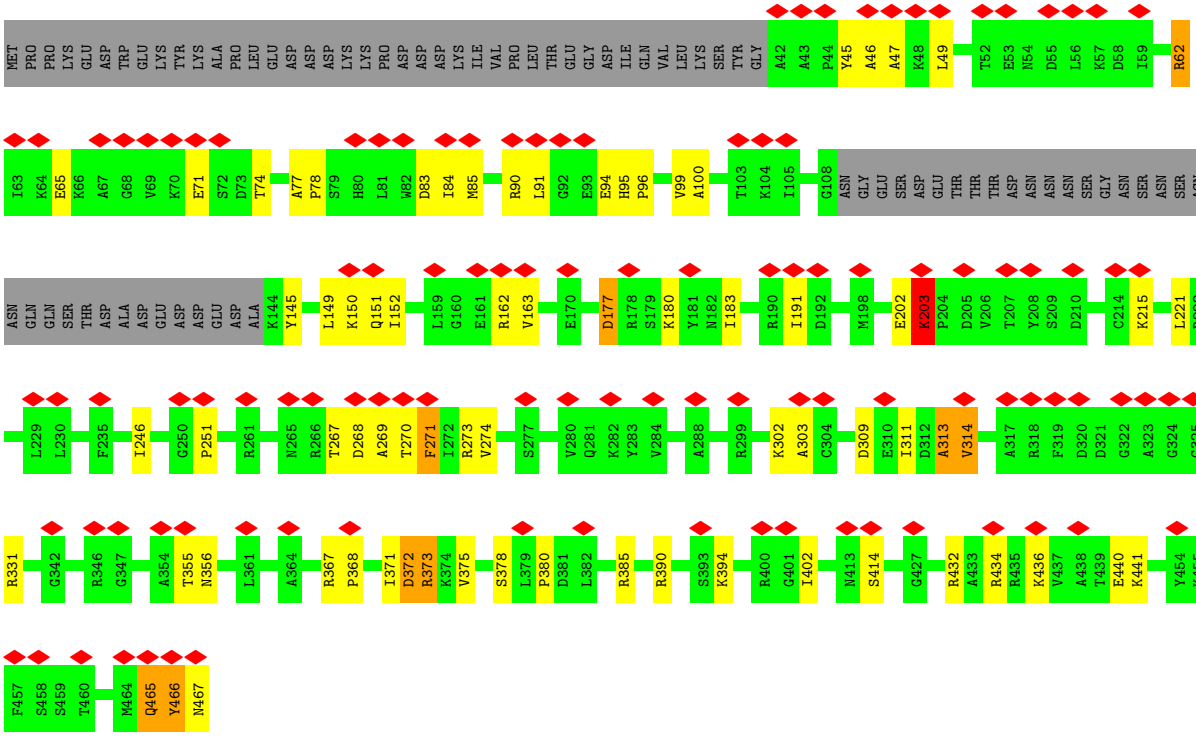
Chain Z:





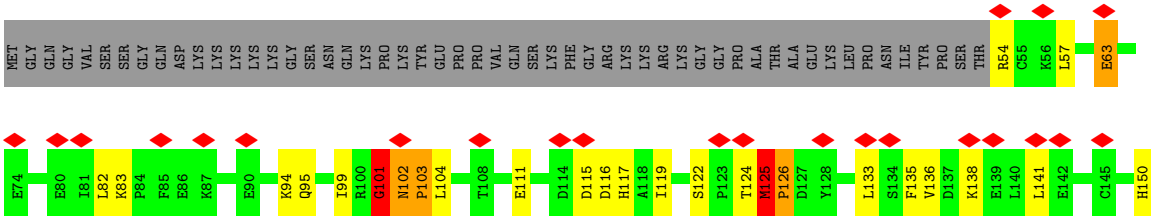
• Molecule 2: RPT1 isoform 1

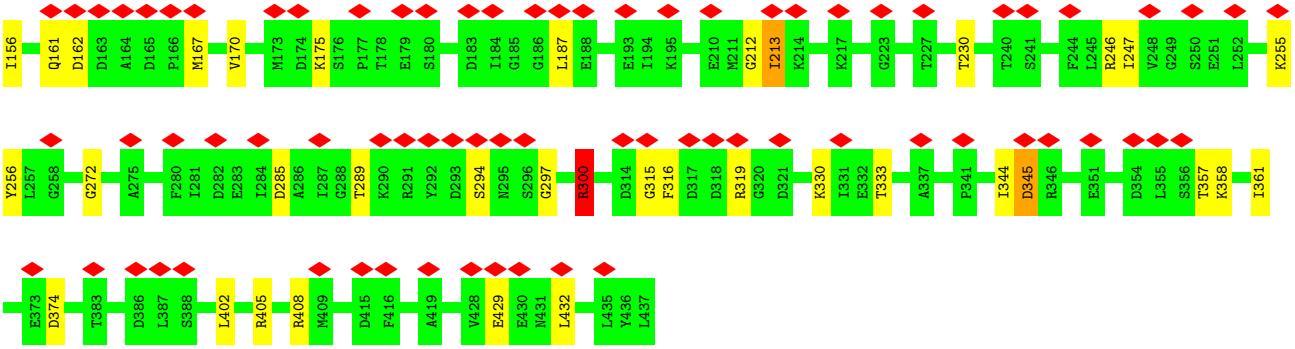
Chain H:



• Molecule 3: RPT2 isoform 1

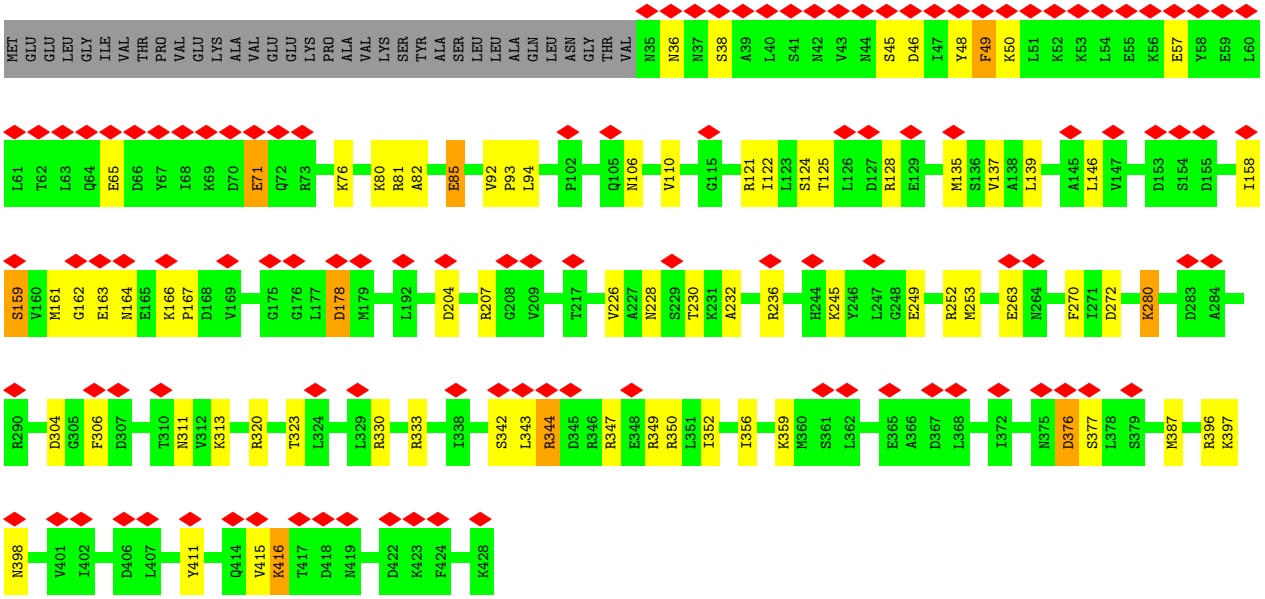
Chain I:





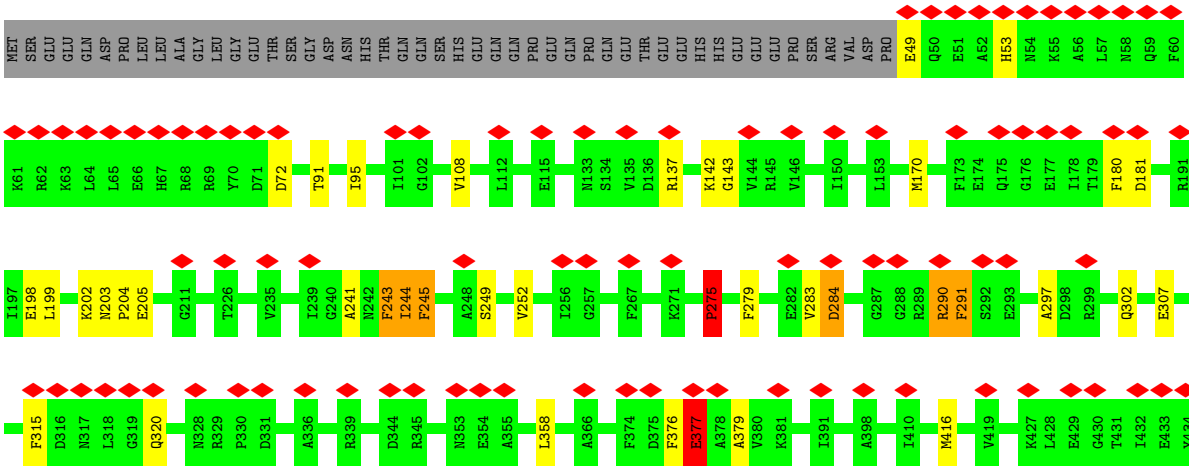
• Molecule 4: RPT3 isoform 1

Chain K:



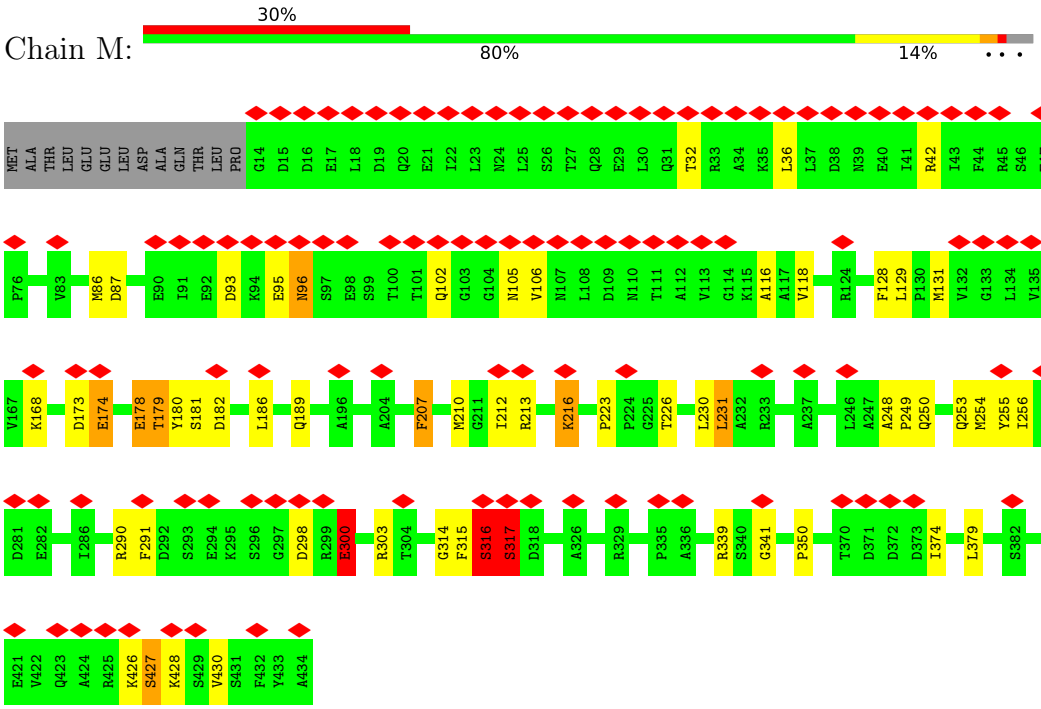
• Molecule 5: RPT4 isoform 1

Chain L:



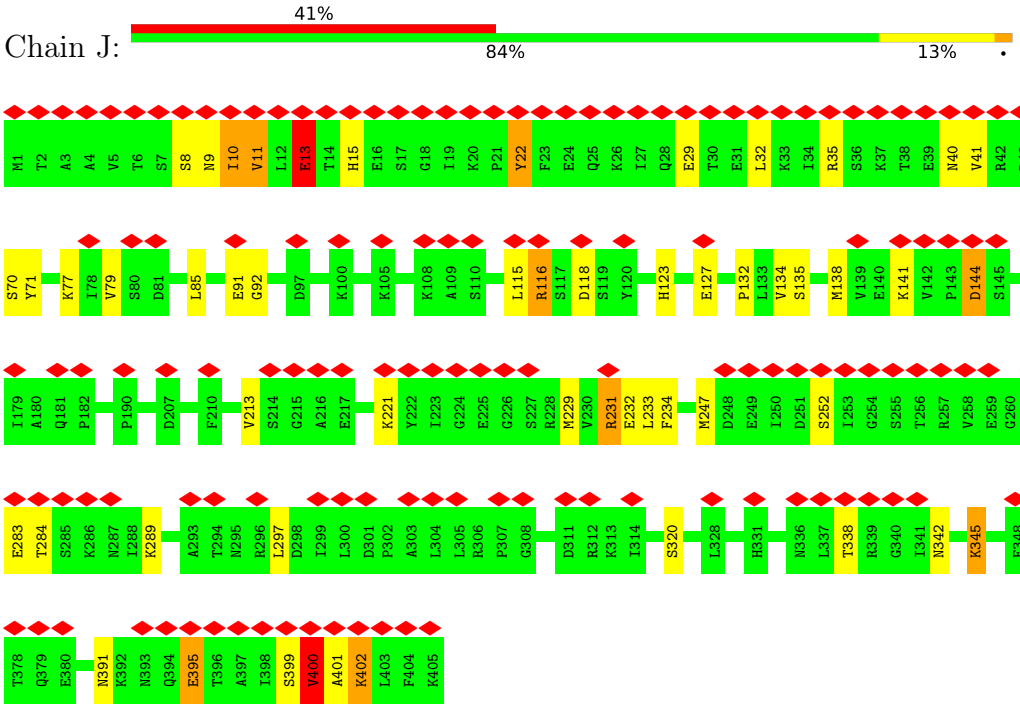
• Molecule 6: RPT5 isoform 1

Chain M:



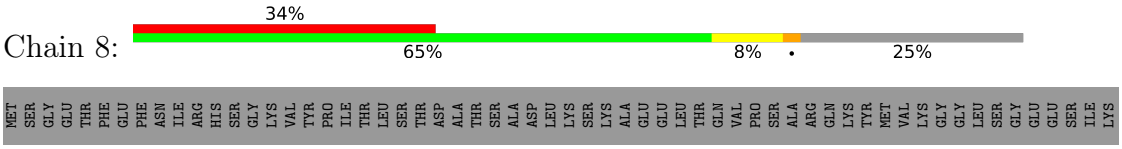
• Molecule 7: RPT6 isoform 1

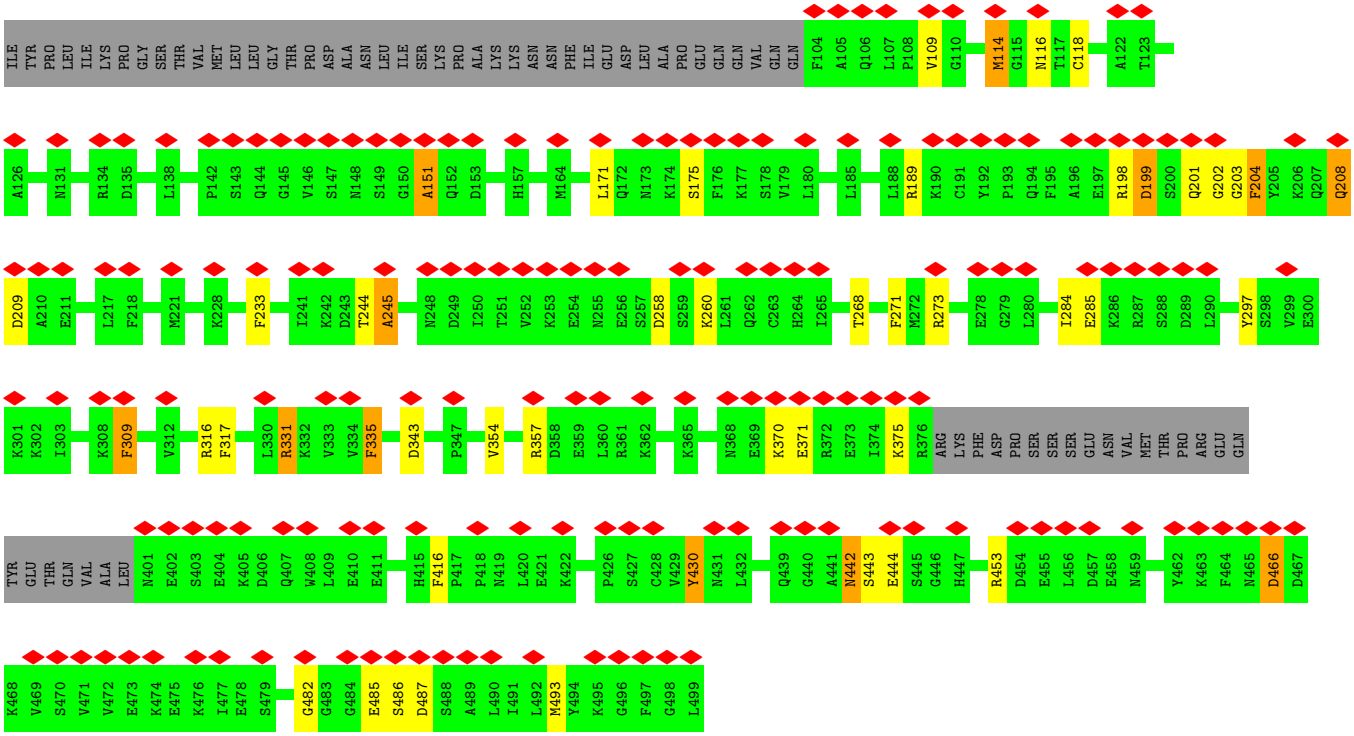
Chain J:



• Molecule 8: Ubiquitin carboxyl-terminal hydrolase

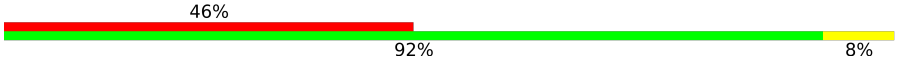
Chain 8:

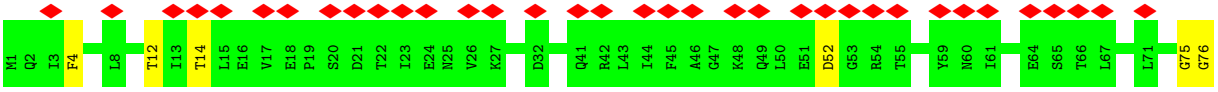




• Molecule 9: Polyubiquitin-B

Chain 9:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88243	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	33.914	Depositor
Minimum map value	-16.285	Depositor
Average map value	-0.023	Depositor
Map value standard deviation	0.792	Depositor
Recommended contour level	6.5	Depositor
Map size (Å)	588.0, 588.0, 588.0	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.1, 2.1, 2.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GLZ, 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	Z	0.66	2/7122 (0.0%)	1.27	74/9645 (0.8%)
2	H	0.49	0/3106	0.89	4/4180 (0.1%)
3	I	0.55	0/3054	0.96	12/4111 (0.3%)
4	K	0.53	0/3156	0.90	5/4261 (0.1%)
5	L	0.56	0/3128	0.92	6/4204 (0.1%)
6	M	0.54	1/3323 (0.0%)	0.89	3/4478 (0.1%)
7	J	0.51	0/3212	0.97	12/4316 (0.3%)
8	8	0.71	1/3089 (0.0%)	1.13	20/4144 (0.5%)
9	9	0.55	0/603	0.93	0/811
All	All	0.58	4/29793 (0.0%)	1.04	136/40150 (0.3%)

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	Z	0	40
2	H	0	4
3	I	0	4
4	K	0	10
5	L	0	6
6	M	0	7
7	J	0	12
8	8	0	11
9	9	0	2
All	All	0	96

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	149	TRP	CB-CG	-7.64	1.36	1.50
6	M	207	PHE	CB-CG	-5.75	1.41	1.51
8	8	198	ARG	NE-CZ	5.68	1.40	1.33
1	Z	44	LYS	CE-NZ	-5.13	1.36	1.49

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	33	GLU	OE1-CD-OE2	-17.74	102.02	123.30
1	Z	366	LYS	CG-CD-CE	16.98	162.82	111.90
8	8	198	ARG	NE-CZ-NH2	-15.06	112.77	120.30
1	Z	366	LYS	CB-CG-CD	15.05	150.73	111.60
8	8	198	ARG	NE-CZ-NH1	14.34	127.47	120.30
7	J	22	TYR	CB-CG-CD2	-13.45	112.93	121.00
1	Z	33	GLU	CG-CD-OE1	11.54	141.38	118.30
1	Z	366	LYS	CD-CE-NZ	-10.34	87.92	111.70
1	Z	33	GLU	CG-CD-OE2	-10.03	98.24	118.30
3	I	167	MET	CG-SD-CE	9.83	115.93	100.20
1	Z	468	GLU	OE1-CD-OE2	-9.16	112.31	123.30
1	Z	321	PHE	CB-CG-CD2	-9.08	114.44	120.80
3	I	54	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	Z	498	ALA	N-CA-CB	-8.60	98.07	110.10
5	L	275	PRO	CA-N-CD	-8.45	99.67	111.50
1	Z	902	TYR	CB-CG-CD2	-8.41	115.95	121.00
1	Z	63	LEU	CB-CG-CD2	8.36	125.20	111.00
3	I	125	MET	C-N-CD	-8.12	102.73	120.60
1	Z	497	PHE	CB-CG-CD2	-8.01	115.20	120.80
3	I	167	MET	CB-CG-SD	7.99	136.38	112.40
7	J	395	GLU	OE1-CD-OE2	-7.98	113.73	123.30
1	Z	759	ARG	NE-CZ-NH2	7.92	124.26	120.30
5	L	377	GLU	CA-CB-CG	7.84	130.64	113.40
1	Z	900	LEU	CB-CG-CD1	7.69	124.07	111.00
8	8	309	PHE	CB-CG-CD2	-7.58	115.49	120.80
7	J	22	TYR	CB-CG-CD1	7.48	125.49	121.00
1	Z	759	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	Z	104	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	Z	30	LYS	CA-CB-CG	7.27	129.39	113.40
6	M	231	LEU	CB-CG-CD1	7.21	123.26	111.00
1	Z	104	ASP	CB-CG-OD1	7.20	124.78	118.30
3	I	63	GLU	OE1-CD-OE2	-7.14	114.73	123.30
8	8	331	ARG	CA-CB-CG	7.13	129.09	113.40
8	8	416	PHE	CB-CG-CD1	7.11	125.77	120.80
1	Z	369	PHE	CB-CG-CD2	-7.02	115.88	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	471	LEU	CA-CB-CG	6.95	131.29	115.30
1	Z	802	ASP	N-CA-CB	-6.94	98.11	110.60
1	Z	374	LEU	CB-CG-CD2	6.90	122.72	111.00
1	Z	430	LEU	CB-CG-CD1	-6.79	99.46	111.00
1	Z	9	GLN	CA-CB-CG	6.75	128.24	113.40
8	8	316	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	Z	557	GLU	CA-CB-CG	6.62	127.97	113.40
1	Z	142	ASP	CB-CG-OD1	6.62	124.25	118.30
1	Z	7	LYS	CD-CE-NZ	6.61	126.89	111.70
8	8	416	PHE	CB-CG-CD2	-6.58	116.19	120.80
1	Z	131	LYS	CB-CG-CD	6.47	128.42	111.60
3	I	125	MET	N-CA-C	-6.47	93.54	111.00
1	Z	287	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	Z	91	PHE	CB-CG-CD2	-6.43	116.30	120.80
8	8	189	ARG	NE-CZ-NH1	6.40	123.50	120.30
8	8	202	GLY	O-C-N	-6.39	112.34	123.20
1	Z	376	SER	N-CA-C	6.37	128.19	111.00
1	Z	497	PHE	CB-CG-CD1	6.36	125.25	120.80
1	Z	244	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	Z	358	TYR	CB-CG-CD1	6.34	124.80	121.00
6	M	300	GLU	OE1-CD-OE2	-6.32	115.72	123.30
1	Z	441	TYR	CB-CG-CD2	-6.26	117.25	121.00
1	Z	592	GLU	OE1-CD-OE2	-6.23	115.83	123.30
1	Z	504	GLU	CA-CB-CG	6.20	127.03	113.40
1	Z	272	TYR	CB-CG-CD2	-6.17	117.30	121.00
8	8	493	MET	CG-SD-CE	-6.17	90.33	100.20
1	Z	84	ALA	C-N-CA	6.17	137.12	121.70
4	K	48	TYR	CB-CG-CD2	-6.14	117.31	121.00
1	Z	85	VAL	C-N-CD	-6.12	107.14	120.60
5	L	291	PHE	N-CA-CB	-6.12	99.58	110.60
1	Z	471	LEU	CB-CG-CD2	-6.09	100.64	111.00
8	8	442	ASN	CB-CA-C	-6.08	98.24	110.40
1	Z	76	LYS	CD-CE-NZ	-6.06	97.77	111.70
1	Z	900	LEU	CA-CB-CG	6.00	129.09	115.30
3	I	101	GLY	CA-C-N	-5.96	104.08	117.20
1	Z	170	GLU	CG-CD-OE1	5.96	130.22	118.30
7	J	400	VAL	N-CA-C	-5.96	94.91	111.00
8	8	114	MET	CB-CG-SD	5.96	130.27	112.40
8	8	316	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	Z	30	LYS	CB-CG-CD	5.91	126.97	111.60
4	K	135	MET	CG-SD-CE	5.89	109.63	100.20
5	L	243	PHE	CB-CG-CD1	5.89	124.92	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	170	GLU	CA-CB-CG	5.88	126.33	113.40
8	8	487	ASP	CB-CG-OD1	5.82	123.53	118.30
3	I	345	ASP	N-CA-CB	-5.80	100.16	110.60
3	I	54	ARG	NE-CZ-NH2	-5.79	117.40	120.30
5	L	137	ARG	NE-CZ-NH2	-5.79	117.40	120.30
2	H	203	LYS	CB-CG-CD	5.78	126.63	111.60
1	Z	108	ASP	CB-CG-OD1	5.76	123.48	118.30
1	Z	287	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	H	314	VAL	CG1-CB-CG2	5.74	120.09	110.90
8	8	189	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	Z	142	ASP	CB-CG-OD2	-5.73	113.15	118.30
1	Z	358	TYR	CB-CG-CD2	-5.73	117.56	121.00
2	H	434	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	Z	7	LYS	CB-CG-CD	5.70	126.43	111.60
7	J	13	GLU	CA-CB-CG	5.69	125.91	113.40
8	8	487	ASP	CB-CG-OD2	-5.67	113.19	118.30
7	J	116	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	Z	140	LEU	CB-CG-CD2	5.56	120.46	111.00
1	Z	108	ASP	CB-CG-OD2	-5.54	113.31	118.30
7	J	32	LEU	CA-CB-CG	5.51	127.98	115.30
1	Z	377	ALA	CB-CA-C	5.48	118.32	110.10
4	K	49	PHE	CB-CG-CD2	-5.48	116.97	120.80
1	Z	909	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	Z	817	LEU	CB-CG-CD2	5.47	120.30	111.00
7	J	116	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	H	432	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	Z	793	PHE	CB-CG-CD2	-5.42	117.00	120.80
1	Z	170	GLU	CG-CD-OE2	-5.42	107.46	118.30
4	K	416	LYS	N-CA-C	-5.42	96.37	111.00
7	J	395	GLU	CG-CD-OE2	-5.41	107.48	118.30
7	J	231	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	Z	837	TYR	CB-CG-CD2	5.36	124.22	121.00
1	Z	9	GLN	CB-CG-CD	5.35	125.52	111.60
1	Z	921	GLU	OE1-CD-OE2	-5.33	116.91	123.30
1	Z	321	PHE	CB-CG-CD1	5.32	124.53	120.80
8	8	331	ARG	CB-CG-CD	5.30	125.38	111.60
1	Z	277	GLU	CA-CB-CG	-5.29	101.76	113.40
3	I	300	ARG	CB-CG-CD	5.27	125.30	111.60
3	I	408	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	Z	356	ASP	CB-CG-OD1	5.26	123.04	118.30
4	K	71	GLU	CG-CD-OE1	5.24	128.78	118.30
1	Z	911	LYS	N-CA-CB	5.24	120.03	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	738	TYR	CA-CB-CG	5.21	123.31	113.40
7	J	35	ARG	CG-CD-NE	-5.19	100.89	111.80
1	Z	376	SER	CB-CA-C	-5.17	100.27	110.10
8	8	453	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	Z	909	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	Z	202	ARG	NE-CZ-NH1	5.10	122.85	120.30
8	8	430	TYR	CB-CG-CD2	-5.10	117.94	121.00
5	L	284	ASP	CB-CG-OD1	5.09	122.88	118.30
3	I	57	LEU	O-C-N	5.07	130.82	122.70
1	Z	759	ARG	CB-CG-CD	5.07	124.77	111.60
8	8	199	ASP	CB-CA-C	-5.07	100.27	110.40
1	Z	30	LYS	CD-CE-NZ	5.06	123.34	111.70
1	Z	512	ILE	CA-CB-CG2	-5.06	100.79	110.90
7	J	175	GLU	CA-CB-CG	5.05	124.52	113.40
1	Z	138	ARG	CD-NE-CZ	5.04	130.66	123.60
1	Z	704	GLU	CG-CD-OE1	5.04	128.37	118.30
6	M	42	ARG	CG-CD-NE	5.00	122.31	111.80

There are no chirality outliers.

