



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:30 PM UTC

PDB ID : 7SVU / pdb_00007svu
EMDB ID : EMD-25453
Title : TnsBctd-TnsC-TniQ complex
Authors : Park, J.; Tsai, A.W.T.; Kellogg, E.H.
Deposited on : 2021-11-19
Resolution : 3.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

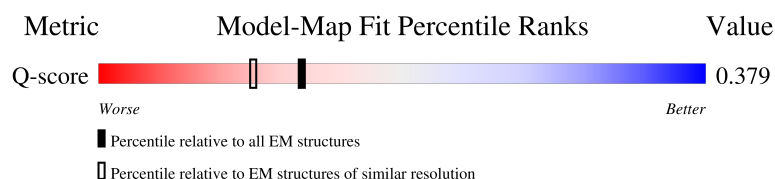
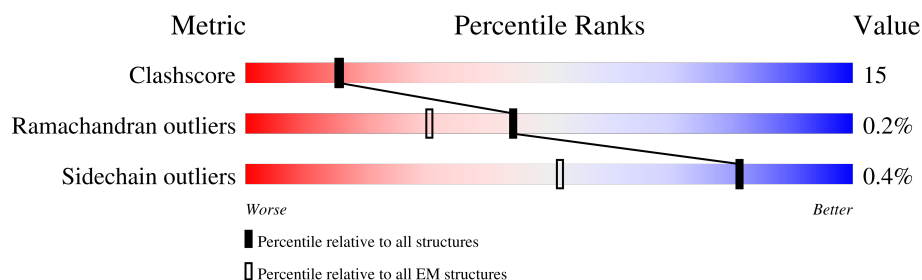
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

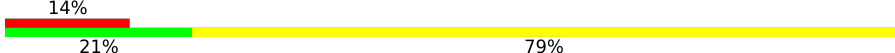
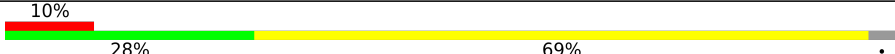
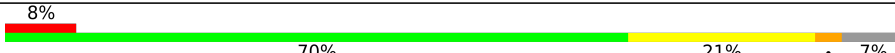
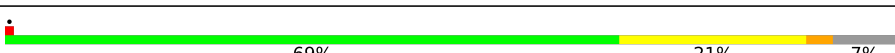
The reported resolution of this entry is 3.50 Å.

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



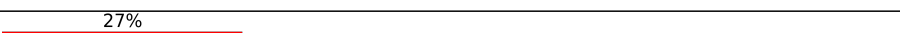
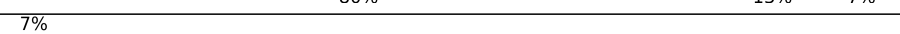
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	28	
2	2	29	
3	A	276	
3	B	276	

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Mol	Chain	Length	Quality of chain
3	C	276	
3	D	276	
3	E	276	
3	F	276	
3	G	276	
3	H	276	
3	I	276	
3	J	276	
3	K	276	
4	a	15	
4	b	15	
4	c	15	
4	d	15	
4	e	15	
4	f	15	
4	h	15	
4	j	15	
4	k	15	
5	X	167	
5	Y	167	

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
7	ATP	J	302	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28015 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 DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	28	Total	C	N	O	P	0	0
			560	280	56	196	28		

- Molecule 2 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	28	Total	C	N	O	P	0	0
			588	280	140	140	28		

- Molecule 3 is a protein called TnsC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
3	B	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
3	C	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
3	D	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
3	E	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
3	F	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
3	G	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
3	H	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
3	I	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
3	J	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		
3	K	257	Total	C	N	O	S	0	0
			2066	1306	377	375	8		

- Molecule 4 is a protein called TnsB-CTD.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	a	14	Total	C	N	O	0	0
			129	83	19	27		
4	b	14	Total	C	N	O	0	0
			129	83	19	27		
4	c	14	Total	C	N	O	0	0
			129	83	19	27		
4	d	14	Total	C	N	O	0	0
			129	83	19	27		
4	e	14	Total	C	N	O	0	0
			129	83	19	27		
4	f	14	Total	C	N	O	0	0
			129	83	19	27		
4	h	14	Total	C	N	O	0	0
			129	83	19	27		
4	j	14	Total	C	N	O	0	0
			129	83	19	27		
4	k	14	Total	C	N	O	0	0
			129	83	19	27		

- Molecule 5 is a protein called TniQ.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	X	165	Total	C	N	O	S	0	0
			1314	838	241	221	14		
5	Y	165	Total	C	N	O	S	0	0
			1314	838	241	221	14		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

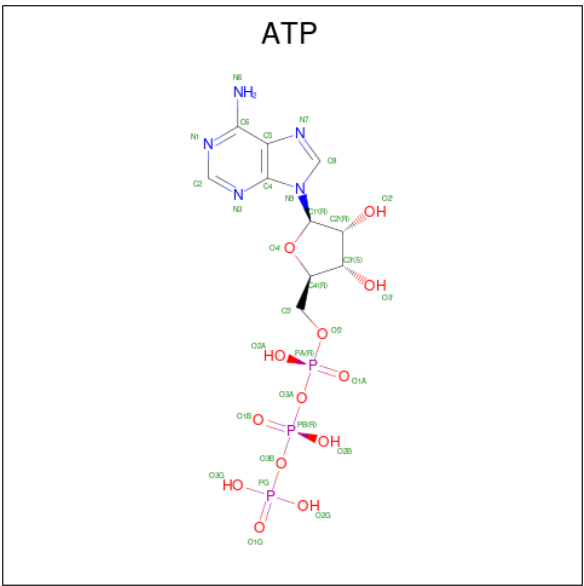
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	Mg	0
			1	1	
6	B	1	Total	Mg	0
			1	1	
6	C	1	Total	Mg	0
			1	1	
6	D	1	Total	Mg	0
			1	1	
6	E	1	Total	Mg	0
			1	1	
6	F	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
6	G	1	Total	Mg	0
			1	1	
6	H	1	Total	Mg	0
			1	1	
6	I	1	Total	Mg	0
			1	1	
6	J	1	Total	Mg	0
			1	1	
6	K	1	Total	Mg	0
			1	1	

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

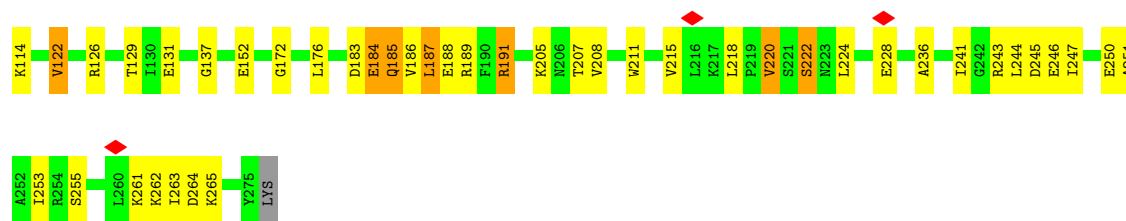


Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	E	1	Total	C	N	O	P	0
			31	10	5	13	3	
7	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

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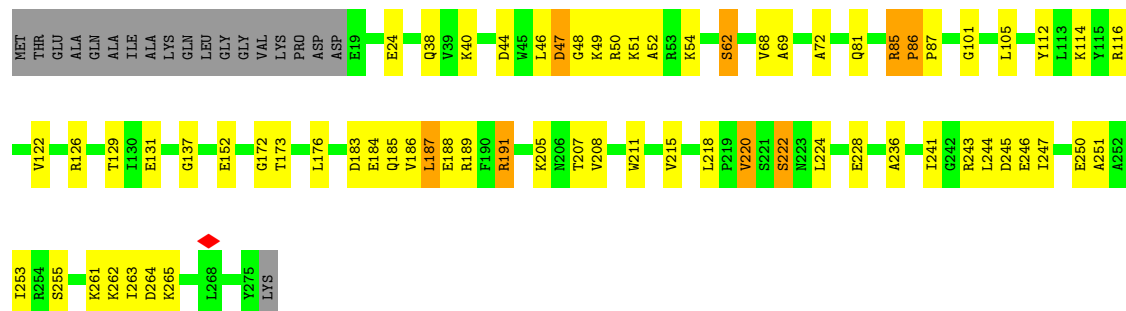
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Mol	Chain	Residues	Atoms					AltConf
7	G	1	Total 31	C 10	N 5	O 13	P 3	0
7	H	1	Total 31	C 10	N 5	O 13	P 3	0
7	I	1	Total 31	C 10	N 5	O 13	P 3	0
7	J	1	Total 31	C 10	N 5	O 13	P 3	0
7	K	1	Total 31	C 10	N 5	O 13	P 3	0



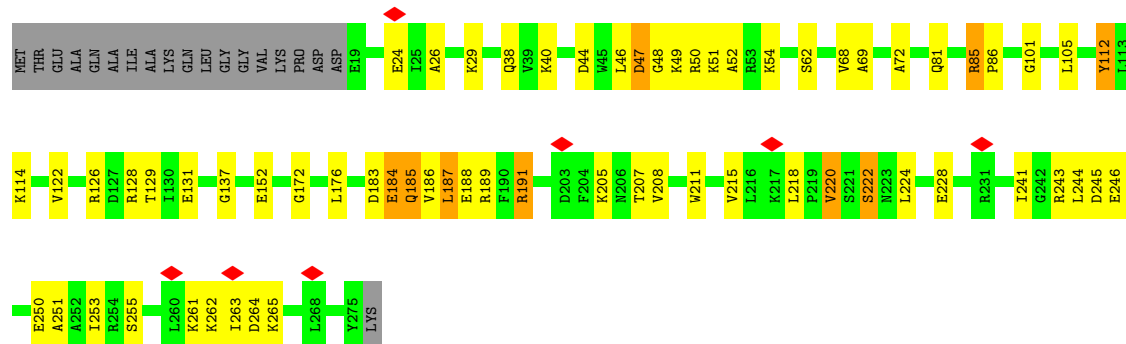
• Molecule 3: TnsC

Chain C: 68% 22% 7%



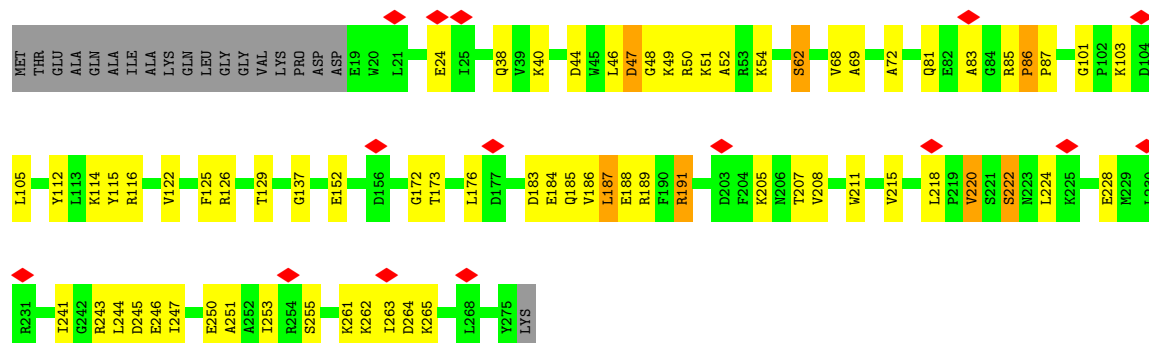
• Molecule 3: TnsC

Chain D: 69% 21% 7%

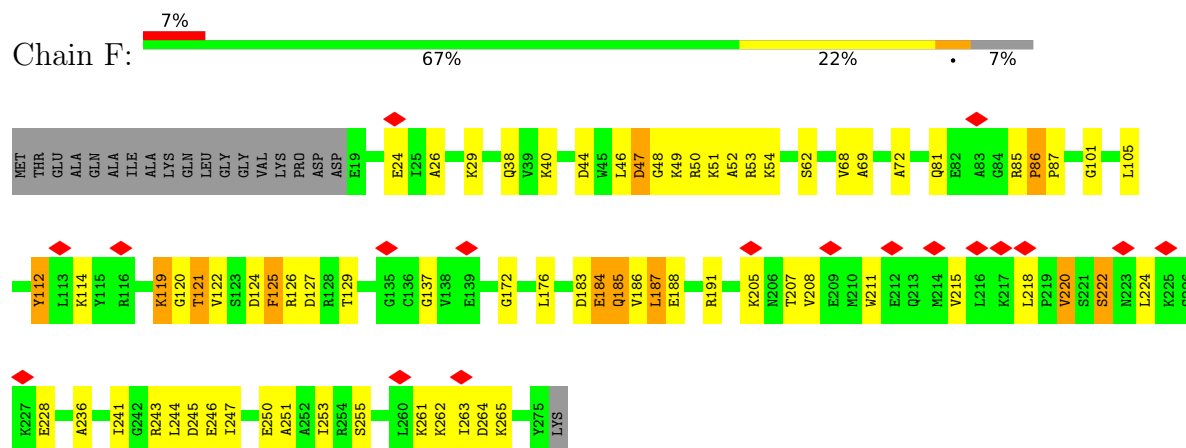


• Molecule 3: TnsC

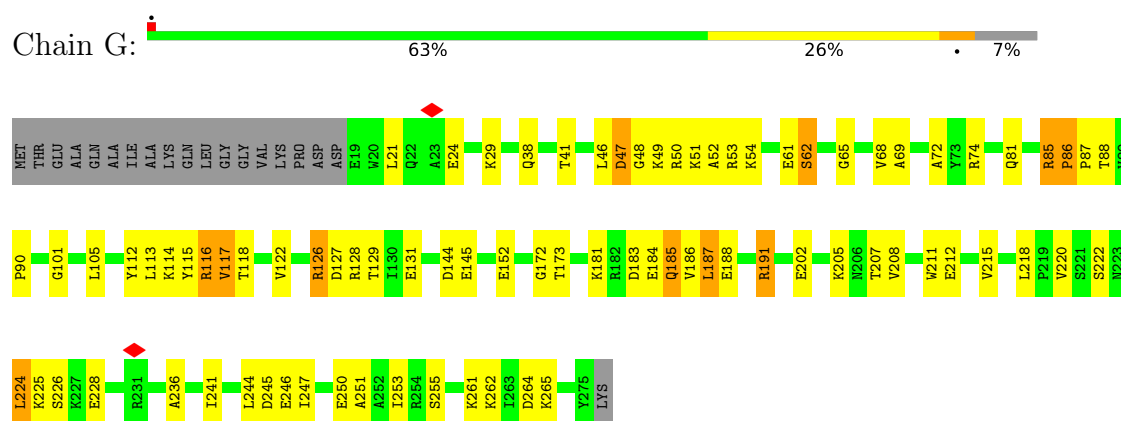
Chain E: 5% 68% 23% 7%



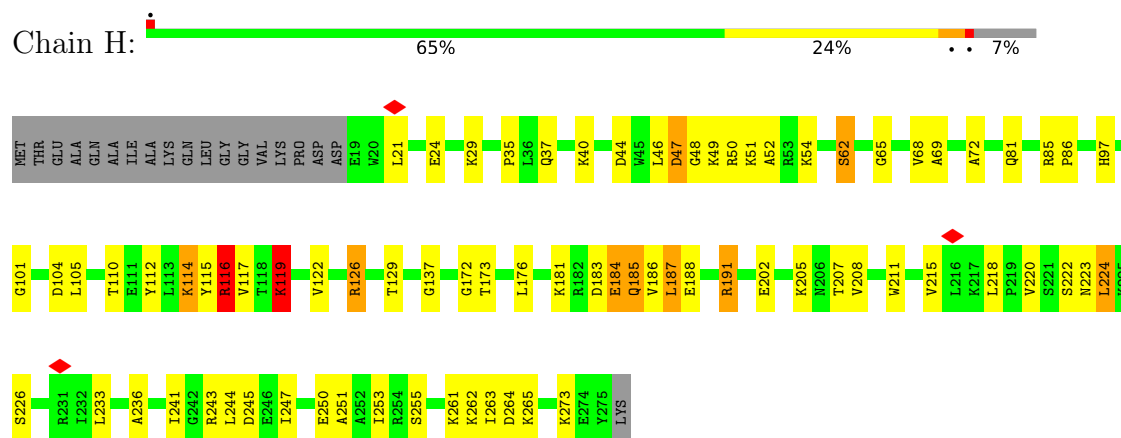
- Molecule 3: TnsC



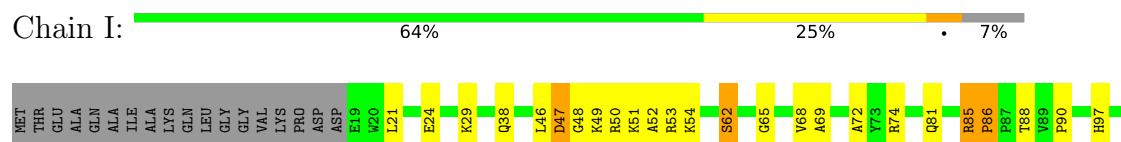
- Molecule 3: TnsC

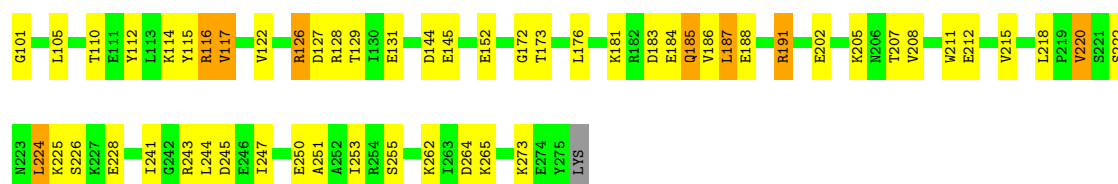


- Molecule 3: TnsC

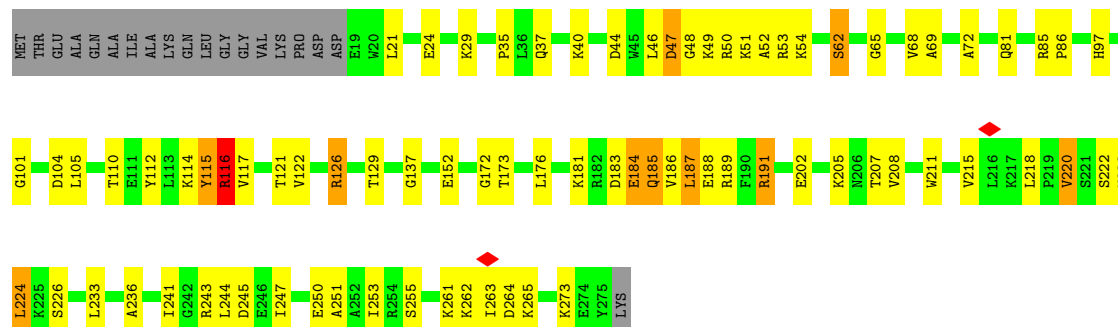


- Molecule 3: TnsC

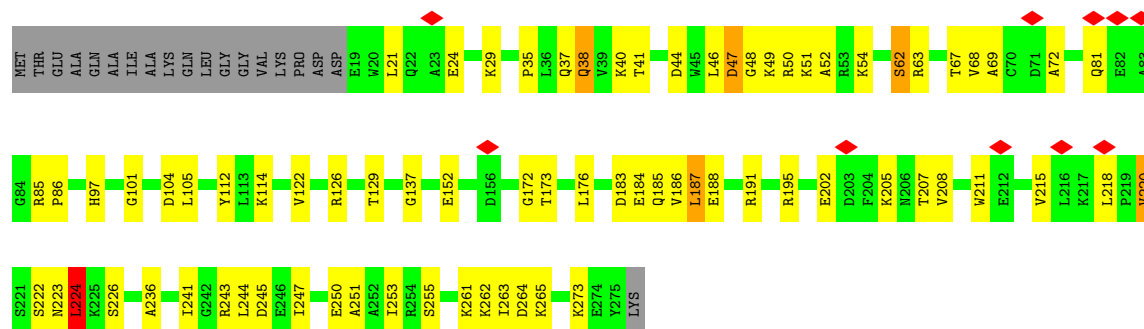




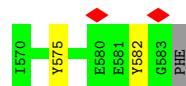
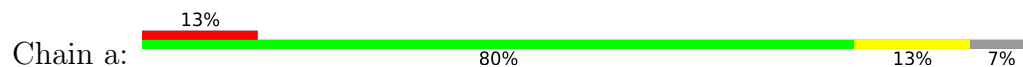
- Molecule 3: TnsC



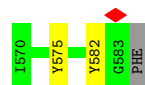
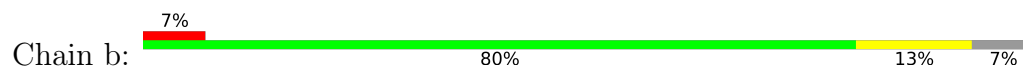
- Molecule 3: TnsC



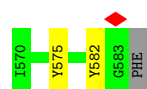
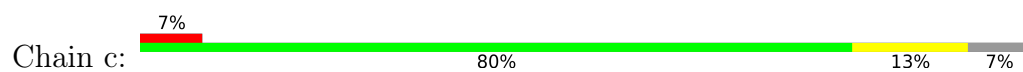
- Molecule 4: TnsB-CTD