All (96) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	8	151	ALA	Mainchain
8	8	175	SER	Peptide
8	8	208	GLN	Peptide
8	8	233	PHE	Sidechain
8	8	244	THR	Peptide
8	8	245	ALA	Mainchain
8	8	271	PHE	Sidechain
8	8	309	PHE	Sidechain
8	8	443	SER	Peptide
8	8	466	ASP	Mainchain
8	8	482	GLY	Peptide
9	9	52	ASP	Sidechain
9	9	75	GLY	Peptide
2	H	151	GLN	Peptide
2	H	313	ALA	Peptide
2	H	94	GLU	Peptide
2	H	96	PRO	Peptide
3	I	101	GLY	Peptide
3	I	344	ILE	Peptide
3	I	429	GLU	Peptide

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Mol	Chain	Res	Type	Group
3	I	63	GLU	Sidechain
7	J	10	ILE	Peptide
7	J	118	ASP	Peptide
7	J	13	GLU	Sidechain
7	J	144	ASP	Sidechain
7	J	22	TYR	Sidechain
7	J	283	GLU	Sidechain
7	J	284	THR	Peptide
7	J	29	GLU	Sidechain
7	J	391	ASN	Sidechain
7	J	395	GLU	Sidechain
7	J	399	SER	Mainchain
7	J	60	ASP	Sidechain
4	K	178	ASP	Sidechain
4	K	204	ASP	Sidechain
4	K	263	GLU	Sidechain
4	K	36	ASN	Sidechain
4	K	376	ASP	Sidechain
4	K	411	TYR	Sidechain
4	K	46	ASP	Sidechain
4	K	49	PHE	Sidechain
4	K	57	GLU	Sidechain
4	K	71	GLU	Sidechain
5	L	181	ASP	Sidechain
5	L	244	ILE	Peptide
5	L	290	ARG	Peptide
5	L	320	GLN	Peptide
5	L	376	PHE	Peptide
5	L	49	GLU	Sidechain
6	M	105	ASN	Peptide
6	M	178	GLU	Peptide
6	M	290	ARG	Peptide
6	M	298	ASP	Sidechain
6	M	300	GLU	Sidechain
6	M	314	GLY	Peptide
6	M	316	SER	Peptide
1	Z	104	ASP	Sidechain
1	Z	108	ASP	Sidechain
1	Z	138	ARG	Sidechain
1	Z	142	ASP	Sidechain,Mainchain
1	Z	174	GLU	Mainchain
1	Z	219	ASP	Sidechain

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Mol	Chain	Res	Type	Group
1	Z	222	ASP	Sidechain
1	Z	239	GLU	Sidechain
1	Z	260	GLU	Sidechain
1	Z	272	TYR	Sidechain
1	Z	321	PHE	Sidechain
1	Z	328	ASP	Sidechain
1	Z	33	GLU	Sidechain
1	Z	356	ASP	Sidechain
1	Z	363	ASP	Sidechain
1	Z	369	PHE	Sidechain
1	Z	394	TYR	Sidechain
1	Z	4	GLU	Peptide
1	Z	408	TYR	Sidechain
1	Z	413	ASP	Sidechain
1	Z	468	GLU	Sidechain
1	Z	503	ASP	Sidechain
1	Z	550	PHE	Sidechain
1	Z	583	ASP	Sidechain
1	Z	592	GLU	Sidechain
1	Z	633	GLU	Sidechain
1	Z	634	ASP	Sidechain
1	Z	65	GLU	Sidechain
1	Z	718	ASP	Sidechain
1	Z	73	GLU	Sidechain
1	Z	750	GLU	Sidechain
1	Z	787	ASP	Sidechain
1	Z	793	PHE	Sidechain
1	Z	799	PHE	Sidechain
1	Z	810	ASN	Sidechain
1	Z	852	GLN	Sidechain
1	Z	9	GLN	Sidechain
1	Z	91	PHE	Sidechain
1	Z	921	GLU	Sidechain

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	Z	7005	0	6932	85	0
2	H	3057	0	3130	58	0
3	I	3015	0	3084	71	0
4	K	3113	0	3169	55	0
5	L	3082	0	3157	35	0
6	M	3285	0	3323	57	0
7	J	3171	0	3313	48	0
8	8	3034	0	3005	30	0
9	9	601	0	630	7	0
10	H	31	0	12	3	0
10	I	31	0	12	1	0
10	K	31	0	12	0	0
10	L	31	0	12	3	0
10	M	31	0	12	2	0
11	H	1	0	0	0	0
11	I	1	0	0	0	0
11	J	1	0	0	0	0
11	K	1	0	0	0	0
11	L	1	0	0	0	0
11	M	1	0	0	0	0
12	J	27	0	12	0	0
All	All	29551	0	29815	393	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 7.

All (393) 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)
4:K:344:ARG:O	4:K:349:ARG:NH1	1.79	1.15
1:Z:40:GLU:HB3	1:Z:44:LYS:HZ1	0.98	1.13
1:Z:30:LYS:HZ2	1:Z:44:LYS:NZ	1.46	1.12
10:L:501:ATP:O3A	6:M:339:ARG:NH2	1.86	1.06
2:H:356:ASN:ND2	10:H:501:ATP:O2G	1.88	1.06
1:Z:40:GLU:HB3	1:Z:44:LYS:NZ	1.80	0.96
3:I:122:SER:OG	3:I:125:MET:O	1.85	0.94
5:L:358:LEU:HD21	5:L:377:GLU:HB3	1.51	0.93
1:Z:748:LEU:CG	3:I:83:LYS:HB2	1.75	0.90
1:Z:748:LEU:HG	3:I:83:LYS:HB2	1.53	0.90
8:8:273:ARG:NH2	8:8:343:ASP:OD1	2.06	0.88
1:Z:145:ASP:HA	1:Z:149:TRP:HE1	1.37	0.88
7:J:342:ASN:O	7:J:345:LYS:HG2	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:30:LYS:HZ2	1:Z:44:LYS:HZ3	1.21	0.84
3:I:115:ASP:CB	8:8:486:SER:HA	2.10	0.82
1:Z:40:GLU:CB	1:Z:44:LYS:HZ1	1.87	0.82
2:H:221:LEU:HD23	2:H:246:ILE:HD13	1.62	0.80
1:Z:30:LYS:NZ	1:Z:44:LYS:HZ3	1.80	0.79
7:J:71:TYR:O	7:J:115:LEU:HD12	1.83	0.79
1:Z:146:PHE:H	1:Z:149:TRP:HE1	1.30	0.79
1:Z:30:LYS:NZ	1:Z:44:LYS:NZ	2.29	0.78
6:M:315:PHE:O	6:M:316:SER:O	2.00	0.78
1:Z:145:ASP:HA	1:Z:149:TRP:NE1	2.00	0.76
1:Z:93:ARG:HG2	1:Z:135:LEU:HD13	1.68	0.76
1:Z:30:LYS:HZ2	1:Z:44:LYS:HZ2	1.34	0.75
2:H:356:ASN:ND2	10:H:501:ATP:PG	2.59	0.74
7:J:401:ALA:O	7:J:402:LYS:HB2	1.89	0.73
7:J:132:PRO:O	7:J:135:SER:OG	2.06	0.73
1:Z:145:ASP:CG	1:Z:149:TRP:HZ2	1.92	0.73
8:8:208:GLN:HG3	8:8:208:GLN:O	1.90	0.72
5:L:108:VAL:O	5:L:142:LYS:HG3	1.89	0.72
3:I:402:LEU:HA	3:I:405:ARG:HD3	1.72	0.71
5:L:243:PHE:HD2	5:L:245:PHE:CE1	2.10	0.69
1:Z:382:ALA:O	1:Z:386:VAL:HG23	1.94	0.68
3:I:230:THR:OG1	10:I:501:ATP:O2B	2.11	0.68
3:I:170:VAL:HA	7:J:231:ARG:HG3	1.76	0.68
6:M:207:PHE:CE1	6:M:212:ILE:HG13	2.29	0.68
4:K:121:ARG:HD3	4:K:122:ILE:N	2.10	0.67
4:K:137:VAL:HG21	4:K:146:LEU:HD11	1.75	0.67
6:M:316:SER:O	6:M:317:SER:OG	2.08	0.67
6:M:426:LYS:HD3	6:M:427:SER:H	1.60	0.67
1:Z:562:TRP:O	1:Z:566:LEU:HD23	1.95	0.67
4:K:252:ARG:NH1	4:K:253:MET:SD	2.68	0.67
1:Z:30:LYS:HZ2	1:Z:44:LYS:CE	2.07	0.66
5:L:243:PHE:CD2	5:L:245:PHE:CE1	2.84	0.66
3:I:115:ASP:HB3	8:8:486:SER:HA	1.77	0.66
7:J:234:PHE:CE1	7:J:279:LEU:HD21	2.31	0.66
2:H:311:ILE:HA	2:H:313:ALA:O	1.97	0.65
2:H:368:PRO:HA	2:H:371:ILE:HG22	1.78	0.65
4:K:306:PHE:CE2	4:K:313:LYS:HA	2.32	0.65
3:I:150:HIS:O	3:I:154:MET:HE2	1.97	0.65
4:K:139:LEU:HD23	4:K:146:LEU:HA	1.77	0.65
1:Z:748:LEU:HD23	3:I:83:LYS:CG	2.27	0.65
4:K:306:PHE:CZ	4:K:311:ASN:HB3	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:8:118:CYS:SG	9:9:76:GLZ:C	2.85	0.64
2:H:371:ILE:O	2:H:372:ASP:O	2.16	0.64
6:M:178:GLU:O	6:M:179:THR:O	2.16	0.63
1:Z:145:ASP:OD2	1:Z:149:TRP:CZ2	2.51	0.63
7:J:77:LYS:HE2	7:J:85:LEU:HD23	1.80	0.63
6:M:173:ASP:O	6:M:174:GLU:HB2	1.97	0.63
6:M:253:GLN:HG3	6:M:255:TYR:H	1.64	0.63
6:M:189:GLN:HE21	6:M:350:PRO:HD3	1.64	0.62
4:K:65:GLU:OE1	7:J:40:ASN:HB3	1.99	0.62
3:I:115:ASP:CG	8:8:486:SER:HB3	2.20	0.62
1:Z:280:ASP:O	1:Z:284:LEU:HD23	1.99	0.62
2:H:372:ASP:O	2:H:373:ARG:O	2.17	0.62
5:L:142:LYS:HG2	5:L:143:GLY:N	2.14	0.62
2:H:465:GLN:O	2:H:466:TYR:HB2	1.99	0.62
5:L:241:ALA:O	5:L:243:PHE:HD1	1.83	0.62
6:M:207:PHE:HZ	6:M:213:ARG:C	2.03	0.62
1:Z:40:GLU:O	1:Z:44:LYS:HD2	2.00	0.62
7:J:134:VAL:O	7:J:138:MET:HG2	2.00	0.62
1:Z:894:MET:O	1:Z:900:LEU:HB3	2.00	0.62
2:H:203:LYS:CD	2:H:269:ALA:O	2.48	0.61
4:K:343:LEU:O	4:K:344:ARG:O	2.18	0.61
1:Z:146:PHE:N	1:Z:149:TRP:HE1	1.96	0.61
3:I:101:GLY:HA3	3:I:102:ASN:O	2.00	0.61
7:J:232:GLU:OE1	7:J:232:GLU:N	2.33	0.61
1:Z:898:HIS:O	1:Z:899:GLN:HB2	2.01	0.61
2:H:273:ARG:HE	3:I:316:PHE:HB2	1.64	0.61
4:K:396:ARG:HH22	5:L:192:GLU:HG3	1.64	0.60
7:J:234:PHE:CZ	7:J:279:LEU:HD21	2.35	0.60
2:H:203:LYS:HD3	2:H:270:THR:HA	1.83	0.60
8:8:354:VAL:HG13	8:8:357:ARG:HH21	1.65	0.60
2:H:62:ARG:O	2:H:65:GLU:HG2	2.02	0.60
3:I:330:LYS:CE	3:I:333:THR:HG21	2.32	0.60
3:I:115:ASP:HB3	8:8:486:SER:CA	2.32	0.60
6:M:210:MET:CE	6:M:212:ILE:HD11	2.31	0.59
3:I:212:GLY:O	3:I:213:ILE:O	2.21	0.59
6:M:116:ALA:HB1	6:M:128:PHE:CE1	2.38	0.59
1:Z:40:GLU:CB	1:Z:44:LYS:NZ	2.55	0.59
1:Z:308:LYS:O	1:Z:309:GLN:O	2.19	0.59
1:Z:763:HIS:CE1	1:Z:795:THR:HG22	2.38	0.59
1:Z:395:CYS:SG	1:Z:842:GLN:NE2	2.70	0.58
1:Z:842:GLN:NE2	1:Z:845:LEU:HD22	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:179:THR:O	6:M:181:SER:N	2.36	0.58
6:M:207:PHE:CE2	6:M:212:ILE:O	2.56	0.58
3:I:115:ASP:HB3	8:8:486:SER:CB	2.33	0.58
3:I:115:ASP:OD1	8:8:486:SER:HB3	2.03	0.58
4:K:139:LEU:CD2	4:K:146:LEU:HA	2.34	0.58
3:I:115:ASP:OD1	8:8:486:SER:CA	2.52	0.58
1:Z:85:VAL:O	1:Z:85:VAL:CG1	2.51	0.58
3:I:289:THR:HB	3:I:330:LYS:NZ	2.18	0.58
1:Z:145:ASP:CA	1:Z:149:TRP:HE1	2.13	0.57
5:L:244:ILE:O	5:L:279:PHE:CD1	2.58	0.57
6:M:426:LYS:CD	6:M:427:SER:H	2.18	0.57
2:H:203:LYS:HD2	2:H:269:ALA:O	2.05	0.57
4:K:320:ARG:HB2	4:K:323:THR:HG23	1.84	0.57
7:J:167:PRO:HD2	7:J:289:LYS:HZ1	1.69	0.57
2:H:302:LYS:HD3	2:H:303:ALA:HB2	1.87	0.57
4:K:356:ILE:HB	4:K:387:MET:HE2	1.87	0.56
4:K:306:PHE:HE2	4:K:313:LYS:HA	1.70	0.56
5:L:244:ILE:HA	5:L:245:PHE:HB2	1.86	0.56
2:H:246:ILE:HD11	2:H:375:VAL:HG12	1.86	0.56
2:H:380:PRO:HD2	2:H:414:SER:O	2.05	0.56
6:M:374:ILE:HD11	6:M:379:LEU:HD11	1.88	0.56
1:Z:442:VAL:O	1:Z:443:ASP:O	2.24	0.56
6:M:95:GLU:O	6:M:96:ASN:O	2.23	0.56
2:H:356:ASN:CG	10:H:501:ATP:O2G	2.43	0.56
2:H:99:VAL:O	2:H:150:LYS:HG2	2.06	0.56
1:Z:842:GLN:O	1:Z:842:GLN:HG2	2.05	0.56
10:L:501:ATP:PA	6:M:339:ARG:HH22	2.29	0.56
6:M:129:LEU:CD1	6:M:131:MET:HA	2.36	0.56
2:H:271:PHE:HB3	2:H:273:ARG:HH11	1.70	0.55
6:M:207:PHE:HZ	6:M:213:ARG:O	1.87	0.55
2:H:441:LYS:HE2	2:H:441:LYS:HA	1.88	0.55
4:K:166:LYS:HD3	4:K:167:PRO:HD2	1.88	0.55
4:K:124:SER:O	4:K:125:THR:OG1	2.20	0.55
2:H:251:PRO:HD2	2:H:378:SER:HA	1.89	0.55
4:K:81:ARG:CD	4:K:85:GLU:OE1	2.54	0.55
2:H:84:ILE:HG23	2:H:85:MET:HG3	1.89	0.55
1:Z:269:TYR:CE2	1:Z:293:MET:HG3	2.42	0.54
2:H:302:LYS:HD3	2:H:303:ALA:N	2.21	0.54
1:Z:748:LEU:CD2	3:I:83:LYS:CG	2.62	0.54
5:L:284:ASP:OD2	6:M:291:PHE:CD1	2.61	0.54
3:I:117:HIS:CE1	8:8:485:GLU:OE2	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:166:LYS:HD2	4:K:228:ASN:OD1	2.07	0.54
7:J:221:LYS:O	7:J:221:LYS:HG2	2.08	0.54
6:M:86:MET:O	6:M:86:MET:SD	2.66	0.53
6:M:230:LEU:HD13	10:M:501:ATP:H2'	1.90	0.53
3:I:117:HIS:NE2	8:8:485:GLU:OE2	2.40	0.53
5:L:243:PHE:CD2	5:L:245:PHE:HE1	2.25	0.53
7:J:8:SER:O	7:J:9:ASN:HB2	2.09	0.53
1:Z:85:VAL:O	1:Z:85:VAL:HG12	2.08	0.53
5:L:290:ARG:HD2	5:L:290:ARG:O	2.09	0.53
6:M:223:PRO:O	6:M:226:THR:HG23	2.09	0.53
1:Z:352:LYS:HG2	1:Z:462:VAL:HG23	1.91	0.53
6:M:168:LYS:HE3	6:M:168:LYS:HA	1.91	0.53
1:Z:93:ARG:HG3	1:Z:135:LEU:HD22	1.90	0.52
5:L:284:ASP:OD2	6:M:291:PHE:HD1	1.92	0.52
6:M:253:GLN:OE1	6:M:254:MET:N	2.41	0.52
1:Z:63:LEU:HD23	1:Z:63:LEU:H	1.73	0.52
1:Z:352:LYS:CG	1:Z:462:VAL:HG23	2.40	0.52
1:Z:145:ASP:CG	1:Z:149:TRP:CZ2	2.79	0.52
1:Z:154:ILE:HD13	2:H:47:ALA:HB2	1.92	0.52
1:Z:305:VAL:HG12	1:Z:307:HIS:H	1.74	0.52
2:H:202:GLU:HG3	2:H:203:LYS:H	1.74	0.52
6:M:69:ILE:O	6:M:73:ARG:HD3	2.09	0.52
1:Z:748:LEU:CD2	3:I:83:LYS:HG2	2.40	0.52
7:J:77:LYS:HE2	7:J:85:LEU:CD2	2.39	0.52
8:8:116:ASN:HA	9:9:76:GLZ:HA1	1.91	0.52
2:H:83:ASP:OD1	3:I:99:ILE:HG21	2.10	0.51
7:J:229:MET:SD	7:J:233:LEU:N	2.83	0.51
2:H:71:GLU:H	7:J:79:VAL:HG23	1.74	0.51
3:I:102:ASN:O	3:I:103:PRO:C	2.48	0.51
7:J:11:VAL:O	7:J:15:HIS:HB2	2.11	0.51
3:I:432:LEU:H	3:I:432:LEU:HD23	1.75	0.51
6:M:179:THR:C	6:M:181:SER:H	2.13	0.51
2:H:311:ILE:C	2:H:311:ILE:HD12	2.31	0.51
5:L:180:PHE:CE1	5:L:194:ARG:NH2	2.79	0.51
5:L:243:PHE:CE2	5:L:245:PHE:HE1	2.29	0.51
1:Z:145:ASP:CB	1:Z:149:TRP:HZ2	2.23	0.51
1:Z:171:LYS:H	1:Z:171:LYS:HD3	1.75	0.51
7:J:57:PHE:N	7:J:57:PHE:CD2	2.74	0.51
2:H:367:ARG:HH11	2:H:367:ARG:HG3	1.75	0.51
4:K:270:PHE:CZ	4:K:272:ASP:HA	2.46	0.51
6:M:207:PHE:CZ	6:M:213:ARG:C	2.83	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:101:GLY:H	3:I:104:LEU:HD21	1.76	0.50
7:J:127:GLU:OE2	7:J:127:GLU:HA	2.12	0.50
7:J:127:GLU:HG3	7:J:127:GLU:O	2.12	0.50
5:L:170:MET:HB2	5:L:244:ILE:HG22	1.94	0.50
1:Z:30:LYS:NZ	1:Z:44:LYS:HD3	2.27	0.49
3:I:150:HIS:O	3:I:154:MET:CE	2.60	0.49
3:I:247:ILE:HA	7:J:231:ARG:NH2	2.27	0.49
4:K:356:ILE:HA	4:K:359:LYS:HG3	1.94	0.49
7:J:231:ARG:HB2	7:J:232:GLU:OE1	2.12	0.49
2:H:271:PHE:HB3	2:H:273:ARG:NH1	2.27	0.49
4:K:306:PHE:CZ	4:K:311:ASN:CB	2.95	0.49
6:M:136:ASP:HB3	6:M:138:ASP:OD1	2.13	0.49
3:I:133:LEU:HD22	3:I:155:SER:OG	2.12	0.49
4:K:330:ARG:NH2	7:J:141:LYS:HE2	2.28	0.49
4:K:330:ARG:NH1	7:J:141:LYS:HE2	2.27	0.49
10:L:501:ATP:PA	6:M:339:ARG:NH2	2.84	0.49
3:I:115:ASP:OD1	8:8:486:SER:CB	2.61	0.49
1:Z:314:LEU:HD12	1:Z:956:LEU:HD21	1.95	0.49
3:I:101:GLY:C	3:I:102:ASN:O	2.51	0.49
5:L:198:GLU:O	5:L:202:LYS:HG2	2.13	0.48
7:J:138:MET:O	7:J:141:LYS:N	2.46	0.48
7:J:297:LEU:H	7:J:297:LEU:HD23	1.78	0.48
1:Z:154:ILE:CD1	2:H:47:ALA:HB2	2.43	0.48
8:8:335:PHE:HD1	8:8:335:PHE:O	1.96	0.48
1:Z:462:VAL:O	1:Z:462:VAL:HG13	2.13	0.48
2:H:191:ILE:HG13	2:H:191:ILE:O	2.13	0.48
2:H:267:THR:O	2:H:268:ASP:CG	2.51	0.48
5:L:108:VAL:O	5:L:142:LYS:CG	2.61	0.48
2:H:274:VAL:O	2:H:309:ASP:HB2	2.13	0.48
2:H:372:ASP:O	2:H:373:ARG:C	2.52	0.48
3:I:141:LEU:H	3:I:141:LEU:HD23	1.78	0.48
4:K:333:ARG:NH2	7:J:141:LYS:HB2	2.29	0.48
6:M:210:MET:HE3	6:M:212:ILE:HD11	1.94	0.48
3:I:125:MET:HB3	3:I:126:PRO:HD3	1.96	0.48
7:J:127:GLU:O	7:J:127:GLU:CG	2.61	0.48
1:Z:748:LEU:HD23	3:I:83:LYS:HG2	1.95	0.48
3:I:170:VAL:O	7:J:231:ARG:HG3	2.13	0.48
8:8:284:ILE:HG12	9:9:12:THR:HG21	1.96	0.48
6:M:129:LEU:C	6:M:129:LEU:HD12	2.34	0.47
1:Z:24:THR:HB	1:Z:25:PRO:CD	2.44	0.47
4:K:65:GLU:HG3	7:J:41:VAL:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:330:ARG:NH2	7:J:141:LYS:O	2.47	0.47
5:L:249:SER:HA	5:L:252:VAL:HG12	1.96	0.47
4:K:249:GLU:O	4:K:253:MET:HG2	2.14	0.47
2:H:371:ILE:O	2:H:371:ILE:HG13	2.15	0.47
4:K:230:THR:HG23	4:K:232:ALA:H	1.80	0.47
7:J:53:ASP:O	7:J:57:PHE:CD2	2.67	0.47
2:H:327:ASN:O	2:H:331:ARG:NH1	2.47	0.47
4:K:106:ASN:HB3	4:K:121:ARG:HH12	1.79	0.47
6:M:118:VAL:HG22	6:M:128:PHE:HD1	1.79	0.47
1:Z:439:TYR:HA	1:Z:442:VAL:HG22	1.97	0.47
3:I:330:LYS:NZ	3:I:333:THR:HG21	2.30	0.47
4:K:330:ARG:CZ	7:J:141:LYS:HE2	2.44	0.47
1:Z:149:TRP:HA	1:Z:152:GLU:HB3	1.96	0.47
1:Z:700:GLU:OE1	1:Z:700:GLU:N	2.48	0.47
2:H:327:ASN:O	2:H:331:ARG:CZ	2.63	0.47
4:K:304:ASP:OD1	7:J:141:LYS:NZ	2.47	0.47
1:Z:788:PRO:O	1:Z:789:GLN:HB2	2.15	0.46
3:I:272:GLY:C	3:I:319:ARG:HH21	2.19	0.46
6:M:230:LEU:HD12	10:M:501:ATP:O3'	2.14	0.46
3:I:150:HIS:O	3:I:154:MET:SD	2.73	0.46
2:H:402:ILE:HG23	2:H:440:GLU:OE2	2.14	0.46
3:I:138:LYS:O	3:I:141:LEU:CD2	2.63	0.46
4:K:137:VAL:HG21	4:K:146:LEU:CD1	2.43	0.46
6:M:248:ALA:HB3	6:M:249:PRO:HD3	1.96	0.46
1:Z:386:VAL:HG13	1:Z:837:TYR:CD2	2.51	0.46
1:Z:748:LEU:CG	3:I:83:LYS:CB	2.64	0.46
6:M:207:PHE:CZ	6:M:212:ILE:HG13	2.50	0.46
4:K:280:LYS:HD2	4:K:280:LYS:C	2.36	0.46
1:Z:30:LYS:HZ2	1:Z:44:LYS:CD	2.28	0.46
4:K:110:VAL:HG21	4:K:139:LEU:HD11	1.96	0.46
2:H:466:TYR:O	2:H:467:ASN:C	2.55	0.45
1:Z:601:VAL:HG23	1:Z:622:HIS:CE1	2.51	0.45
5:L:91:THR:O	5:L:95:ILE:HG12	2.15	0.45
7:J:221:LYS:O	7:J:221:LYS:CG	2.64	0.45
1:Z:386:VAL:CG1	1:Z:837:TYR:CD2	3.00	0.45
2:H:74:THR:OG1	3:I:136:VAL:HB	2.17	0.45
6:M:166:ARG:HD3	6:M:250:GLN:HE21	1.81	0.45
3:I:115:ASP:HB2	8:8:486:SER:HA	1.95	0.45
3:I:358:LYS:HA	3:I:361:ILE:HD12	1.99	0.45
5:L:244:ILE:O	5:L:279:PHE:HD1	1.97	0.45
8:8:335:PHE:O	8:8:335:PHE:CD1	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:759:ARG:HH11	1:Z:759:ARG:HD3	1.46	0.45
3:I:115:ASP:CB	8:8:486:SER:CA	2.87	0.45
2:H:465:GLN:O	2:H:466:TYR:CB	2.64	0.45
5:L:283:VAL:O	5:L:284:ASP:OD1	2.35	0.45
3:I:111:GLU:OE2	3:I:119:ILE:HD12	2.17	0.45
6:M:254:MET:HE1	6:M:254:MET:O	2.16	0.45
1:Z:81:SER:HA	1:Z:88:PRO:HB2	1.99	0.45
1:Z:879:ALA:O	1:Z:883:THR:HG23	2.16	0.45
3:I:187:LEU:H	3:I:357:THR:HG23	1.82	0.45
6:M:143:ASN:OD1	6:M:143:ASN:N	2.50	0.45
3:I:95:GLN:O	3:I:95:GLN:HG2	2.15	0.44
3:I:116:ASP:HA	3:I:138:LYS:HE3	1.99	0.44
3:I:289:THR:HB	3:I:330:LYS:HZ3	1.81	0.44
1:Z:80:SER:O	1:Z:81:SER:HB2	2.17	0.44
5:L:202:LYS:HG3	5:L:203:ASN:N	2.33	0.44
6:M:163:PHE:HB2	6:M:168:LYS:HD3	2.00	0.44
6:M:189:GLN:HE21	6:M:350:PRO:CD	2.29	0.44
1:Z:30:LYS:NZ	1:Z:44:LYS:CE	2.77	0.44
1:Z:135:LEU:CD1	1:Z:138:ARG:HH21	2.30	0.44
2:H:77:ALA:HB3	2:H:78:PRO:HD3	2.00	0.44
3:I:255:LYS:HG3	3:I:256:TYR:CE1	2.52	0.44
5:L:379:ALA:CB	5:L:416:MET:SD	3.06	0.44
7:J:229:MET:HE2	7:J:232:GLU:HB2	1.99	0.44
8:8:114:MET:H	8:8:114:MET:HG2	1.52	0.44
3:I:124:THR:O	3:I:125:MET:HB2	2.18	0.44
4:K:128:ARG:HG3	4:K:128:ARG:HH11	1.82	0.44
3:I:115:ASP:OD2	3:I:117:HIS:HB2	2.17	0.44
7:J:70:SER:O	7:J:115:LEU:HB2	2.17	0.44
6:M:63:LYS:O	6:M:67:GLU:HG2	2.17	0.44
6:M:186:LEU:HB3	6:M:189:GLN:OE1	2.18	0.44
7:J:229:MET:CE	7:J:232:GLU:HB2	2.47	0.43
2:H:267:THR:O	2:H:268:ASP:OD1	2.36	0.43
3:I:330:LYS:HE3	3:I:333:THR:HG21	2.00	0.43
7:J:167:PRO:HD2	7:J:289:LYS:NZ	2.31	0.43
4:K:306:PHE:CD2	4:K:313:LYS:HG3	2.53	0.43
1:Z:24:THR:HB	1:Z:25:PRO:HD3	1.99	0.43
1:Z:829:GLN:O	1:Z:833:GLN:HG3	2.17	0.43
3:I:125:MET:HB3	3:I:126:PRO:CD	2.48	0.43
4:K:82:ALA:O	4:K:85:GLU:HB2	2.18	0.43
4:K:162:GLY:O	4:K:163:GLU:HG2	2.18	0.43
6:M:69:ILE:HG22	6:M:73:ARG:HD3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:73:ARG:HD2	6:M:156:LEU:HD11	2.00	0.43
1:Z:591:ILE:HD12	1:Z:591:ILE:H	1.83	0.43
2:H:100:ALA:HB2	2:H:149:LEU:HD23	2.00	0.43
5:L:297:ALA:CB	6:M:300:GLU:HG3	2.48	0.43
7:J:229:MET:SD	7:J:233:LEU:HB2	2.59	0.43
8:8:118:CYS:SG	9:9:76:GLZ:CA	3.07	0.43
2:H:203:LYS:HD3	2:H:269:ALA:O	2.18	0.43
3:I:115:ASP:OD1	8:8:486:SER:N	2.52	0.43
1:Z:748:LEU:HD13	3:I:82:LEU:O	2.19	0.43
6:M:32:THR:O	6:M:36:LEU:HD12	2.18	0.43
7:J:116:ARG:HE	7:J:123:HIS:CG	2.37	0.43
2:H:380:PRO:HB2	2:H:385:ARG:CG	2.49	0.43
1:Z:560:THR:O	1:Z:563:VAL:HG22	2.19	0.43
7:J:372:GLU:O	7:J:373:ARG:HB2	2.19	0.43
1:Z:386:VAL:HG13	1:Z:837:TYR:CG	2.54	0.43
2:H:302:LYS:HD3	2:H:303:ALA:CB	2.49	0.43
4:K:236:ARG:NH2	5:L:315:PHE:N	2.67	0.43
4:K:166:LYS:HD3	4:K:167:PRO:CD	2.48	0.42
5:L:142:LYS:HG2	5:L:143:GLY:H	1.84	0.42
4:K:159:SER:O	4:K:161:MET:SD	2.77	0.42
8:8:208:GLN:O	8:8:208:GLN:CG	2.61	0.42
1:Z:31:LYS:HE3	1:Z:79:THR:HA	2.02	0.42
3:I:285:ASP:O	3:I:289:THR:HG22	2.20	0.42
5:L:199:LEU:HA	5:L:202:LYS:CE	2.49	0.42
5:L:358:LEU:CD2	5:L:377:GLU:HB3	2.35	0.42
1:Z:68:LEU:HA	1:Z:71:LEU:HD12	2.00	0.42
3:I:101:GLY:CA	3:I:102:ASN:O	2.64	0.42
5:L:307:GLU:O	5:L:310:THR:HG22	2.20	0.42
4:K:306:PHE:CD2	4:K:313:LYS:HA	2.54	0.42
4:K:306:PHE:HZ	4:K:311:ASN:HB3	1.82	0.42
8:8:109:VAL:CG2	8:8:171:LEU:HA	2.49	0.42
1:Z:546:ILE:HG22	1:Z:574:TYR:OH	2.20	0.42
2:H:311:ILE:H	2:H:311:ILE:HG13	1.75	0.42
3:I:133:LEU:HD23	3:I:156:ILE:O	2.19	0.42
1:Z:443:ASP:O	1:Z:444:GLU:O	2.38	0.42
4:K:333:ARG:HH21	7:J:141:LYS:HB2	1.85	0.41
5:L:53:HIS:O	5:L:53:HIS:CG	2.73	0.41
6:M:216:LYS:HG2	6:M:341:GLY:O	2.20	0.41
7:J:213:VAL:HB	7:J:247:MET:HA	2.02	0.41
2:H:46:ALA:HA	2:H:49:LEU:HG	2.01	0.41
2:H:177:ASP:OD1	2:H:180:LYS:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:226:VAL:O	4:K:230:THR:HG22	2.19	0.41
4:K:397:LYS:O	4:K:398:ASN:HB2	2.20	0.41
6:M:207:PHE:HA	6:M:210:MET:HE2	2.03	0.41
1:Z:314:LEU:CD1	1:Z:956:LEU:HD21	2.50	0.41
3:I:289:THR:HB	3:I:330:LYS:HZ1	1.83	0.41
4:K:92:VAL:HB	4:K:93:PRO:HA	2.01	0.41
6:M:261:LYS:HG3	6:M:264:ARG:HH21	1.85	0.41
2:H:311:ILE:HD12	2:H:311:ILE:O	2.20	0.41
3:I:102:ASN:HB3	3:I:103:PRO:CD	2.51	0.41
3:I:175:LYS:CE	7:J:278:GLN:O	2.69	0.41
3:I:297:GLY:O	3:I:300:ARG:NH1	2.53	0.41
4:K:352:ILE:O	4:K:356:ILE:CD1	2.68	0.41
1:Z:495:ILE:HD13	1:Z:884:THR:HG21	2.03	0.41
1:Z:287:ARG:HB2	1:Z:855:LEU:HD11	2.03	0.41
4:K:76:LYS:O	4:K:80:LYS:HG2	2.21	0.41
4:K:106:ASN:HB3	4:K:121:ARG:HH22	1.86	0.41
5:L:290:ARG:HA	5:L:302:GLN:OE1	2.21	0.41
6:M:73:ARG:NH1	6:M:156:LEU:HD12	2.35	0.41
1:Z:123:ALA:HB1	1:Z:132:HIS:CE1	2.56	0.41
2:H:163:VAL:HG11	2:H:183:ILE:HG22	2.03	0.41
2:H:390:ARG:O	2:H:394:LYS:HD2	2.21	0.41
4:K:207:ARG:O	4:K:313:LYS:HB2	2.20	0.41
4:K:347:ARG:HG2	4:K:350:ARG:HH21	1.85	0.41
7:J:91:GLU:HB3	7:J:92:GLY:H	1.71	0.41
8:8:285:GLU:O	9:9:14:THR:HG23	2.20	0.41
1:Z:165:TYR:HA	1:Z:168:GLN:HE21	1.86	0.41
2:H:311:ILE:HD11	2:H:355:THR:CG2	2.50	0.41
3:I:99:ILE:HD11	3:I:135:PHE:CE1	2.55	0.41
4:K:92:VAL:HA	4:K:94:LEU:HG	2.02	0.41
6:M:163:PHE:HB2	6:M:168:LYS:CD	2.51	0.41
5:L:202:LYS:HG3	5:L:203:ASN:H	1.86	0.41
6:M:118:VAL:CG2	6:M:128:PHE:HD1	2.33	0.41
3:I:94:LYS:O	3:I:95:GLN:CB	2.69	0.40
4:K:121:ARG:HD3	4:K:122:ILE:O	2.21	0.40
5:L:199:LEU:HA	5:L:202:LYS:HE3	2.03	0.40
6:M:189:GLN:OE1	6:M:189:GLN:N	2.44	0.40
1:Z:842:GLN:HE22	1:Z:845:LEU:HD22	1.84	0.40
3:I:161:GLN:O	3:I:162:ASP:HB3	2.21	0.40
3:I:246:ARG:HH12	7:J:275:LEU:HA	1.86	0.40
6:M:256:ILE:HD11	6:M:303:ARG:HB2	2.03	0.40
8:8:199:ASP:HB2	8:8:203:GLY:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:9:4:PHE:HB3	9:9:12:THR:CG2	2.51	0.40
1:Z:249:MET:HB3	1:Z:265:LEU:HD21	2.03	0.40
2:H:203:LYS:HD3	2:H:270:THR:CA	2.51	0.40
5:L:204:PRO:HG2	5:L:205:GLU:OE1	2.21	0.40
8:8:371:GLU:O	8:8:375:LYS:HG2	2.20	0.40
3:I:300:ARG:HG3	3:I:300:ARG:HH11	1.86	0.40
4:K:158:ILE:HD12	4:K:158:ILE:HA	1.92	0.40
8:8:118:CYS:HB3	9:9:76:GLZ:O	2.21	0.40
2:H:62:ARG:HA	2:H:65:GLU:OE2	2.20	0.40
2:H:91:LEU:O	2:H:91:LEU:HG	2.21	0.40
3:I:115:ASP:OD1	8:8:486:SER:HA	2.21	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	Z	902/993 (91%)	817 (91%)	71 (8%)	14 (2%)	9 44
2	H	387/467 (83%)	350 (90%)	30 (8%)	7 (2%)	8 40
3	I	382/437 (87%)	333 (87%)	42 (11%)	7 (2%)	8 40
4	K	392/428 (92%)	358 (91%)	31 (8%)	3 (1%)	19 60
5	L	386/437 (88%)	364 (94%)	19 (5%)	3 (1%)	19 60
6	M	419/434 (96%)	376 (90%)	33 (8%)	10 (2%)	6 33
7	J	403/405 (100%)	357 (89%)	43 (11%)	3 (1%)	22 63
8	8	368/499 (74%)	336 (91%)	24 (6%)	8 (2%)	6 35
9	9	74/76 (97%)	67 (90%)	7 (10%)	0	100 100
All	All	3713/4176 (89%)	3358 (90%)	300 (8%)	55 (2%)	14 46