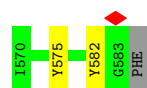
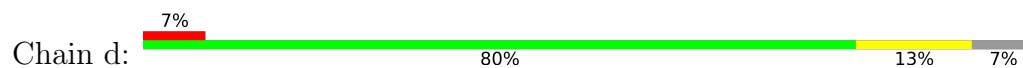
- Molecule 4: TnsB-CTD



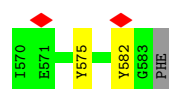
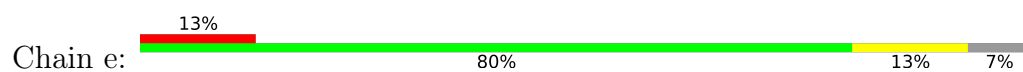
- Molecule 4: TnsB-CTD



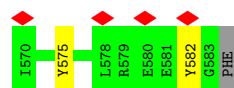
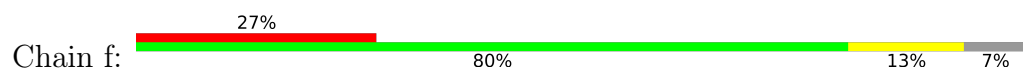
- Molecule 4: TnsB-CTD



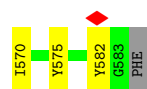
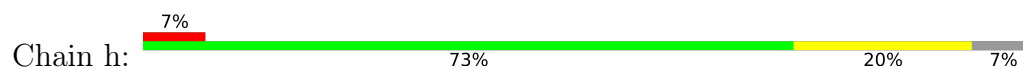
- Molecule 4: TnsB-CTD



- Molecule 4: TnsB-CTD



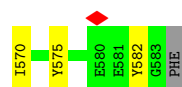
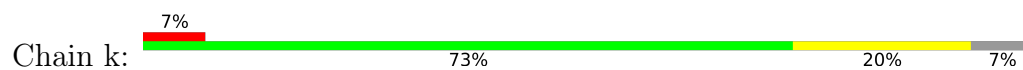
- Molecule 4: TnsB-CTD



- Molecule 4: TnsB-CTD

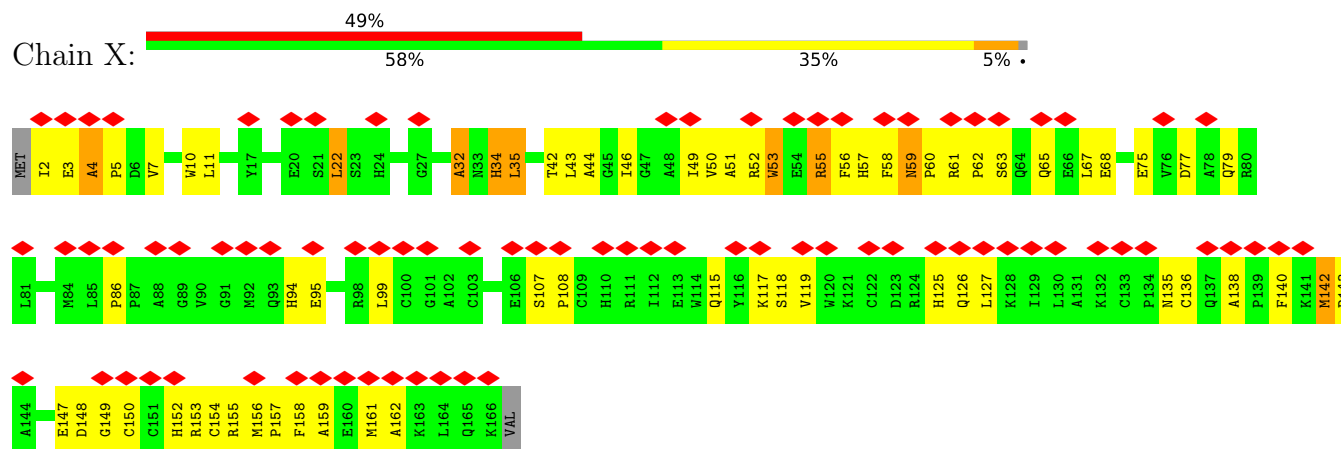


- Molecule 4: TnsB-CTD



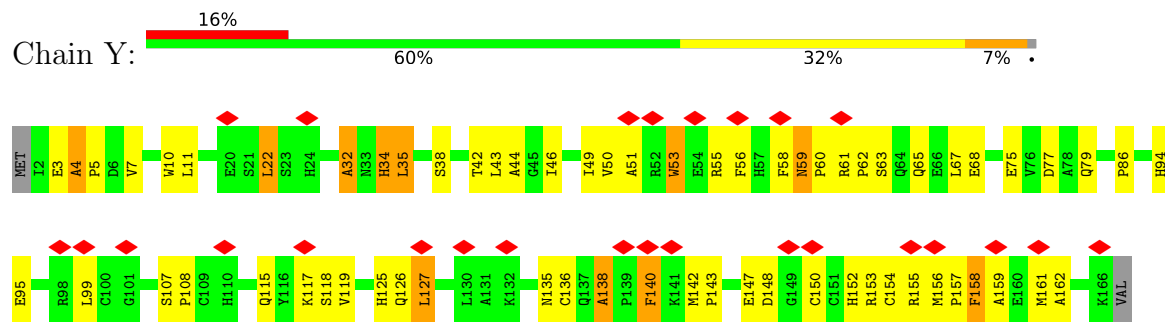
● Molecule 5: ThiQ

Chain X:



● Molecule 5: ThiQ

Chain Y:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61515	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	21.737	Depositor
Minimum map value	0.000	Depositor
Average map value	0.176	Depositor
Map value standard deviation	0.689	Depositor
Recommended contour level	3.5	Depositor
Map size ($\text{\AA}$)	340.48, 340.48, 340.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.33, 1.33, 1.33	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.23	0/615	0.57	0/948
2	2	0.16	0/670	0.28	0/1028
3	A	1.46	27/2097 (1.3%)	1.35	34/2817 (1.2%)
3	B	1.46	27/2097 (1.3%)	1.35	34/2817 (1.2%)
3	C	1.46	27/2097 (1.3%)	1.35	34/2817 (1.2%)
3	D	1.46	29/2097 (1.4%)	1.35	33/2817 (1.2%)
3	E	1.46	27/2097 (1.3%)	1.35	33/2817 (1.2%)
3	F	1.46	26/2097 (1.2%)	1.37	37/2817 (1.3%)
3	G	1.48	28/2097 (1.3%)	1.44	32/2817 (1.1%)
3	H	1.50	25/2097 (1.2%)	1.37	32/2817 (1.1%)
3	I	1.48	27/2097 (1.3%)	1.44	32/2817 (1.1%)
3	J	1.50	25/2097 (1.2%)	1.38	35/2817 (1.2%)
3	K	1.48	24/2097 (1.1%)	1.36	33/2817 (1.2%)
4	a	1.25	0/132	1.29	2/178 (1.1%)
4	b	1.24	0/132	1.30	2/178 (1.1%)
4	c	1.24	0/132	1.29	2/178 (1.1%)
4	d	1.24	0/132	1.29	2/178 (1.1%)
4	e	1.24	0/132	1.30	2/178 (1.1%)
4	f	1.24	0/132	1.30	2/178 (1.1%)
4	h	1.23	0/132	1.28	2/178 (1.1%)
4	j	1.23	0/132	1.27	2/178 (1.1%)
4	k	1.23	0/132	1.27	2/178 (1.1%)
5	X	1.18	3/1353 (0.2%)	1.82	51/1830 (2.8%)
5	Y	1.18	3/1353 (0.2%)	1.82	51/1830 (2.8%)
All	All	1.41	298/28246 (1.1%)	1.39	489/38225 (1.3%)

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
3	A	0	1
3	B	0	1
3	C	0	1
3	D	0	1
3	E	0	1
3	F	0	1
3	G	0	1
3	H	0	1
3	I	0	1
3	J	0	1
3	K	0	1
All	All	0	11

All (298) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	38	GLN	C-O	-7.16	1.15	1.24
3	G	105	LEU	C-O	-7.13	1.15	1.24
3	C	38	GLN	C-O	-7.13	1.15	1.24
3	D	184	GLU	C-O	-7.13	1.15	1.24
3	D	38	GLN	C-O	-7.12	1.15	1.24
3	J	105	LEU	C-O	-7.12	1.15	1.24
3	H	105	LEU	C-O	-7.11	1.15	1.24
3	E	184	GLU	C-O	-7.11	1.15	1.24
3	B	38	GLN	C-O	-7.10	1.15	1.24
3	K	105	LEU	C-O	-7.10	1.15	1.24
3	F	184	GLU	C-O	-7.09	1.15	1.24
3	A	38	GLN	C-O	-7.09	1.15	1.24
3	E	38	GLN	C-O	-7.07	1.15	1.24
3	A	184	GLU	C-O	-7.07	1.15	1.24
3	I	38	GLN	C-O	-7.07	1.15	1.24
3	I	105	LEU	C-O	-7.07	1.15	1.24
3	B	184	GLU	C-O	-7.05	1.15	1.24
3	C	184	GLU	C-O	-7.04	1.15	1.24
3	G	38	GLN	C-O	-7.04	1.15	1.24
3	B	105	LEU	C-O	-7.02	1.16	1.24
3	E	105	LEU	C-O	-7.02	1.16	1.24
3	A	105	LEU	C-O	-7.01	1.16	1.24
3	H	247	ILE	C-O	-7.00	1.16	1.24
3	J	247	ILE	C-O	-6.99	1.16	1.24
3	C	105	LEU	C-O	-6.99	1.16	1.24
3	D	105	LEU	C-O	-6.99	1.16	1.24
3	G	247	ILE	C-O	-6.99	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	247	ILE	C-O	-6.98	1.16	1.24
3	K	247	ILE	C-O	-6.95	1.16	1.24
3	D	247	ILE	C-O	-6.94	1.16	1.24
3	F	105	LEU	C-O	-6.93	1.16	1.24
3	F	247	ILE	C-O	-6.93	1.16	1.24
3	B	247	ILE	C-O	-6.91	1.16	1.24
3	A	247	ILE	C-O	-6.91	1.16	1.24
3	A	244	LEU	C-O	-6.83	1.16	1.24
3	C	247	ILE	C-O	-6.83	1.16	1.24
3	E	247	ILE	C-O	-6.83	1.16	1.24
3	K	244	LEU	C-O	-6.82	1.16	1.24
3	J	244	LEU	C-O	-6.78	1.16	1.24
3	B	244	LEU	C-O	-6.77	1.16	1.24
3	I	244	LEU	C-O	-6.77	1.16	1.24
3	H	244	LEU	C-O	-6.77	1.16	1.24
3	E	244	LEU	C-O	-6.76	1.16	1.24
3	G	244	LEU	C-O	-6.76	1.16	1.24
3	D	244	LEU	C-O	-6.76	1.16	1.24
3	F	244	LEU	C-O	-6.75	1.16	1.24
3	C	244	LEU	C-O	-6.75	1.16	1.24
3	B	186	VAL	C-O	-6.72	1.15	1.24
3	D	186	VAL	C-O	-6.70	1.15	1.24
3	E	186	VAL	C-O	-6.70	1.15	1.24
3	C	186	VAL	C-O	-6.69	1.15	1.24
3	G	184	GLU	C-O	-6.68	1.15	1.24
3	I	186	VAL	C-O	-6.68	1.15	1.24
3	G	186	VAL	C-O	-6.67	1.15	1.24
3	I	184	GLU	C-O	-6.67	1.15	1.24
3	A	186	VAL	C-O	-6.67	1.15	1.24
3	F	186	VAL	C-O	-6.66	1.15	1.24
3	K	184	GLU	C-O	-6.65	1.15	1.24
3	J	184	GLU	C-O	-6.65	1.15	1.24
3	I	50	ARG	C-O	-6.65	1.16	1.24
3	G	50	ARG	C-O	-6.65	1.16	1.24
3	H	186	VAL	C-O	-6.64	1.15	1.24
3	K	186	VAL	C-O	-6.62	1.16	1.24
3	H	184	GLU	C-O	-6.62	1.15	1.24
3	J	50	ARG	C-O	-6.61	1.16	1.24
3	J	186	VAL	C-O	-6.61	1.16	1.24
3	K	50	ARG	C-O	-6.60	1.16	1.24
3	B	50	ARG	C-O	-6.59	1.16	1.24
3	D	50	ARG	C-O	-6.58	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	50	ARG	C-O	-6.58	1.16	1.24
3	E	50	ARG	C-O	-6.57	1.16	1.24
3	A	50	ARG	C-O	-6.54	1.16	1.24
3	F	50	ARG	C-O	-6.53	1.16	1.24
3	C	50	ARG	C-O	-6.51	1.16	1.24
3	G	122	VAL	C-O	-6.45	1.16	1.24
3	D	122	VAL	C-O	-6.43	1.16	1.24
3	B	122	VAL	C-O	-6.43	1.16	1.24
3	I	122	VAL	C-O	-6.43	1.16	1.24
3	C	122	VAL	C-O	-6.42	1.16	1.24
3	G	129	THR	C-O	-6.42	1.16	1.24
3	E	122	VAL	C-O	-6.41	1.16	1.24
3	A	122	VAL	C-O	-6.40	1.16	1.24
3	I	129	THR	C-O	-6.39	1.16	1.24
3	B	129	THR	C-O	-6.38	1.16	1.24
3	K	122	VAL	C-O	-6.38	1.16	1.24
3	E	129	THR	C-O	-6.37	1.16	1.24
3	H	122	VAL	C-O	-6.36	1.16	1.24
5	Y	42	THR	CA-C	-6.36	1.44	1.52
3	F	129	THR	C-O	-6.35	1.16	1.24
3	H	129	THR	C-O	-6.35	1.16	1.24
3	A	129	THR	C-O	-6.34	1.16	1.24
3	J	122	VAL	C-O	-6.34	1.16	1.24
3	C	129	THR	C-O	-6.34	1.16	1.24
5	X	42	THR	CA-C	-6.31	1.44	1.52
3	D	129	THR	C-O	-6.30	1.16	1.24
3	J	129	THR	C-O	-6.30	1.16	1.24
3	K	129	THR	C-O	-6.27	1.16	1.24
3	C	245	ASP	C-O	-6.26	1.17	1.24
3	A	245	ASP	C-O	-6.22	1.17	1.24
3	E	245	ASP	C-O	-6.22	1.17	1.24
3	B	245	ASP	C-O	-6.16	1.17	1.24
3	A	38	GLN	CA-C	-6.16	1.44	1.52
3	K	245	ASP	C-O	-6.14	1.17	1.24
3	F	245	ASP	C-O	-6.13	1.17	1.24
3	G	245	ASP	C-O	-6.13	1.17	1.24
3	C	38	GLN	CA-C	-6.13	1.44	1.52
3	J	245	ASP	C-O	-6.13	1.17	1.24
3	I	245	ASP	C-O	-6.12	1.17	1.24
3	B	38	GLN	CA-C	-6.12	1.45	1.52
3	I	38	GLN	CA-C	-6.11	1.45	1.52
3	D	245	ASP	C-O	-6.10	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	245	ASP	C-O	-6.10	1.17	1.24
3	E	38	GLN	CA-C	-6.09	1.45	1.52
3	F	38	GLN	CA-C	-6.09	1.45	1.52
3	G	38	GLN	CA-C	-6.09	1.45	1.52
3	D	38	GLN	CA-C	-6.08	1.45	1.52
3	K	241	ILE	C-O	-6.08	1.16	1.24
3	I	241	ILE	C-O	-6.08	1.16	1.24
3	J	185	GLN	C-O	-6.07	1.17	1.24
3	K	185	GLN	C-O	-6.07	1.17	1.24
3	G	241	ILE	C-O	-6.04	1.16	1.24
3	I	54	LYS	C-O	-6.03	1.16	1.24
3	J	241	ILE	C-O	-6.02	1.16	1.24
3	H	185	GLN	C-O	-6.01	1.17	1.24
3	G	187	LEU	C-O	-6.01	1.17	1.24
3	H	241	ILE	C-O	-6.00	1.16	1.24
3	G	54	LYS	C-O	-5.98	1.16	1.24
3	I	187	LEU	C-O	-5.95	1.17	1.24
3	G	185	GLN	C-O	-5.92	1.17	1.24
3	I	185	GLN	C-O	-5.88	1.17	1.24
3	E	54	LYS	C-O	-5.87	1.16	1.24
3	K	183	ASP	C-O	-5.85	1.17	1.23
3	A	54	LYS	C-O	-5.85	1.16	1.24
3	J	183	ASP	C-O	-5.85	1.17	1.23
3	H	183	ASP	C-O	-5.84	1.17	1.23
3	D	54	LYS	C-O	-5.84	1.16	1.24
3	C	54	LYS	C-O	-5.84	1.16	1.24
3	B	54	LYS	C-O	-5.80	1.16	1.24
3	B	187	LEU	C-O	-5.79	1.17	1.24
3	D	187	LEU	C-O	-5.78	1.17	1.24
3	K	187	LEU	C-O	-5.78	1.17	1.24
3	K	54	LYS	C-O	-5.78	1.16	1.23
3	F	54	LYS	C-O	-5.78	1.16	1.24
3	C	187	LEU	C-O	-5.77	1.17	1.24
3	F	187	LEU	C-O	-5.77	1.17	1.24
3	C	183	ASP	C-O	-5.77	1.17	1.24
3	A	241	ILE	C-O	-5.76	1.16	1.24
3	H	187	LEU	C-O	-5.75	1.17	1.24
3	C	241	ILE	C-O	-5.75	1.16	1.24
3	E	187	LEU	C-O	-5.75	1.17	1.24
3	H	54	LYS	C-O	-5.75	1.16	1.23
3	J	187	LEU	C-O	-5.75	1.17	1.24
3	E	241	ILE	C-O	-5.75	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	54	LYS	C-O	-5.74	1.16	1.23
3	B	241	ILE	C-O	-5.74	1.16	1.24
3	A	185	GLN	C-O	-5.73	1.17	1.24
3	C	185	GLN	C-O	-5.73	1.17	1.24
3	F	49	LYS	N-CA	-5.73	1.39	1.46
3	A	187	LEU	C-O	-5.72	1.17	1.24
3	A	49	LYS	N-CA	-5.72	1.39	1.46
3	C	49	LYS	N-CA	-5.71	1.39	1.46
3	F	241	ILE	C-O	-5.70	1.16	1.24
3	E	185	GLN	C-O	-5.70	1.17	1.24
3	E	183	ASP	C-O	-5.68	1.17	1.24
3	B	185	GLN	C-O	-5.68	1.17	1.24
3	D	183	ASP	C-O	-5.68	1.17	1.24
3	D	241	ILE	C-O	-5.67	1.16	1.24
3	D	185	GLN	C-O	-5.66	1.17	1.24
3	B	183	ASP	C-O	-5.66	1.17	1.24
3	A	183	ASP	C-O	-5.65	1.17	1.24
3	F	185	GLN	C-O	-5.65	1.17	1.24
3	F	183	ASP	C-O	-5.65	1.17	1.24
3	E	49	LYS	N-CA	-5.64	1.39	1.46
3	I	49	LYS	N-CA	-5.63	1.39	1.46
3	H	47	ASP	C-O	-5.63	1.17	1.24
3	G	49	LYS	N-CA	-5.63	1.39	1.46
3	H	49	LYS	N-CA	-5.63	1.39	1.46
3	B	49	LYS	N-CA	-5.62	1.39	1.46
3	D	47	ASP	C-O	-5.62	1.17	1.24
3	J	49	LYS	N-CA	-5.62	1.39	1.46
3	D	49	LYS	N-CA	-5.62	1.39	1.46
3	E	47	ASP	C-O	-5.61	1.17	1.24
3	K	47	ASP	C-O	-5.61	1.17	1.24
3	A	47	ASP	C-O	-5.61	1.17	1.24
3	J	47	ASP	C-O	-5.60	1.17	1.24
3	G	183	ASP	C-O	-5.60	1.17	1.24
3	K	49	LYS	N-CA	-5.60	1.39	1.46
3	K	126	ARG	C-O	-5.59	1.17	1.24
3	C	47	ASP	C-O	-5.59	1.17	1.24
3	B	126	ARG	C-O	-5.59	1.17	1.24
3	I	183	ASP	C-O	-5.59	1.17	1.24
3	B	47	ASP	C-O	-5.58	1.17	1.24
3	F	47	ASP	C-O	-5.57	1.17	1.24
3	J	126	ARG	C-O	-5.57	1.17	1.24
3	H	126	ARG	C-O	-5.55	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	126	ARG	C-O	-5.55	1.17	1.24
3	I	47	ASP	C-O	-5.55	1.17	1.24
3	G	47	ASP	C-O	-5.54	1.17	1.24
3	E	126	ARG	C-O	-5.52	1.17	1.24
3	D	126	ARG	C-O	-5.51	1.17	1.24
3	G	126	ARG	C-O	-5.51	1.17	1.24
3	I	126	ARG	C-O	-5.51	1.17	1.24
3	C	126	ARG	C-O	-5.50	1.17	1.24
3	A	46	LEU	C-O	-5.46	1.17	1.24
3	F	46	LEU	C-O	-5.41	1.17	1.24
3	D	46	LEU	C-O	-5.40	1.17	1.24
5	Y	62	PRO	CA-C	-5.39	1.48	1.52
3	G	46	LEU	C-O	-5.39	1.17	1.24
3	I	46	LEU	C-O	-5.37	1.17	1.24
5	X	62	PRO	CA-C	-5.36	1.48	1.52
3	E	46	LEU	C-O	-5.36	1.17	1.24
3	B	46	LEU	C-O	-5.35	1.17	1.24
3	H	46	LEU	C-O	-5.34	1.17	1.24
3	C	46	LEU	C-O	-5.34	1.17	1.24
3	K	46	LEU	C-O	-5.33	1.17	1.24
3	F	50	ARG	CA-C	-5.32	1.45	1.52
3	H	50	ARG	CA-C	-5.31	1.45	1.52
3	H	253	ILE	C-O	-5.31	1.18	1.24
3	J	50	ARG	CA-C	-5.31	1.45	1.52
3	J	46	LEU	C-O	-5.30	1.18	1.24
3	K	211	TRP	CA-C	-5.30	1.45	1.52
3	H	211	TRP	CA-C	-5.29	1.45	1.52
3	J	253	ILE	C-O	-5.29	1.18	1.24
3	C	211	TRP	CA-C	-5.29	1.45	1.52
3	D	211	TRP	CA-C	-5.29	1.45	1.52
3	K	253	ILE	C-O	-5.28	1.18	1.24
3	B	50	ARG	CA-C	-5.28	1.46	1.52
3	K	50	ARG	CA-C	-5.27	1.46	1.52
3	D	253	ILE	C-O	-5.26	1.18	1.24
3	G	50	ARG	CA-C	-5.26	1.46	1.52
3	C	253	ILE	C-O	-5.25	1.18	1.24
3	I	50	ARG	CA-C	-5.25	1.46	1.52
3	B	211	TRP	CA-C	-5.25	1.45	1.52
3	E	253	ILE	C-O	-5.25	1.18	1.24
3	J	211	TRP	CA-C	-5.25	1.45	1.52
3	D	50	ARG	CA-C	-5.24	1.46	1.52
3	I	253	ILE	C-O	-5.24	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	253	ILE	C-O	-5.23	1.18	1.24
3	C	24	GLU	CA-C	-5.23	1.46	1.52
3	A	211	TRP	CA-C	-5.22	1.45	1.52
3	D	24	GLU	CA-C	-5.22	1.46	1.52
3	F	211	TRP	CA-C	-5.22	1.45	1.52
3	A	253	ILE	C-O	-5.20	1.18	1.24
3	C	50	ARG	CA-C	-5.20	1.46	1.52
3	E	211	TRP	CA-C	-5.20	1.45	1.52
3	H	24	GLU	CA-C	-5.20	1.46	1.52
3	F	24	GLU	CA-C	-5.20	1.46	1.52
3	E	50	ARG	CA-C	-5.20	1.46	1.52
3	F	253	ILE	C-O	-5.20	1.18	1.24
3	G	253	ILE	C-O	-5.19	1.18	1.24
3	A	50	ARG	CA-C	-5.19	1.46	1.52
3	E	24	GLU	CA-C	-5.18	1.46	1.52
3	E	176	LEU	C-O	-5.18	1.18	1.24
3	B	24	GLU	CA-C	-5.18	1.46	1.52
3	A	24	GLU	CA-C	-5.17	1.46	1.52
3	K	24	GLU	CA-C	-5.17	1.46	1.52
3	H	116	ARG	CA-C	-5.17	1.46	1.52
3	J	24	GLU	CA-C	-5.16	1.46	1.52
3	A	176	LEU	C-O	-5.16	1.18	1.24
3	C	176	LEU	C-O	-5.16	1.18	1.24
3	G	24	GLU	CA-C	-5.15	1.46	1.52
3	D	49	LYS	CA-C	-5.15	1.45	1.52
3	I	24	GLU	CA-C	-5.15	1.46	1.52
3	I	211	TRP	CA-C	-5.14	1.45	1.52
3	A	49	LYS	CA-C	-5.13	1.45	1.52
3	C	246	GLU	CA-C	-5.13	1.46	1.52
3	E	246	GLU	CA-C	-5.13	1.46	1.52
3	B	49	LYS	CA-C	-5.12	1.45	1.52
3	G	211	TRP	CA-C	-5.12	1.45	1.52
3	H	49	LYS	CA-C	-5.12	1.45	1.52
3	D	246	GLU	CA-C	-5.11	1.46	1.52
3	E	49	LYS	CA-C	-5.11	1.45	1.52
3	G	49	LYS	CA-C	-5.11	1.45	1.52
3	J	49	LYS	CA-C	-5.11	1.45	1.52
3	A	246	GLU	CA-C	-5.11	1.46	1.52
5	X	32	ALA	C-O	-5.11	1.18	1.24
3	F	49	LYS	CA-C	-5.09	1.45	1.52
3	D	176	LEU	C-O	-5.09	1.18	1.24
3	I	49	LYS	CA-C	-5.09	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	32	ALA	C-O	-5.08	1.18	1.24
3	B	246	GLU	CA-C	-5.07	1.46	1.52
3	F	176	LEU	C-O	-5.07	1.18	1.24
3	C	49	LYS	CA-C	-5.07	1.45	1.52
3	G	188	GLU	C-O	-5.06	1.17	1.24
3	F	112	TYR	C-O	-5.06	1.18	1.24
3	F	246	GLU	CA-C	-5.05	1.46	1.52
3	K	49	LYS	CA-C	-5.05	1.45	1.52
3	B	176	LEU	C-O	-5.04	1.18	1.24
3	J	116	ARG	CA-C	-5.04	1.45	1.53
3	H	176	LEU	C-O	-5.04	1.18	1.24
3	J	176	LEU	C-O	-5.02	1.18	1.24
3	I	188	GLU	C-O	-5.02	1.17	1.24
3	D	188	GLU	C-O	-5.02	1.17	1.24
3	G	251	ALA	C-O	-5.01	1.18	1.24
3	I	176	LEU	C-O	-5.01	1.18	1.24
3	D	112	TYR	C-O	-5.01	1.18	1.24
3	G	246	GLU	CA-C	-5.01	1.46	1.52
3	K	176	LEU	C-O	-5.01	1.18	1.24