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Z	5	SER
1	Z	85	VAL
1	Z	142	ASP
1	Z	173	ALA
1	Z	174	GLU
1	Z	309	GLN
1	Z	366	LYS
1	Z	377	ALA
1	Z	443	ASP
1	Z	444	GLU
1	Z	498	ALA
1	Z	802	ASP
1	Z	926	ASN
2	H	95	HIS
2	H	152	ILE
2	H	314	VAL
2	H	372	ASP
2	H	466	TYR
3	I	102	ASN
3	I	125	MET
3	I	213	ILE
4	K	344	ARG
4	K	416	LYS
5	L	245	PHE
5	L	275	PRO
6	M	96	ASN
6	M	179	THR
6	M	316	SER
6	M	427	SER
7	J	11	VAL
7	J	400	VAL
8	8	201	GLN
8	8	209	ASP
8	8	245	ALA
2	H	373	ARG
4	K	415	VAL
5	L	291	PHE
6	M	106	VAL
6	M	317	SER
6	M	430	VAL
8	8	204	PHE
3	I	126	PRO
3	I	345	ASP

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Mol	Chain	Res	Type
6	M	180	TYR
8	8	151	ALA
8	8	442	ASN
8	8	444	GLU
2	H	465	GLN
6	M	174	GLU
8	8	466	ASP
1	Z	24	THR
6	M	87	ASP
3	I	315	GLY
3	I	103	PRO
7	J	10	ILE

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	Z	773/850 (91%)	735 (95%)	38 (5%)	25	50
2	H	330/399 (83%)	319 (97%)	11 (3%)	38	61
3	I	341/385 (89%)	338 (99%)	3 (1%)	78	87
4	K	346/374 (92%)	334 (96%)	12 (4%)	36	59
5	L	332/377 (88%)	329 (99%)	3 (1%)	78	87
6	M	364/375 (97%)	357 (98%)	7 (2%)	57	75
7	J	352/352 (100%)	342 (97%)	10 (3%)	43	65
8	8	337/449 (75%)	327 (97%)	10 (3%)	41	63
9	9	68/68 (100%)	68 (100%)	0	100	100
All	All	3243/3629 (89%)	3149 (97%)	94 (3%)	45	64

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	2	VAL
1	Z	7	LYS

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Mol	Chain	Res	Type
1	Z	9	GLN
1	Z	16	SER
1	Z	32	LYS
1	Z	63	LEU
1	Z	74	SER
1	Z	86	PRO
1	Z	131	LYS
1	Z	170	GLU
1	Z	171	LYS
1	Z	179	SER
1	Z	210	TYR
1	Z	239	GLU
1	Z	267	THR
1	Z	290	GLU
1	Z	293	MET
1	Z	376	SER
1	Z	387	ASN
1	Z	402	ASP
1	Z	431	ASP
1	Z	471	LEU
1	Z	479	THR
1	Z	557	GLU
1	Z	561	ASP
1	Z	583	ASP
1	Z	589	SER
1	Z	627	LYS
1	Z	728	LYS
1	Z	738	TYR
1	Z	751	ASP
1	Z	811	SER
1	Z	822	THR
1	Z	840	ARG
1	Z	848	THR
1	Z	869	ASP
1	Z	880	SER
1	Z	899	GLN
2	H	45	TYR
2	H	62	ARG
2	H	90	ARG
2	H	145	TYR
2	H	162	ARG
2	H	177	ASP

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Mol	Chain	Res	Type
2	H	203	LYS
2	H	215	LYS
2	H	271	PHE
2	H	328	GLU
2	H	436	LYS
3	I	294	SER
3	I	300	ARG
3	I	374	ASP
4	K	38	SER
4	K	45	SER
4	K	50	LYS
4	K	85	GLU
4	K	159	SER
4	K	164	ASN
4	K	178	ASP
4	K	245	LYS
4	K	280	LYS
4	K	342	SER
4	K	376	ASP
4	K	377	SER
5	L	72	ASP
5	L	275	PRO
5	L	377	GLU
6	M	93	ASP
6	M	102	GLN
6	M	182	ASP
6	M	216	LYS
6	M	231	LEU
6	M	317	SER
6	M	428	LYS
7	J	13	GLU
7	J	144	ASP
7	J	149	MET
7	J	252	SER
7	J	320	SER
7	J	338	THR
7	J	345	LYS
7	J	353	CYS
7	J	400	VAL
7	J	402	LYS
8	8	204	PHE
8	8	258	ASP

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Mol	Chain	Res	Type
8	8	260	LYS
8	8	268	THR
8	8	297	TYR
8	8	317	PHE
8	8	331	ARG
8	8	335	PHE
8	8	370	LYS
8	8	430	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	Z	37	GLN
1	Z	168	GLN
1	Z	364	ASN
1	Z	379	GLN
1	Z	622	HIS
1	Z	763	HIS
1	Z	766	HIS
4	K	164	ASN
6	M	28	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	GLZ	9	76	9	3,3,3	0.77	0	0,2,2	-	-

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	GLZ	9	76	9	-	0/0/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	9	76	GLZ	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
10	ATP	K	501	-	26,33,33	0.89	1 (3%)	31,52,52	1.23	3 (9%)
12	ADP	J	501	11	24,29,29	0.92	2 (8%)	29,45,45	1.11	2 (6%)
10	ATP	M	501	11	26,33,33	0.92	1 (3%)	31,52,52	1.23	3 (9%)
10	ATP	L	501	11	26,33,33	0.94	1 (3%)	31,52,52	1.08	1 (3%)
10	ATP	I	501	11	26,33,33	0.90	1 (3%)	31,52,52	1.34	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	ATP	H	501	-	26,33,33	0.88	1 (3%)	31,52,52	1.25	4 (12%)

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
10	ATP	K	501	-	-	3/18/38/38	0/3/3/3
12	ADP	J	501	11	-	2/12/32/32	0/3/3/3
10	ATP	M	501	11	-	9/18/38/38	0/3/3/3
10	ATP	L	501	11	-	4/18/38/38	0/3/3/3
10	ATP	I	501	11	-	7/18/38/38	0/3/3/3
10	ATP	H	501	-	-	5/18/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	J	501	ADP	C5-C4	2.20	1.46	1.40
10	K	501	ATP	C5-C4	2.18	1.46	1.40
12	J	501	ADP	C2-N3	2.07	1.35	1.32
10	H	501	ATP	C5-C4	2.06	1.46	1.40
10	M	501	ATP	C5-C4	2.05	1.46	1.40
10	L	501	ATP	C5-C4	2.05	1.46	1.40
10	I	501	ATP	C5-C4	2.01	1.46	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	I	501	ATP	N3-C2-N1	-3.73	122.85	128.68
10	M	501	ATP	N3-C2-N1	-3.44	123.30	128.68
10	H	501	ATP	N3-C2-N1	-3.24	123.61	128.68
10	L	501	ATP	N3-C2-N1	-3.23	123.63	128.68
12	J	501	ADP	N3-C2-N1	-2.99	124.01	128.68
10	H	501	ATP	N6-C6-N1	2.84	124.47	118.57
10	I	501	ATP	C1'-N9-C4	-2.80	121.72	126.64
10	I	501	ATP	N6-C6-N1	2.77	124.33	118.57
10	K	501	ATP	N3-C2-N1	-2.73	124.41	128.68
10	K	501	ATP	C4-C5-N7	-2.37	106.92	109.40
10	M	501	ATP	C4-C5-N7	-2.31	106.99	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	K	501	ATP	C3'-C2'-C1'	2.28	104.41	100.98
10	I	501	ATP	C2-N1-C6	2.24	122.59	118.75
10	M	501	ATP	O5'-C5'-C4'	2.20	116.58	108.99
10	H	501	ATP	C5-C6-N6	-2.20	117.01	120.35
12	J	501	ADP	C3'-C2'-C1'	2.11	104.16	100.98
10	H	501	ATP	C3'-C2'-C1'	2.08	104.11	100.98