All (489) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	86	PRO	CA-C-N	15.30	134.90	120.21
3	I	86	PRO	C-N-CA	15.30	134.90	120.21
3	G	86	PRO	CA-C-N	15.28	134.88	120.21
3	G	86	PRO	C-N-CA	15.28	134.88	120.21
5	Y	4	ALA	CA-C-N	14.83	134.83	119.85
5	Y	4	ALA	C-N-CA	14.83	134.83	119.85
5	X	4	ALA	CA-C-N	14.80	134.79	119.85
5	X	4	ALA	C-N-CA	14.80	134.79	119.85
5	Y	59	ASN	CA-C-N	13.95	137.27	119.84
5	Y	59	ASN	C-N-CA	13.95	137.27	119.84
5	X	59	ASN	CA-C-N	13.92	137.24	119.84
5	X	59	ASN	C-N-CA	13.92	137.24	119.84
5	X	56	PHE	N-CA-C	12.72	128.52	112.24
5	Y	56	PHE	N-CA-C	12.71	128.50	112.24
3	I	85	ARG	CA-C-N	12.64	128.76	119.66
3	I	85	ARG	C-N-CA	12.64	128.76	119.66
3	G	85	ARG	CA-C-N	12.59	128.72	119.66
3	G	85	ARG	C-N-CA	12.59	128.72	119.66
3	G	222	SER	N-CA-C	11.52	123.83	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	222	SER	N-CA-C	11.51	123.83	111.28
5	X	126	GLN	N-CA-C	10.49	125.87	111.39
5	Y	126	GLN	N-CA-C	10.48	125.86	111.39
5	Y	67	LEU	N-CA-C	9.65	121.87	111.36
5	X	67	LEU	N-CA-C	9.63	121.86	111.36
3	K	224	LEU	N-CA-C	9.42	122.75	111.82
3	J	224	LEU	N-CA-C	9.38	122.70	111.82
3	H	224	LEU	N-CA-C	9.38	122.70	111.82
5	X	94	HIS	N-CA-C	9.10	124.89	111.34
5	Y	94	HIS	N-CA-C	9.07	124.85	111.34
3	H	205	LYS	N-CA-C	8.76	120.44	111.07
3	J	205	LYS	N-CA-C	8.75	120.43	111.07
3	K	205	LYS	N-CA-C	8.74	120.42	111.07
5	X	42	THR	N-CA-C	8.54	120.67	111.36
5	Y	42	THR	N-CA-C	8.54	120.67	111.36
3	E	208	VAL	N-CA-C	-8.43	102.32	110.42
3	K	86	PRO	CA-C-N	8.42	128.47	119.89
3	K	86	PRO	C-N-CA	8.42	128.47	119.89
3	D	86	PRO	CA-C-N	8.41	128.46	119.89
3	D	86	PRO	C-N-CA	8.41	128.46	119.89
3	B	208	VAL	N-CA-C	-8.40	102.36	110.42
3	J	86	PRO	CA-C-N	8.40	128.46	119.89
3	J	86	PRO	C-N-CA	8.40	128.46	119.89
3	F	208	VAL	N-CA-C	-8.39	102.37	110.42
3	H	86	PRO	CA-C-N	8.38	128.44	119.89
3	H	86	PRO	C-N-CA	8.38	128.44	119.89
3	A	208	VAL	N-CA-C	-8.38	102.38	110.42
3	C	86	PRO	CA-C-N	8.37	128.43	119.89
3	C	86	PRO	C-N-CA	8.37	128.43	119.89
5	X	95	GLU	N-CA-C	8.37	123.55	112.17
3	F	86	PRO	CA-C-N	8.36	128.42	119.89
3	F	86	PRO	C-N-CA	8.36	128.42	119.89
3	B	86	PRO	CA-C-N	8.36	128.42	119.89
3	B	86	PRO	C-N-CA	8.36	128.42	119.89
3	J	208	VAL	N-CA-C	-8.36	102.40	110.42
3	K	208	VAL	N-CA-C	-8.35	102.40	110.42
3	C	208	VAL	N-CA-C	-8.35	102.40	110.42
3	A	86	PRO	CA-C-N	8.34	128.40	119.89
3	A	86	PRO	C-N-CA	8.34	128.40	119.89
5	X	34	HIS	N-CA-C	8.34	122.88	111.54
5	Y	95	GLU	N-CA-C	8.34	123.51	112.17
3	D	208	VAL	N-CA-C	-8.33	102.42	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	86	PRO	CA-C-N	8.32	128.37	119.89
3	E	86	PRO	C-N-CA	8.32	128.37	119.89
5	Y	34	HIS	N-CA-C	8.32	122.85	111.54
3	G	208	VAL	N-CA-C	-8.31	102.44	110.42
3	H	208	VAL	N-CA-C	-8.31	102.44	110.42
3	I	208	VAL	N-CA-C	-8.29	102.46	110.42
3	K	215	VAL	N-CA-C	8.26	118.67	111.56
3	B	215	VAL	N-CA-C	8.25	118.65	111.56
3	J	215	VAL	N-CA-C	8.25	118.65	111.56
3	E	215	VAL	N-CA-C	8.24	118.65	111.56
3	D	215	VAL	N-CA-C	8.22	118.63	111.56
3	F	215	VAL	N-CA-C	8.22	118.63	111.56
3	H	215	VAL	N-CA-C	8.21	118.62	111.56
3	A	215	VAL	N-CA-C	8.20	118.61	111.56
3	C	215	VAL	N-CA-C	8.20	118.61	111.56
3	G	215	VAL	N-CA-C	8.19	118.60	111.56
3	I	215	VAL	N-CA-C	8.18	118.60	111.56
5	X	140	PHE	N-CA-C	8.15	123.27	110.32
3	E	191	ARG	N-CA-C	8.14	120.15	111.28
3	D	191	ARG	N-CA-C	8.12	120.13	111.28
3	F	191	ARG	N-CA-C	8.12	120.13	111.28
5	Y	140	PHE	N-CA-C	8.12	123.23	110.32
3	B	191	ARG	N-CA-C	8.11	120.12	111.28
3	C	265	LYS	N-CA-C	8.10	120.83	111.11
3	C	191	ARG	N-CA-C	8.10	120.11	111.28
3	G	265	LYS	N-CA-C	8.10	120.83	111.11
3	A	191	ARG	N-CA-C	8.10	120.11	111.28
3	H	191	ARG	N-CA-C	8.10	120.10	111.28
3	E	265	LYS	N-CA-C	8.09	120.82	111.11
3	J	191	ARG	N-CA-C	8.09	120.10	111.28
3	A	265	LYS	N-CA-C	8.09	120.81	111.11
3	G	191	ARG	N-CA-C	8.08	120.09	111.28
3	B	265	LYS	N-CA-C	8.08	120.81	111.11
3	I	265	LYS	N-CA-C	8.08	120.81	111.11
3	I	191	ARG	N-CA-C	8.07	120.08	111.28
3	D	265	LYS	N-CA-C	8.05	120.77	111.11
3	K	191	ARG	N-CA-C	8.05	120.06	111.28
3	K	265	LYS	N-CA-C	8.05	120.77	111.11
3	H	265	LYS	N-CA-C	8.05	120.77	111.11
3	F	265	LYS	N-CA-C	8.02	120.73	111.11
3	J	265	LYS	N-CA-C	8.02	120.73	111.11
3	K	48	GLY	N-CA-C	-7.83	103.42	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	220	VAL	N-CA-C	7.80	118.58	110.62
3	H	48	GLY	N-CA-C	-7.80	103.45	112.50
3	J	48	GLY	N-CA-C	-7.80	103.45	112.50
3	F	48	GLY	N-CA-C	-7.79	103.46	112.50
3	G	48	GLY	N-CA-C	-7.79	103.46	112.50
3	I	48	GLY	N-CA-C	-7.79	103.46	112.50
3	B	48	GLY	N-CA-C	-7.79	103.46	112.50
3	D	205	LYS	N-CA-C	7.78	120.45	111.11
3	D	48	GLY	N-CA-C	-7.78	103.47	112.50
3	E	220	VAL	N-CA-C	7.78	118.56	110.62
3	F	220	VAL	N-CA-C	7.77	118.55	110.62
3	A	48	GLY	N-CA-C	-7.77	103.49	112.50
3	B	205	LYS	N-CA-C	7.77	120.43	111.11
3	E	48	GLY	N-CA-C	-7.76	103.49	112.50
3	C	220	VAL	N-CA-C	7.76	118.54	110.62
3	D	85	ARG	CA-C-N	7.76	128.37	120.38
3	D	85	ARG	C-N-CA	7.76	128.37	120.38
3	F	85	ARG	CA-C-N	7.76	128.37	120.38
3	F	85	ARG	C-N-CA	7.76	128.37	120.38
3	B	220	VAL	N-CA-C	7.76	118.53	110.62
3	B	85	ARG	CA-C-N	7.76	128.37	120.38
3	B	85	ARG	C-N-CA	7.76	128.37	120.38
3	A	205	LYS	N-CA-C	7.75	120.42	111.11
3	C	48	GLY	N-CA-C	-7.75	103.50	112.50
3	A	220	VAL	N-CA-C	7.75	118.52	110.62
3	C	205	LYS	N-CA-C	7.75	120.41	111.11
3	J	85	ARG	CA-C-N	7.74	128.35	120.38
3	J	85	ARG	C-N-CA	7.74	128.35	120.38
3	E	85	ARG	CA-C-N	7.74	128.35	120.38
3	E	85	ARG	C-N-CA	7.74	128.35	120.38
3	E	205	LYS	N-CA-C	7.73	120.39	111.11
3	F	205	LYS	N-CA-C	7.73	120.38	111.11
3	A	85	ARG	CA-C-N	7.72	128.33	120.38
3	A	85	ARG	C-N-CA	7.72	128.33	120.38
3	C	85	ARG	CA-C-N	7.72	128.33	120.38
3	C	85	ARG	C-N-CA	7.72	128.33	120.38
3	H	85	ARG	CA-C-N	7.71	128.33	120.38
3	H	85	ARG	C-N-CA	7.71	128.33	120.38
3	K	85	ARG	CA-C-N	7.68	128.29	120.38
3	K	85	ARG	C-N-CA	7.68	128.29	120.38
3	G	62	SER	N-CA-C	7.51	121.54	112.38
3	I	205	LYS	N-CA-C	7.50	120.40	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	118	SER	N-CA-C	7.48	121.98	113.01
3	I	62	SER	N-CA-C	7.47	121.50	112.38
3	G	205	LYS	N-CA-C	7.47	120.37	111.33
5	Y	118	SER	N-CA-C	7.47	121.97	113.01
3	F	62	SER	N-CA-C	7.47	121.49	112.38
3	D	62	SER	N-CA-C	7.46	121.49	112.38
5	Y	108	PRO	N-CA-C	-7.45	99.37	111.21
5	X	108	PRO	N-CA-C	-7.44	99.37	111.21
3	J	62	SER	N-CA-C	7.43	121.45	112.38
3	H	62	SER	N-CA-C	7.43	121.44	112.38
3	B	62	SER	N-CA-C	7.43	121.44	112.38
3	K	62	SER	N-CA-C	7.42	121.43	112.38
3	C	62	SER	N-CA-C	7.41	121.42	112.38
3	E	62	SER	N-CA-C	7.40	121.41	112.38
3	A	62	SER	N-CA-C	7.37	121.37	112.38
5	X	119	VAL	N-CA-C	7.30	119.13	109.21
5	Y	119	VAL	N-CA-C	7.28	119.10	109.21
3	I	224	LEU	N-CA-C	7.14	119.15	111.36
3	G	224	LEU	N-CA-C	7.12	119.12	111.36
3	C	52	ALA	N-CA-C	-7.11	104.57	113.18
5	Y	50	VAL	N-CA-C	7.10	119.92	111.05
5	X	50	VAL	N-CA-C	7.09	119.91	111.05
3	A	52	ALA	N-CA-C	-7.07	104.62	113.18
3	G	52	ALA	N-CA-C	-7.07	104.63	113.18
3	J	52	ALA	N-CA-C	-7.06	104.64	113.18
3	F	52	ALA	N-CA-C	-7.05	104.64	113.18
3	D	52	ALA	N-CA-C	-7.05	104.65	113.18
3	E	52	ALA	N-CA-C	-7.05	104.65	113.18
3	I	52	ALA	N-CA-C	-7.05	104.65	113.18
3	K	52	ALA	N-CA-C	-7.04	104.66	113.18
3	H	52	ALA	N-CA-C	-7.04	104.67	113.18
3	B	52	ALA	N-CA-C	-7.03	104.67	113.18
4	f	582	TYR	N-CA-C	6.97	120.32	110.50
4	e	582	TYR	N-CA-C	6.93	120.28	110.50
4	j	582	TYR	N-CA-C	6.93	120.28	110.50
4	k	582	TYR	N-CA-C	6.93	120.27	110.50
4	c	582	TYR	N-CA-C	6.92	120.27	110.50
4	b	582	TYR	N-CA-C	6.92	120.26	110.50
4	h	582	TYR	N-CA-C	6.92	120.26	110.50
4	d	582	TYR	N-CA-C	6.91	120.25	110.50
4	a	582	TYR	N-CA-C	6.91	120.25	110.50
5	X	86	PRO	CA-C-N	6.87	126.85	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	86	PRO	C-N-CA	6.87	126.85	119.78
5	Y	86	PRO	CA-C-N	6.86	126.85	119.78
5	Y	86	PRO	C-N-CA	6.86	126.85	119.78
5	Y	117	LYS	N-CA-C	6.85	119.62	111.33
3	G	188	GLU	N-CA-C	6.84	119.76	111.82
5	X	117	LYS	N-CA-C	6.84	119.60	111.33
3	C	188	GLU	N-CA-C	6.81	119.72	111.82
3	I	188	GLU	N-CA-C	6.81	119.72	111.82
3	A	188	GLU	N-CA-C	6.80	119.71	111.82
3	H	188	GLU	N-CA-C	6.79	119.70	111.82
3	B	188	GLU	N-CA-C	6.79	119.70	111.82
3	E	188	GLU	N-CA-C	6.79	119.70	111.82
3	D	188	GLU	N-CA-C	6.78	119.69	111.82
3	J	188	GLU	N-CA-C	6.78	119.68	111.82
3	F	188	GLU	N-CA-C	6.76	119.66	111.82
3	K	188	GLU	N-CA-C	6.75	119.65	111.82
3	F	122	VAL	CB-CA-C	-6.74	103.21	112.04
5	Y	127	LEU	N-CA-C	6.61	118.24	108.60
5	X	127	LEU	N-CA-C	6.59	118.22	108.60
3	H	223	ASN	N-CA-C	6.57	120.45	111.39
3	J	223	ASN	N-CA-C	6.55	120.43	111.39
5	X	53	TRP	N-CA-C	-6.54	104.23	111.82
5	Y	53	TRP	N-CA-C	-6.54	104.24	111.82
3	K	223	ASN	N-CA-C	6.53	120.39	111.39
5	Y	138	ALA	CA-C-N	6.53	126.49	120.03
5	Y	138	ALA	C-N-CA	6.53	126.49	120.03
5	X	138	ALA	CA-C-N	6.51	126.48	120.03
5	X	138	ALA	C-N-CA	6.51	126.48	120.03
5	X	142	MET	CA-C-N	6.51	126.74	119.32
5	X	142	MET	C-N-CA	6.51	126.74	119.32
5	Y	142	MET	CA-C-N	6.48	126.71	119.32
5	Y	142	MET	C-N-CA	6.48	126.71	119.32
3	J	116	ARG	N-CA-CB	6.46	120.79	110.46
5	Y	68	GLU	CA-C-N	6.29	128.99	120.44
5	Y	68	GLU	C-N-CA	6.29	128.99	120.44
5	X	35	LEU	N-CA-C	6.25	119.21	109.52
5	X	68	GLU	CA-C-N	6.25	128.94	120.44
5	X	68	GLU	C-N-CA	6.25	128.94	120.44
5	Y	49	ILE	N-CA-C	6.23	117.72	110.62
5	Y	35	LEU	N-CA-C	6.23	119.17	109.52
5	X	49	ILE	N-CA-C	6.22	117.71	110.62
3	J	115	TYR	N-CA-C	-6.22	96.95	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	121	THR	N-CA-CB	6.22	121.04	111.22
3	G	50	ARG	N-CA-C	6.20	118.04	111.28
3	J	50	ARG	N-CA-C	6.20	118.04	111.28
3	K	50	ARG	N-CA-C	6.17	118.01	111.28
3	H	50	ARG	N-CA-C	6.17	118.00	111.28
3	I	50	ARG	N-CA-C	6.16	118.00	111.28
5	Y	58	PHE	N-CA-C	6.16	120.55	107.67
3	I	172	GLY	N-CA-C	6.16	119.49	110.80
3	J	172	GLY	N-CA-C	6.16	119.48	110.80
3	G	172	GLY	N-CA-C	6.16	119.48	110.80
3	K	172	GLY	N-CA-C	6.16	119.48	110.80
3	D	50	ARG	N-CA-C	6.15	117.99	111.28
5	X	58	PHE	N-CA-C	6.15	120.53	107.67
3	B	50	ARG	N-CA-C	6.15	117.98	111.28
3	H	172	GLY	N-CA-C	6.14	119.45	110.80
3	F	50	ARG	N-CA-C	6.13	117.96	111.28
3	E	50	ARG	N-CA-C	6.13	117.96	111.28
3	F	172	GLY	N-CA-C	6.12	119.54	110.42
5	Y	22	LEU	N-CA-C	6.11	118.73	111.33
3	D	172	GLY	N-CA-C	6.11	119.53	110.42
3	A	50	ARG	N-CA-C	6.11	117.94	111.28
3	E	172	GLY	N-CA-C	6.10	119.51	110.42
3	C	172	GLY	N-CA-C	6.10	119.50	110.42
5	X	22	LEU	N-CA-C	6.10	118.71	111.33
3	A	172	GLY	N-CA-C	6.09	119.50	110.42
3	C	50	ARG	N-CA-C	6.09	117.92	111.28
3	B	172	GLY	N-CA-C	6.08	119.47	110.42
3	D	222	SER	N-CA-C	6.02	120.48	113.20
3	C	222	SER	N-CA-C	6.01	120.47	113.20
3	F	222	SER	N-CA-C	5.99	120.44	113.20
3	B	222	SER	N-CA-C	5.99	120.44	113.20
3	A	222	SER	N-CA-C	5.97	120.43	113.20
3	C	207	THR	O-C-N	5.96	128.43	122.12
3	E	207	THR	O-C-N	5.95	128.43	122.12
3	E	222	SER	N-CA-C	5.93	120.38	113.20
3	A	105	LEU	N-CA-C	5.93	117.74	111.28
3	C	105	LEU	N-CA-C	5.93	117.74	111.28
3	H	105	LEU	N-CA-C	5.93	117.74	111.28
3	F	207	THR	O-C-N	5.93	128.40	122.12
3	H	207	THR	O-C-N	5.93	128.40	122.12
3	J	105	LEU	N-CA-C	5.91	117.72	111.28
3	K	105	LEU	N-CA-C	5.91	117.72	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	105	LEU	N-CA-C	5.91	117.72	111.28
3	D	207	THR	O-C-N	5.90	128.37	122.12
3	B	105	LEU	N-CA-C	5.90	117.71	111.28
3	A	207	THR	O-C-N	5.89	128.37	122.12
3	I	207	THR	O-C-N	5.89	128.37	122.12
3	J	207	THR	O-C-N	5.89	128.36	122.12
3	D	105	LEU	N-CA-C	5.88	117.69	111.28
3	F	105	LEU	N-CA-C	5.87	117.68	111.28
3	G	207	THR	O-C-N	5.85	128.32	122.12
3	B	207	THR	O-C-N	5.85	128.32	122.12
3	G	105	LEU	N-CA-C	5.85	117.65	111.28
4	f	575	TYR	N-CA-C	5.85	118.43	111.71
4	d	575	TYR	N-CA-C	5.84	118.43	111.71
3	I	105	LEU	N-CA-C	5.84	117.64	111.28
4	a	575	TYR	N-CA-C	5.82	118.41	111.71
3	K	207	THR	O-C-N	5.82	128.29	122.12
4	e	575	TYR	N-CA-C	5.81	118.39	111.71
4	b	575	TYR	N-CA-C	5.81	118.39	111.71
4	c	575	TYR	N-CA-C	5.80	118.38	111.71
5	X	107	SER	CA-C-N	-5.80	113.81	119.78
5	X	107	SER	C-N-CA	-5.80	113.81	119.78
5	X	44	ALA	N-CA-C	5.78	118.36	111.71
5	Y	44	ALA	N-CA-C	5.77	118.35	111.71
5	Y	107	SER	CA-C-N	-5.77	113.83	119.78
5	Y	107	SER	C-N-CA	-5.77	113.83	119.78
3	I	101	GLY	CA-C-N	5.74	125.42	119.56
3	I	101	GLY	C-N-CA	5.74	125.42	119.56
5	X	43	LEU	N-CA-C	-5.74	105.02	111.28
5	Y	43	LEU	N-CA-C	-5.73	105.04	111.28
3	G	101	GLY	CA-C-N	5.71	125.38	119.56
3	G	101	GLY	C-N-CA	5.71	125.38	119.56
3	F	101	GLY	CA-C-N	5.63	125.47	119.28
3	F	101	GLY	C-N-CA	5.63	125.47	119.28
4	k	575	TYR	N-CA-C	5.63	118.35	111.82
4	j	575	TYR	N-CA-C	5.62	118.34	111.82
3	D	101	GLY	CA-C-N	5.62	125.46	119.28
3	D	101	GLY	C-N-CA	5.62	125.46	119.28
3	E	101	GLY	CA-C-N	5.61	125.45	119.28
3	E	101	GLY	C-N-CA	5.61	125.45	119.28
3	J	101	GLY	CA-C-N	5.60	125.44	119.28
3	J	101	GLY	C-N-CA	5.60	125.44	119.28
5	X	77	ASP	N-CA-C	5.60	117.92	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	77	ASP	N-CA-C	5.60	117.92	110.53
5	X	162	ALA	N-CA-C	5.59	119.20	112.38
4	h	575	TYR	N-CA-C	5.59	118.30	111.82
3	C	101	GLY	CA-C-N	5.59	125.42	119.28
3	C	101	GLY	C-N-CA	5.59	125.42	119.28
3	E	68	VAL	N-CA-C	5.59	116.32	110.62
3	K	101	GLY	CA-C-N	5.59	125.43	119.28
3	K	101	GLY	C-N-CA	5.59	125.43	119.28
3	A	68	VAL	N-CA-C	5.58	116.31	110.62
3	B	68	VAL	N-CA-C	5.58	116.32	110.62
3	C	68	VAL	N-CA-C	5.58	116.32	110.62
3	A	101	GLY	CA-C-N	5.58	125.42	119.28
3	A	101	GLY	C-N-CA	5.58	125.42	119.28