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	H	501	ATP	C5'-O5'-PA-O1A
10	H	501	ATP	C5'-O5'-PA-O2A
10	I	501	ATP	C5'-O5'-PA-O3A
10	K	501	ATP	C5'-O5'-PA-O1A
10	K	501	ATP	C5'-O5'-PA-O2A
10	L	501	ATP	C5'-O5'-PA-O3A
10	M	501	ATP	C5'-O5'-PA-O3A
12	J	501	ADP	C5'-O5'-PA-O1A
12	J	501	ADP	C5'-O5'-PA-O3A
10	M	501	ATP	PB-O3A-PA-O1A
10	I	501	ATP	O4'-C4'-C5'-O5'
10	I	501	ATP	PG-O3B-PB-O3A
10	H	501	ATP	PB-O3A-PA-O2A
10	I	501	ATP	C5'-O5'-PA-O1A
10	L	501	ATP	C5'-O5'-PA-O2A
10	M	501	ATP	C5'-O5'-PA-O1A
10	M	501	ATP	C5'-O5'-PA-O2A
10	M	501	ATP	PA-O3A-PB-O3B
10	L	501	ATP	O4'-C4'-C5'-O5'
10	M	501	ATP	PG-O3B-PB-O2B
10	M	501	ATP	C4'-C5'-O5'-PA
10	I	501	ATP	C3'-C4'-C5'-O5'
10	M	501	ATP	O4'-C4'-C5'-O5'
10	H	501	ATP	C5'-O5'-PA-O3A
10	K	501	ATP	C5'-O5'-PA-O3A
10	H	501	ATP	PB-O3A-PA-O1A
10	I	501	ATP	PG-O3B-PB-O1B
10	I	501	ATP	PB-O3A-PA-O1A
10	M	501	ATP	PB-O3A-PA-O2A
10	L	501	ATP	C3'-C4'-C5'-O5'

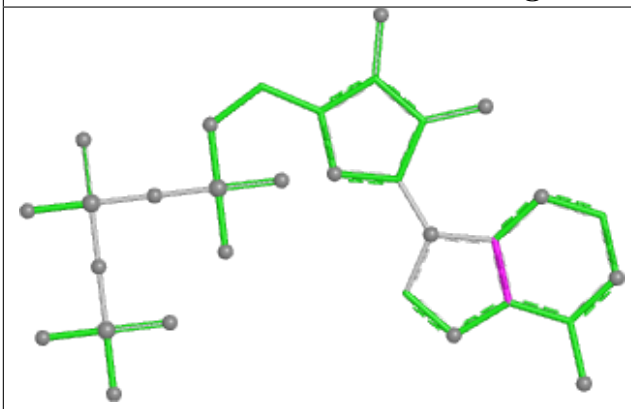
There are no ring outliers.

4 monomers are involved in 9 short contacts:

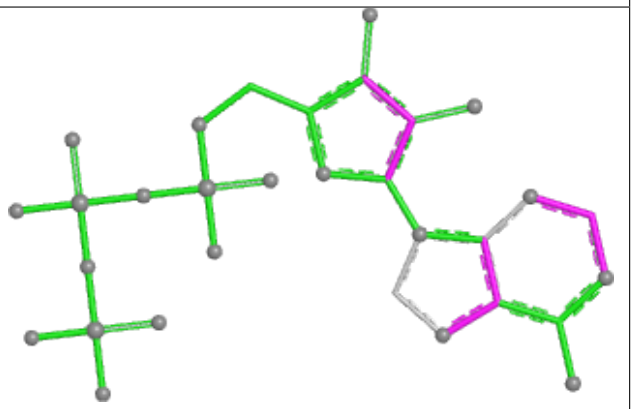
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	M	501	ATP	2	0
10	L	501	ATP	3	0
10	I	501	ATP	1	0
10	H	501	ATP	3	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

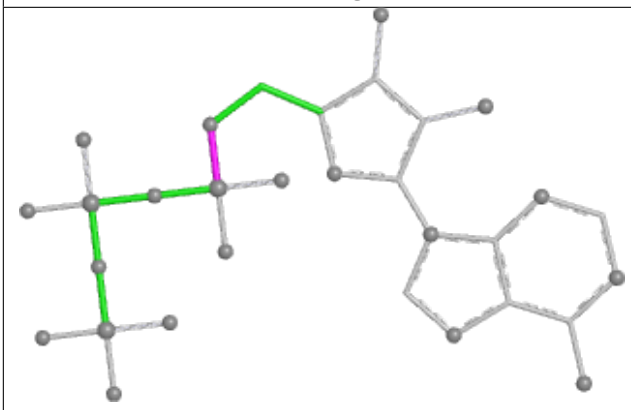
Ligand ATP K 501



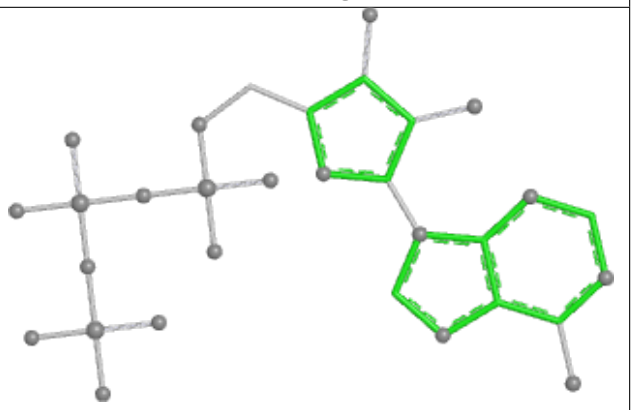
Bond lengths



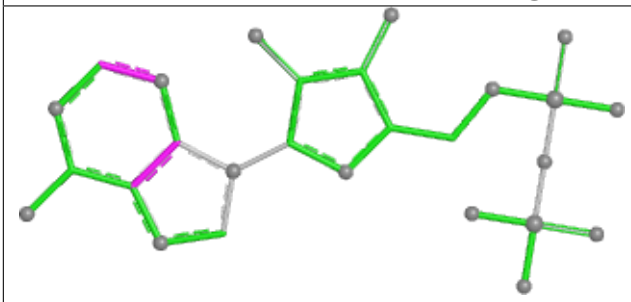
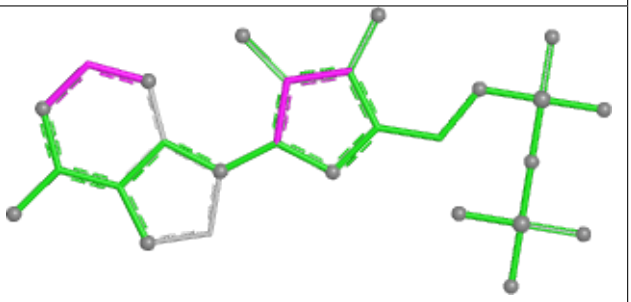
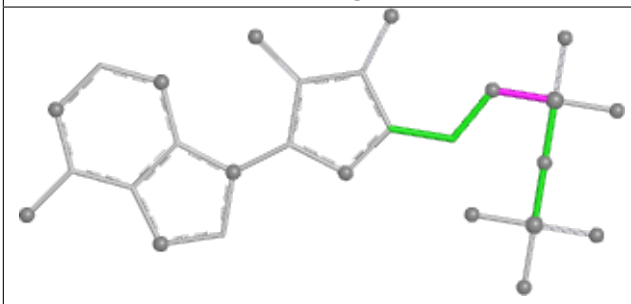
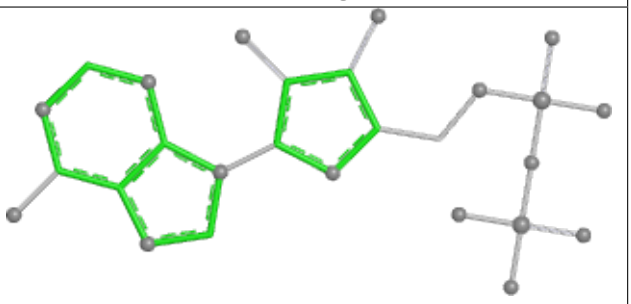
Bond angles

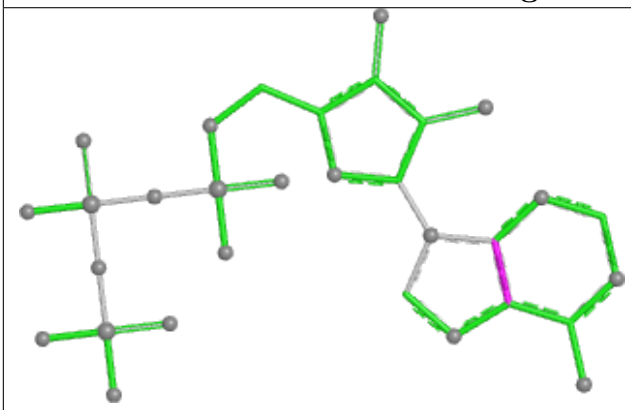
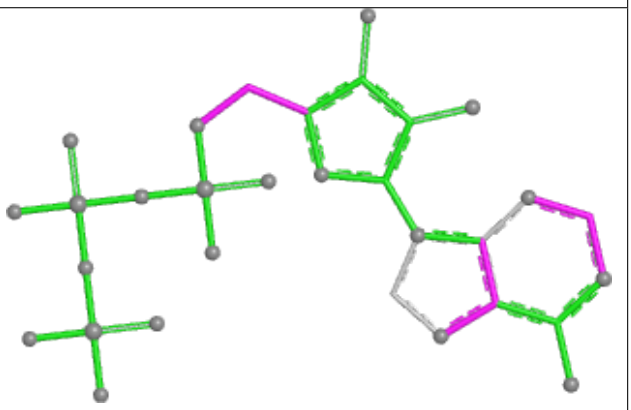
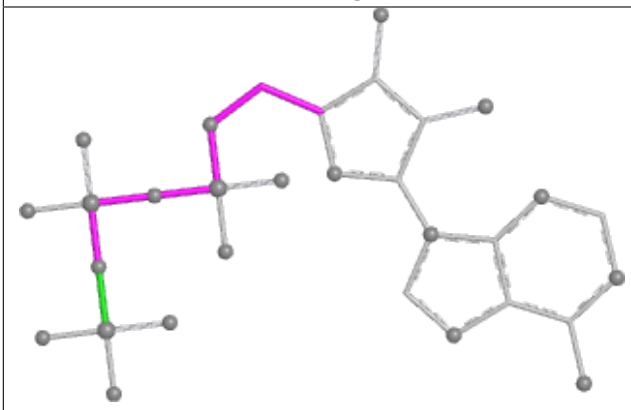
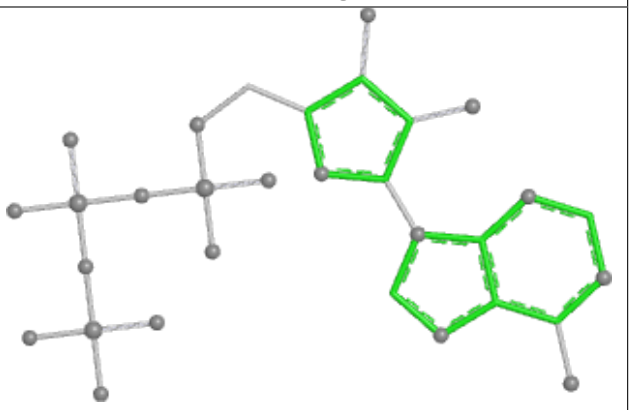


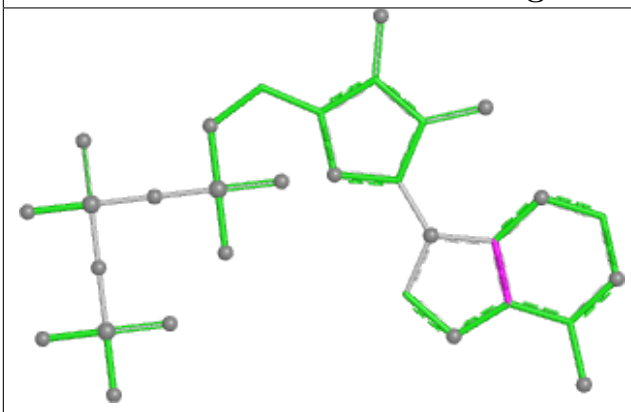
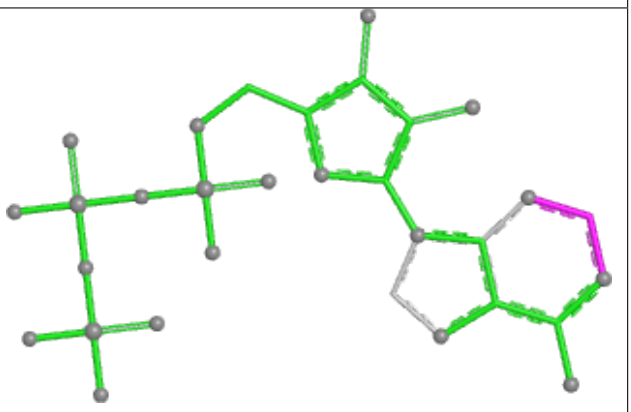
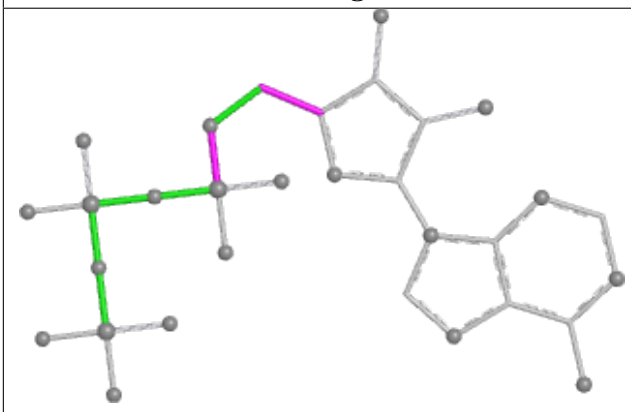
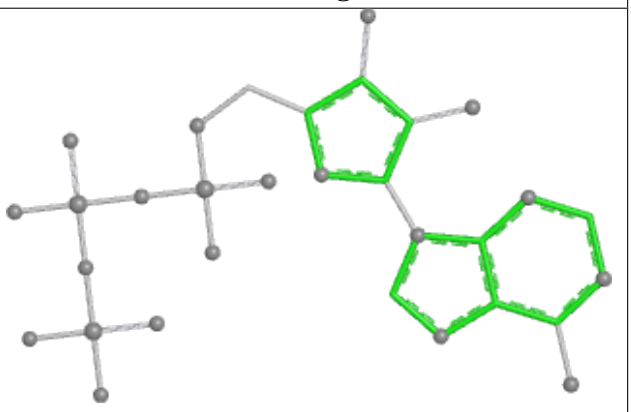
Torsions