3	B	101	GLY	CA-C-N	5.57	125.40	119.28
3	B	101	GLY	C-N-CA	5.57	125.40	119.28
3	G	68	VAL	N-CA-C	5.56	116.29	110.62
3	H	101	GLY	CA-C-N	5.56	125.40	119.28
3	H	101	GLY	C-N-CA	5.56	125.40	119.28
3	F	68	VAL	N-CA-C	5.56	116.29	110.62
3	I	68	VAL	N-CA-C	5.55	116.29	110.62
5	Y	162	ALA	N-CA-C	5.54	119.14	112.38
3	D	68	VAL	N-CA-C	5.53	116.26	110.62
3	H	104	ASP	N-CA-C	5.53	117.38	111.36
3	J	104	ASP	N-CA-C	5.51	117.37	111.36
3	J	68	VAL	N-CA-C	5.48	116.26	110.72
3	I	116	ARG	N-CA-C	5.48	117.63	109.25
3	H	68	VAL	N-CA-C	5.47	116.24	110.72
3	K	68	VAL	N-CA-C	5.47	116.24	110.72
3	G	116	ARG	N-CA-C	5.46	117.61	109.25
3	K	104	ASP	N-CA-C	5.46	117.31	111.36
3	I	69	ALA	CA-C-N	5.44	127.84	120.44
3	I	69	ALA	C-N-CA	5.44	127.84	120.44
3	H	114	LYS	N-CA-C	5.43	119.49	112.86
3	G	69	ALA	CA-C-N	5.42	127.81	120.44
3	G	69	ALA	C-N-CA	5.42	127.81	120.44
3	J	69	ALA	CA-C-N	5.41	127.98	120.29
3	J	69	ALA	C-N-CA	5.41	127.98	120.29
5	X	95	GLU	CA-C-N	-5.41	114.35	119.76
5	X	95	GLU	C-N-CA	-5.41	114.35	119.76
3	H	69	ALA	CA-C-N	5.41	127.97	120.29
3	H	69	ALA	C-N-CA	5.41	127.97	120.29
5	Y	95	GLU	CA-C-N	-5.40	114.36	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	95	GLU	C-N-CA	-5.40	114.36	119.76
3	A	69	ALA	CA-C-N	5.40	127.95	120.29
3	A	69	ALA	C-N-CA	5.40	127.95	120.29
3	I	81	GLN	N-CA-C	5.38	118.16	108.48
3	C	69	ALA	CA-C-N	5.38	127.92	120.29
3	C	69	ALA	C-N-CA	5.38	127.92	120.29
3	K	69	ALA	CA-C-N	5.37	127.91	120.29
3	K	69	ALA	C-N-CA	5.37	127.91	120.29
3	G	81	GLN	N-CA-C	5.37	118.14	108.48
5	X	55	ARG	CA-C-N	5.37	130.18	122.40
5	X	55	ARG	C-N-CA	5.37	130.18	122.40
5	X	43	LEU	CA-C-N	5.36	128.00	120.28
5	X	43	LEU	C-N-CA	5.36	128.00	120.28
3	E	81	GLN	N-CA-C	5.36	118.17	108.69
3	H	72	ALA	N-CA-C	-5.36	105.44	111.28
5	Y	55	ARG	CA-C-N	5.36	130.17	122.40
5	Y	55	ARG	C-N-CA	5.36	130.17	122.40
3	D	69	ALA	CA-C-N	5.35	127.89	120.29
3	D	69	ALA	C-N-CA	5.35	127.89	120.29
3	E	72	ALA	N-CA-C	-5.35	105.44	111.28
3	B	69	ALA	CA-C-N	5.35	127.89	120.29
3	B	69	ALA	C-N-CA	5.35	127.89	120.29
5	Y	43	LEU	CA-C-N	5.35	127.98	120.28
5	Y	43	LEU	C-N-CA	5.35	127.98	120.28
3	H	81	GLN	N-CA-C	5.34	118.15	108.69
3	H	137	GLY	N-CA-C	-5.34	103.55	111.03
3	J	72	ALA	N-CA-C	-5.34	105.45	111.28
3	J	137	GLY	N-CA-C	-5.34	103.55	111.03
3	E	137	GLY	N-CA-C	-5.34	103.55	111.03
3	A	81	GLN	N-CA-C	5.34	118.15	108.69
3	C	72	ALA	N-CA-C	-5.34	105.46	111.28
3	F	81	GLN	N-CA-C	5.34	118.14	108.69
3	F	137	GLY	N-CA-C	-5.34	103.56	111.03
3	B	137	GLY	N-CA-C	-5.34	103.56	111.03
3	D	81	GLN	N-CA-C	5.34	118.14	108.69
3	D	137	GLY	N-CA-C	-5.33	103.56	111.03
3	E	69	ALA	CA-C-N	5.33	127.86	120.29
3	E	69	ALA	C-N-CA	5.33	127.86	120.29
3	A	72	ALA	N-CA-C	-5.33	105.47	111.28
3	K	137	GLY	N-CA-C	-5.33	103.57	111.03
3	C	81	GLN	N-CA-C	5.33	118.12	108.69
3	F	69	ALA	CA-C-N	5.33	127.85	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	69	ALA	C-N-CA	5.33	127.85	120.29
3	A	137	GLY	N-CA-C	-5.33	103.58	111.03
3	J	81	GLN	N-CA-C	5.33	118.11	108.69
3	K	81	GLN	N-CA-C	5.32	118.11	108.69
3	G	72	ALA	N-CA-C	-5.32	105.48	111.28
3	K	72	ALA	N-CA-C	-5.32	105.48	111.28
3	B	81	GLN	N-CA-C	5.32	118.11	108.69
3	E	218	LEU	CB-CA-C	5.32	117.09	109.11
3	A	218	LEU	CB-CA-C	5.31	117.08	109.11
3	C	137	GLY	N-CA-C	-5.31	103.59	111.03
3	B	72	ALA	N-CA-C	-5.31	105.49	111.28
3	C	218	LEU	CB-CA-C	5.30	117.06	109.11
3	B	218	LEU	CB-CA-C	5.30	117.06	109.11
3	F	119	LYS	N-CA-C	5.30	122.09	110.80
3	F	72	ALA	N-CA-C	-5.29	105.51	111.28
3	I	72	ALA	N-CA-C	-5.28	105.52	111.28
3	D	72	ALA	N-CA-C	-5.28	105.52	111.28
3	F	218	LEU	CB-CA-C	5.28	117.03	109.11
3	D	218	LEU	CB-CA-C	5.27	117.01	109.11
3	K	250	GLU	N-CA-C	-5.26	105.63	111.36
3	I	38	GLN	N-CA-C	-5.23	105.66	111.36
3	G	38	GLN	N-CA-C	-5.23	105.66	111.36
3	F	250	GLU	N-CA-C	-5.23	105.66	111.36
3	D	38	GLN	N-CA-C	-5.22	105.67	111.36
3	I	250	GLU	N-CA-C	-5.22	105.67	111.36
3	B	38	GLN	N-CA-C	-5.22	105.67	111.36
3	E	38	GLN	N-CA-C	-5.22	105.67	111.36
5	X	62	PRO	N-CA-C	-5.21	102.58	112.33
5	X	51	ALA	N-CA-C	5.21	118.74	112.38
3	H	251	ALA	N-CA-C	5.21	116.64	111.07
5	X	125	HIS	CA-C-N	5.21	129.75	122.36
5	X	125	HIS	C-N-CA	5.21	129.75	122.36
3	A	250	GLU	N-CA-C	-5.21	105.69	111.36
3	C	250	GLU	N-CA-C	-5.21	105.69	111.36
3	D	251	ALA	N-CA-C	5.20	116.63	111.07
3	F	38	GLN	N-CA-C	-5.20	105.70	111.36
3	B	250	GLU	N-CA-C	-5.20	105.70	111.36
3	D	250	GLU	N-CA-C	-5.20	105.70	111.36
5	Y	125	HIS	CA-C-N	5.20	129.74	122.36
5	Y	125	HIS	C-N-CA	5.20	129.74	122.36
3	A	38	GLN	N-CA-C	-5.19	105.70	111.36
5	Y	62	PRO	N-CA-C	-5.19	102.62	112.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	38	GLN	N-CA-C	-5.18	105.71	111.36
3	J	251	ALA	N-CA-C	5.18	116.61	111.07
3	B	114	LYS	N-CA-C	5.18	118.73	111.74
3	D	114	LYS	N-CA-C	5.18	118.73	111.74
5	Y	51	ALA	N-CA-C	5.17	118.69	112.38
3	I	117	VAL	N-CA-C	5.17	115.81	108.42
3	H	250	GLU	N-CA-C	-5.17	105.65	111.28
5	Y	59	ASN	C-N-CD	-5.17	103.81	125.00
3	A	114	LYS	N-CA-C	5.16	118.71	111.74
3	J	250	GLU	N-CA-C	-5.16	105.65	111.28
3	A	251	ALA	N-CA-C	5.16	116.59	111.07
3	E	250	GLU	N-CA-C	-5.16	105.74	111.36
3	F	251	ALA	N-CA-C	5.16	116.59	111.07
3	K	251	ALA	N-CA-C	5.16	116.59	111.07
3	C	114	LYS	N-CA-C	5.15	118.70	111.74
3	E	251	ALA	N-CA-C	5.15	116.58	111.07
3	C	251	ALA	N-CA-C	5.15	116.58	111.07
3	F	114	LYS	N-CA-C	5.14	118.69	111.74
3	E	114	LYS	N-CA-C	5.14	118.68	111.74
3	I	251	ALA	N-CA-C	5.14	116.57	111.07
5	X	59	ASN	C-N-CD	-5.14	103.92	125.00
3	B	251	ALA	N-CA-C	5.14	116.57	111.07
5	Y	143	PRO	CA-C-N	5.13	127.67	120.28
5	Y	143	PRO	C-N-CA	5.13	127.67	120.28
3	G	117	VAL	N-CA-C	5.13	115.75	108.42
3	G	251	ALA	N-CA-C	5.12	116.55	111.07
3	G	250	GLU	N-CA-C	-5.12	105.70	111.28
5	X	143	PRO	CA-C-N	5.12	127.64	120.28
5	X	143	PRO	C-N-CA	5.12	127.64	120.28
3	F	247	ILE	CA-C-O	-5.09	115.78	121.17
3	J	114	LYS	N-CA-C	5.08	118.63	111.52
3	B	247	ILE	CA-C-O	-5.06	115.80	121.17
3	K	114	LYS	N-CA-C	5.06	118.60	111.52
3	H	236	ALA	N-CA-C	5.05	116.79	111.28
3	C	247	ILE	CA-C-O	-5.05	115.81	121.17
3	A	236	ALA	N-CA-C	5.04	116.78	111.28
3	E	247	ILE	CA-C-O	-5.04	115.83	121.17
3	K	247	ILE	CA-C-O	-5.04	115.83	121.17
3	C	236	ALA	N-CA-C	5.03	116.77	111.28
3	D	247	ILE	CA-C-O	-5.03	115.84	121.17
3	I	247	ILE	CA-C-O	-5.03	115.84	121.17
3	J	236	ALA	N-CA-C	5.03	116.76	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	115	GLN	N-CA-C	5.03	118.89	112.26
3	K	236	ALA	N-CA-C	5.02	116.75	111.28
3	A	247	ILE	CA-C-O	-5.02	115.85	121.17
3	F	236	ALA	N-CA-C	5.02	116.75	111.28
3	J	247	ILE	CA-C-O	-5.01	115.86	121.17
5	Y	115	GLN	N-CA-C	5.01	118.88	112.26
3	G	236	ALA	N-CA-C	5.01	116.74	111.28
3	B	236	ALA	N-CA-C	5.01	116.74	111.28