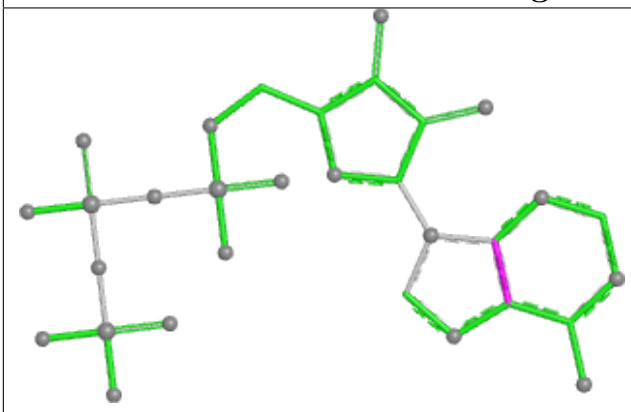
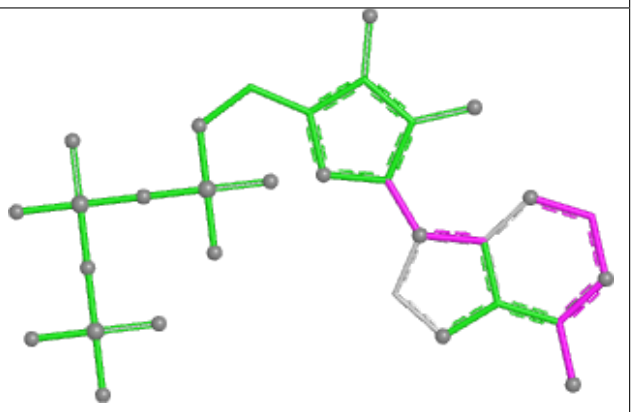
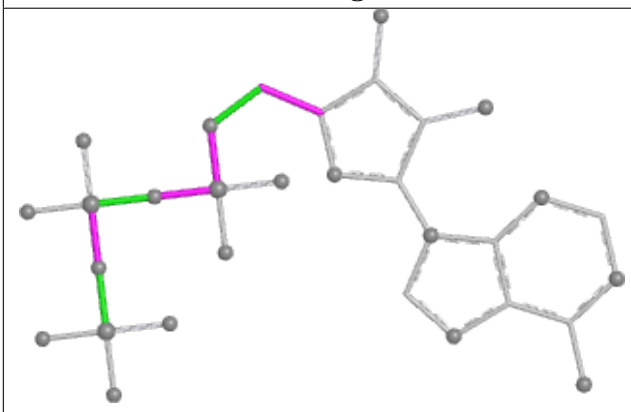
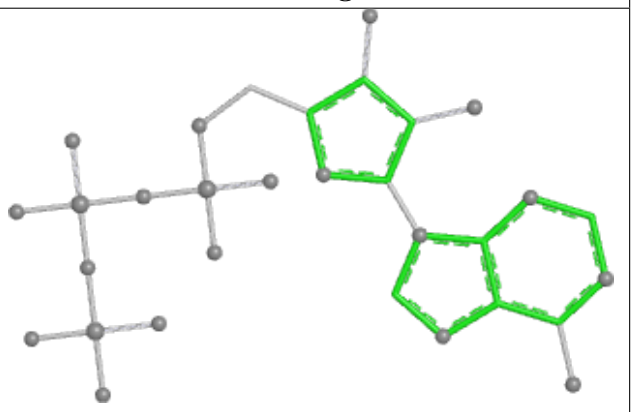


Rings

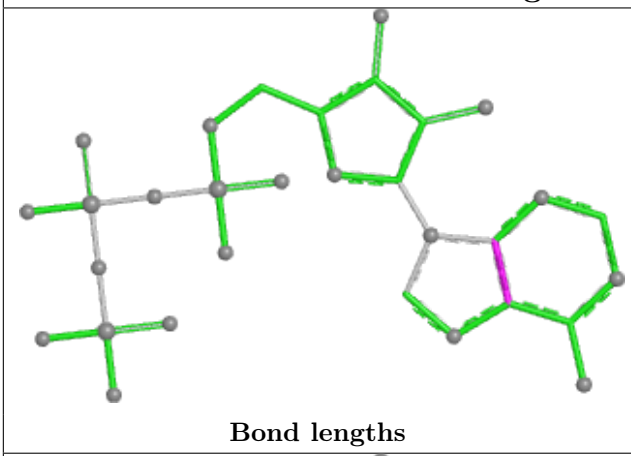
Ligand ADP J 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP M 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

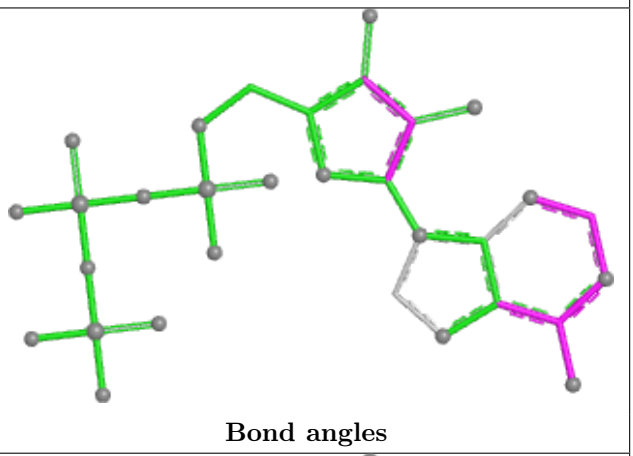
Ligand ATP L 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP I 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

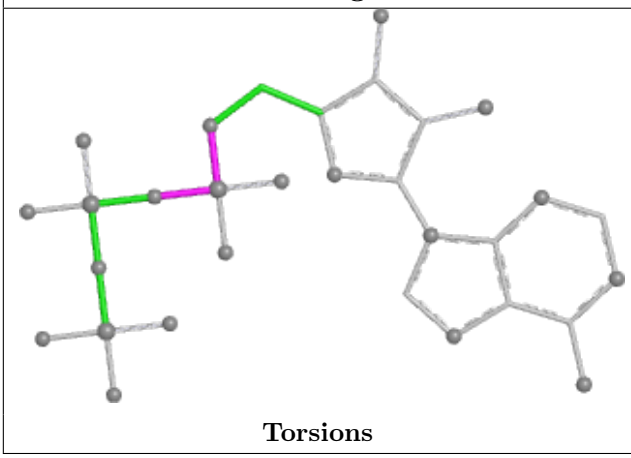
Ligand ATP H 501



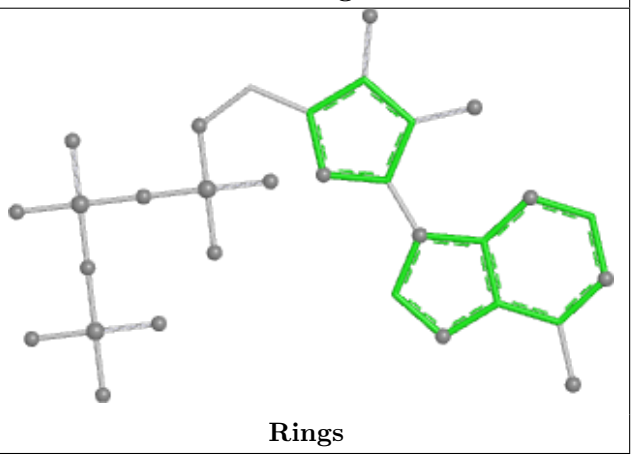
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

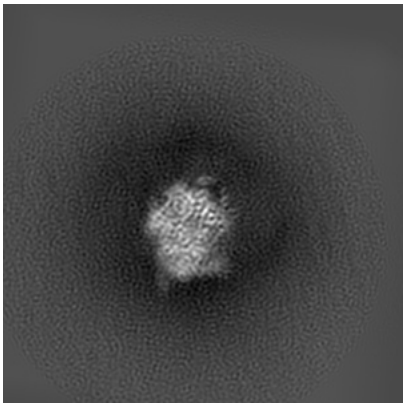
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14083. These allow visual inspection of the internal detail of the map and identification of artifacts.

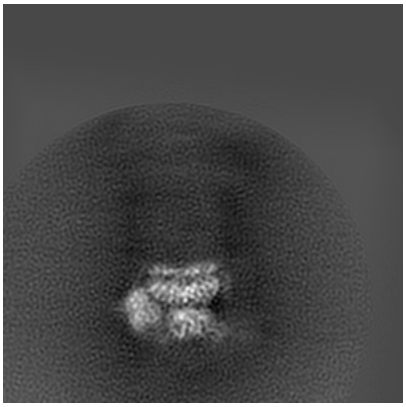
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

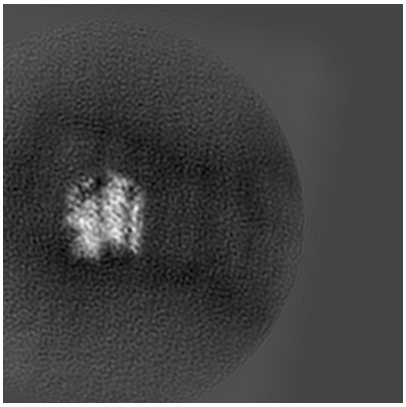
6.1.1 Primary map



X



Y

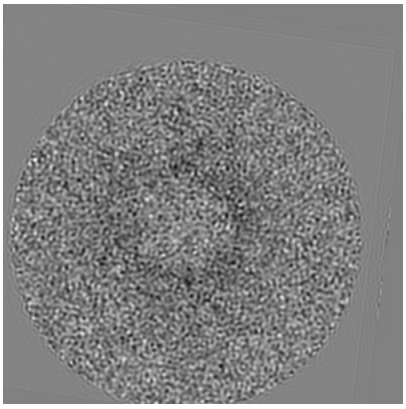


Z

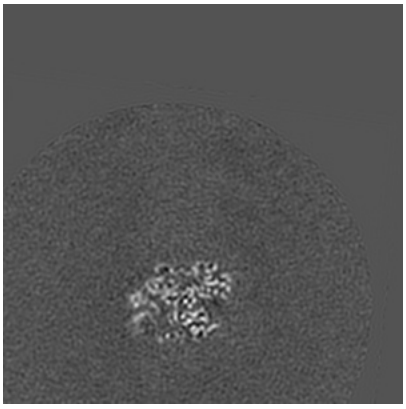
The images above show the map projected in three orthogonal directions.

6.2 Central slices

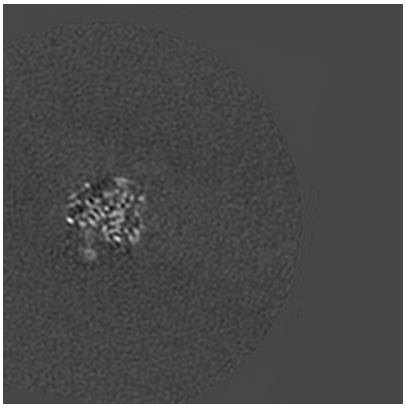
6.2.1 Primary map



X Index: 140



Y Index: 140

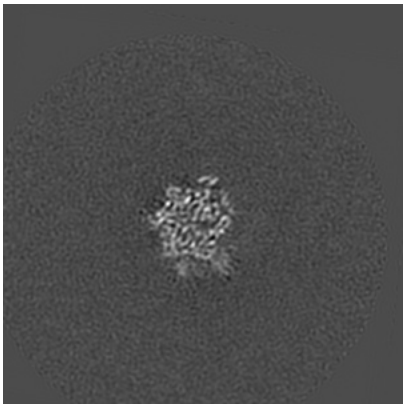


Z Index: 140

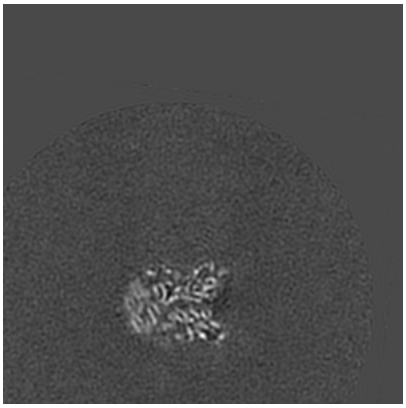
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

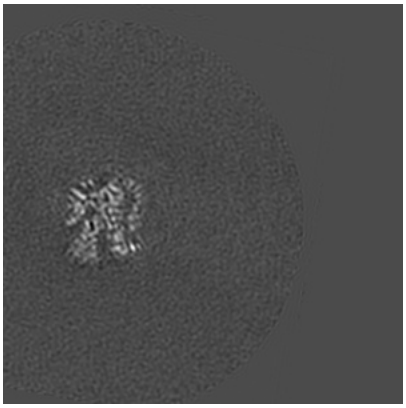
6.3.1 Primary map



X Index: 80



Y Index: 127

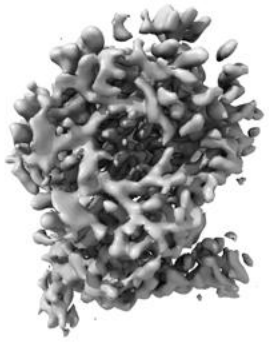


Z Index: 132

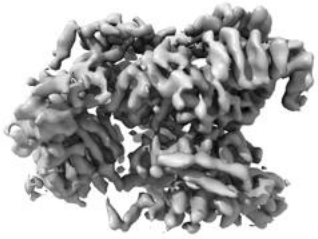
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

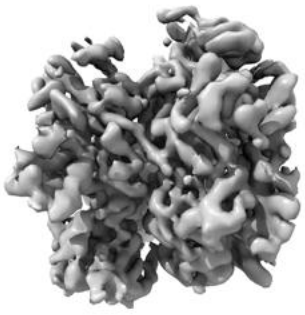
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

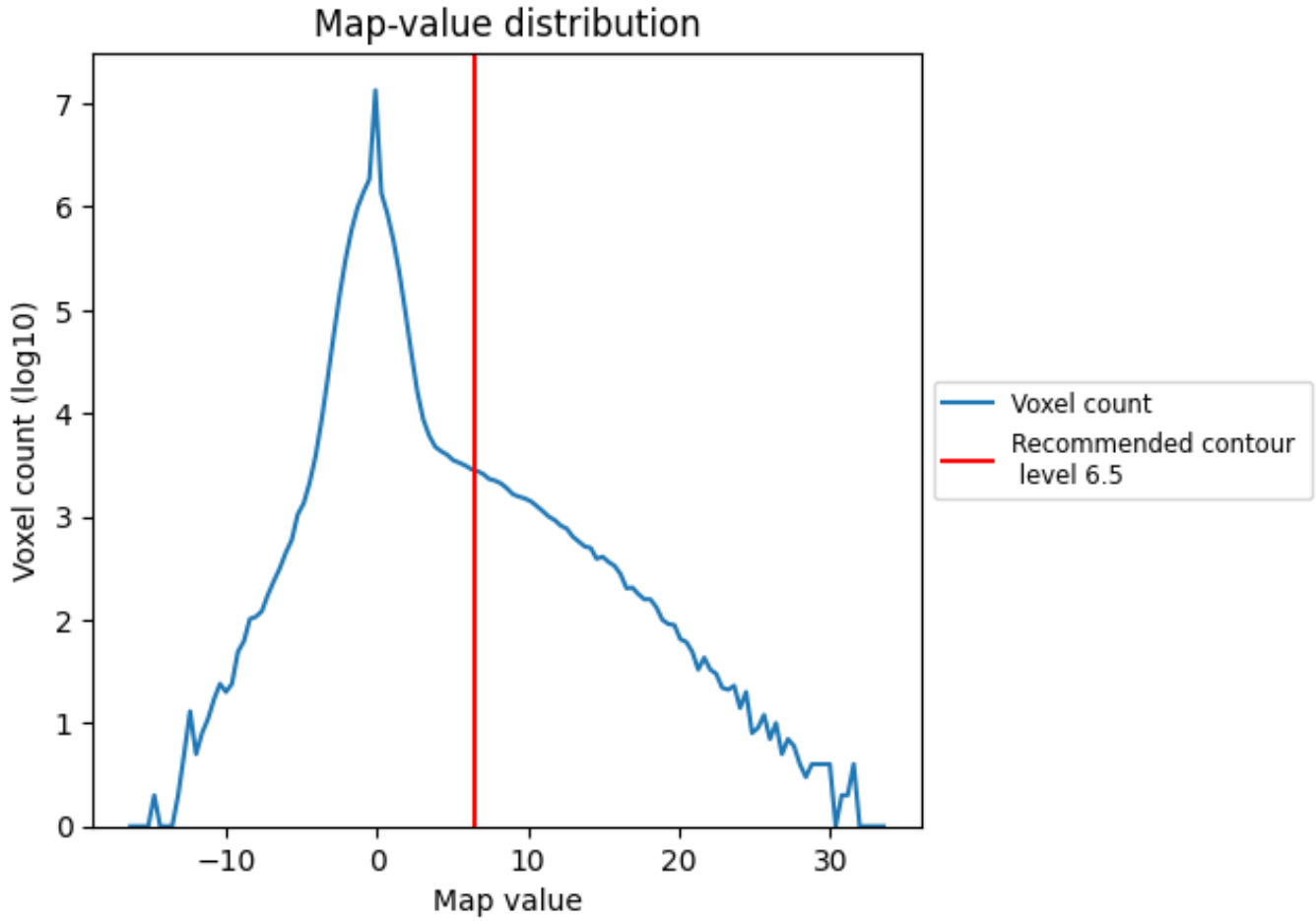
6.5 Mask visualisation (i)

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

7 Map analysis

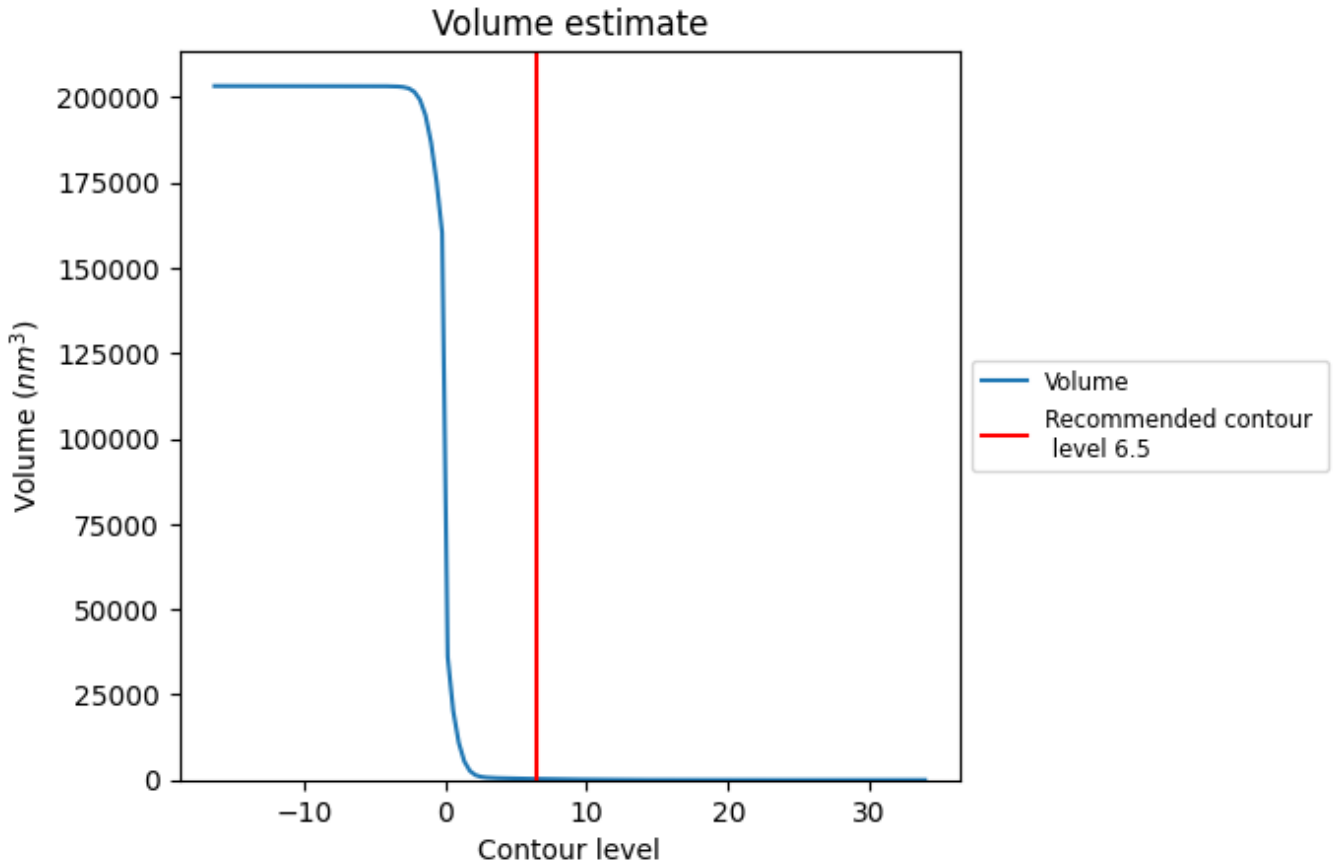
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

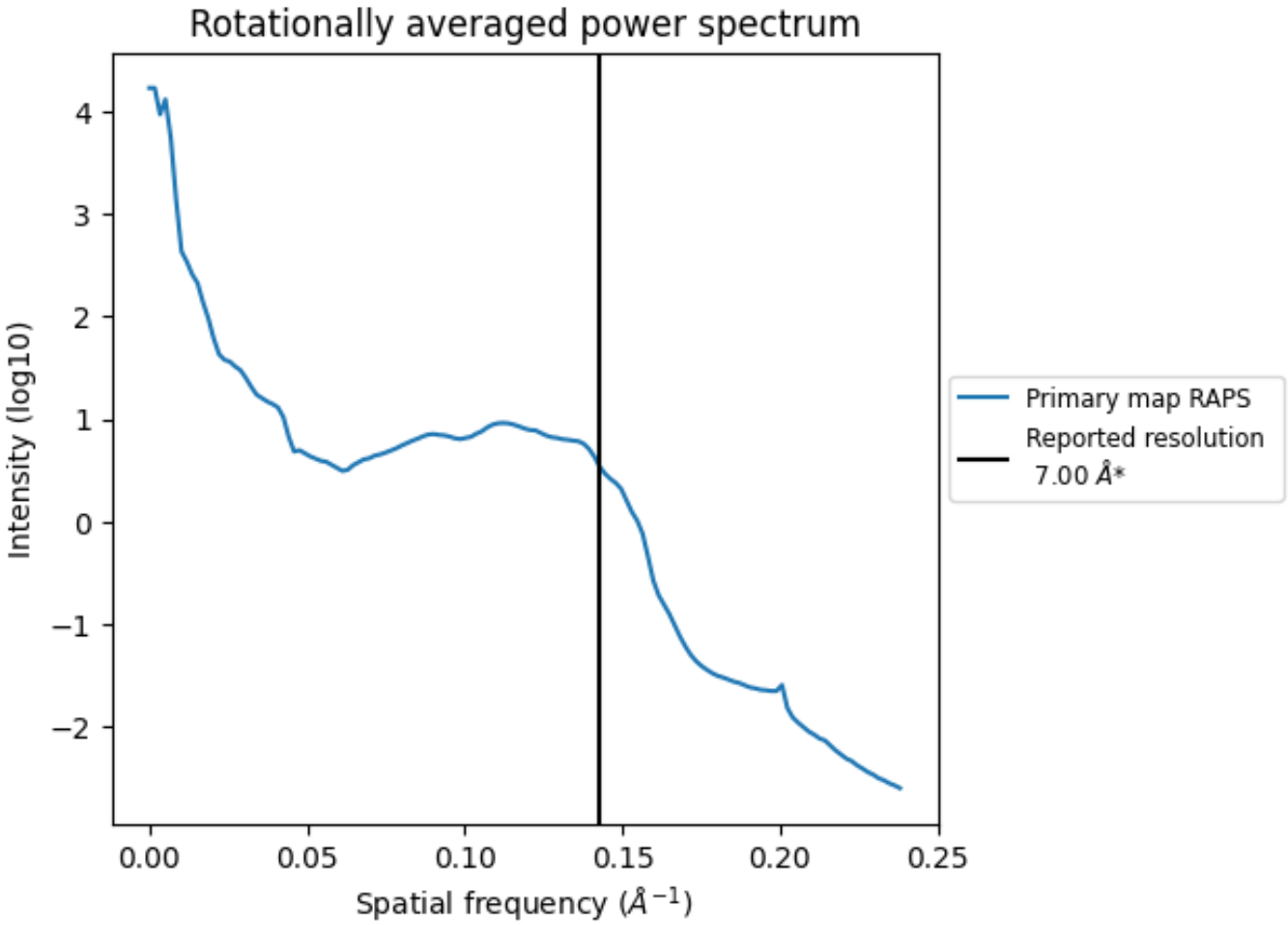
7.2 Volume estimate



The volume at the recommended contour level is 302 nm^3; this corresponds to an approximate mass of 273 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 0.143 Å^{-1}

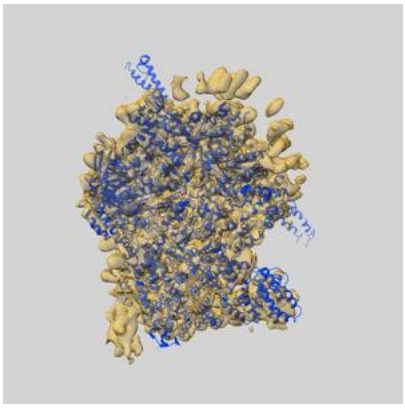
8 Fourier-Shell correlation

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

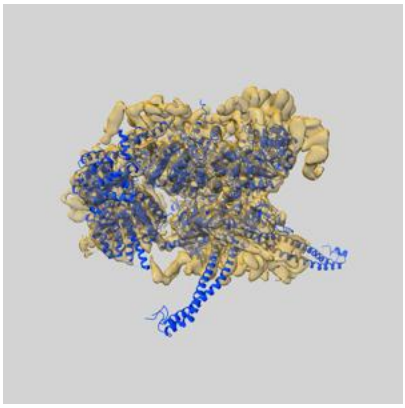
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14083 and PDB model 7QO4. Per-residue inclusion information can be found in section 3 on page 7.

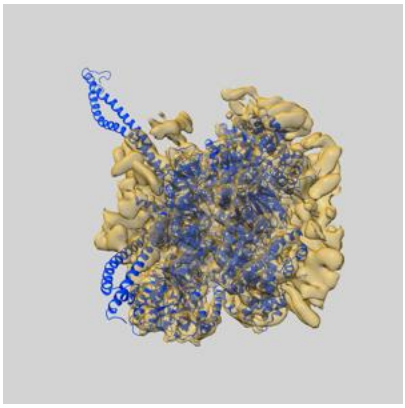
9.1 Map-model overlay



X



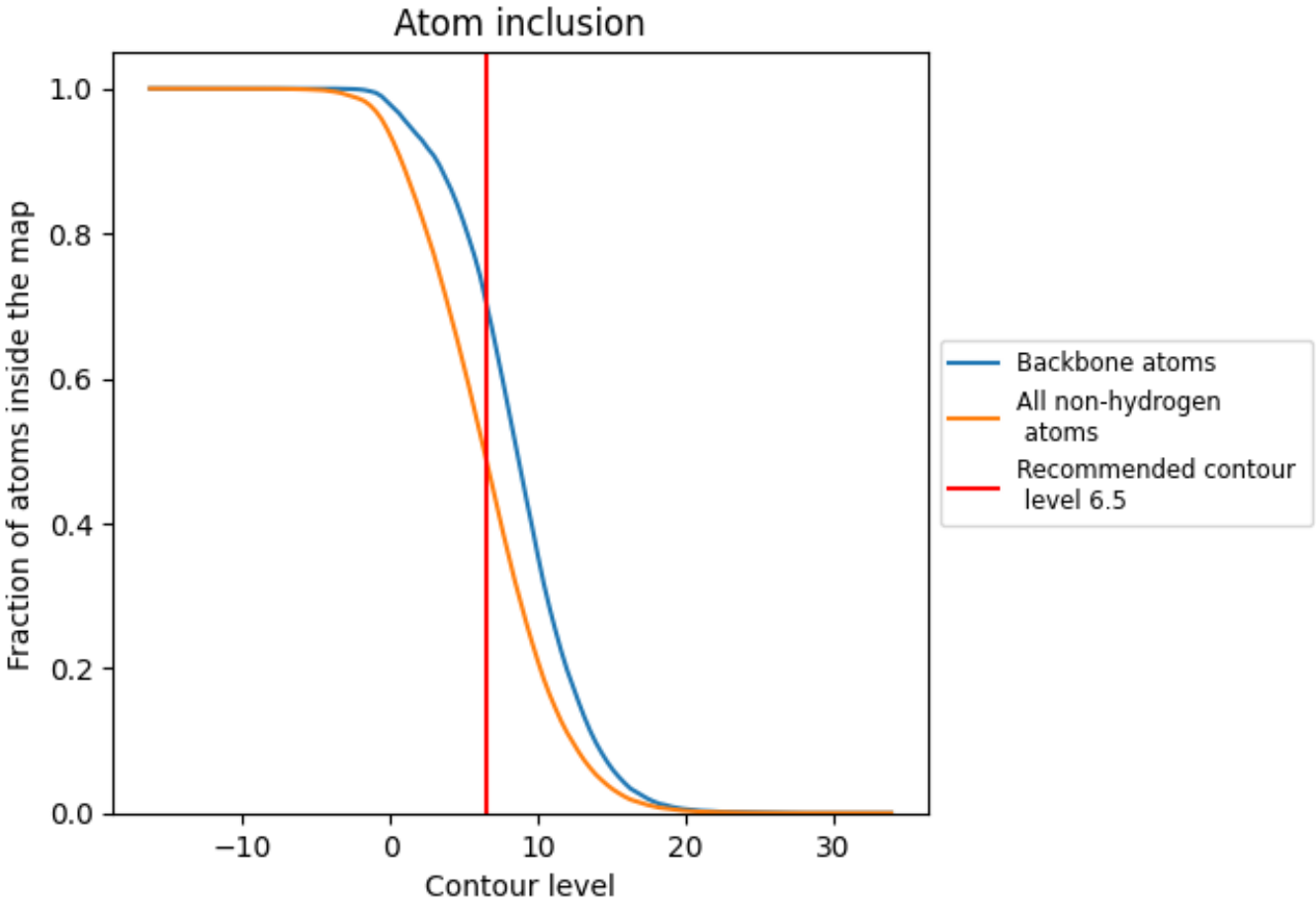
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 6.5 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 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 49% of all non-hydrogen atoms, are inside the map.