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	255	SER	Mainchain
3	B	255	SER	Mainchain
3	C	255	SER	Mainchain
3	D	255	SER	Mainchain
3	E	255	SER	Mainchain
3	F	255	SER	Mainchain
3	G	255	SER	Mainchain
3	H	255	SER	Mainchain
3	I	255	SER	Mainchain
3	J	255	SER	Mainchain
3	K	255	SER	Mainchain

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	1	560	0	337	23	0
2	2	588	0	310	18	0
3	A	2066	0	2153	52	0
3	B	2066	0	2153	76	0
3	C	2066	0	2153	71	0
3	D	2066	0	2153	67	0
3	E	2066	0	2157	73	0
3	F	2066	0	2156	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	2066	0	2155	109	0
3	H	2066	0	2157	83	0
3	I	2066	0	2154	93	0
3	J	2066	0	2155	74	0
3	K	2066	0	2154	54	0
4	a	129	0	110	0	0
4	b	129	0	110	0	0
4	c	129	0	110	0	0
4	d	129	0	110	0	0
4	e	129	0	110	0	0
4	f	129	0	110	0	0
4	h	129	0	110	2	0
4	j	129	0	110	2	0
4	k	129	0	110	2	0
5	X	1314	0	1303	78	0
5	Y	1314	0	1303	71	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
7	A	31	0	12	0	0
7	B	31	0	12	3	0
7	C	31	0	12	3	0
7	D	31	0	12	3	0
7	E	31	0	12	1	0
7	F	31	0	12	3	0
7	G	31	0	12	3	0
7	H	31	0	12	3	0
7	I	31	0	12	4	0
7	J	31	0	12	9	0
7	K	31	0	12	4	0
All	All	28015	0	28075	822	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 15.

All (822) 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)
5:Y:156:MET:HE3	5:Y:161:MET:CE	1.14	1.58
5:X:156:MET:HE3	5:X:161:MET:CE	1.14	1.58
5:Y:156:MET:CE	5:Y:161:MET:HE2	1.21	1.57
5:X:156:MET:CE	5:X:161:MET:HE2	1.21	1.54
3:I:220:VAL:CG2	3:I:262:LYS:HB3	1.07	1.52
5:Y:138:ALA:CB	5:Y:153:ARG:NH1	1.72	1.52
3:I:220:VAL:HG21	3:I:262:LYS:CB	1.06	1.50
3:G:220:VAL:CG1	3:G:262:LYS:HB3	1.41	1.48
3:D:220:VAL:HG11	3:D:262:LYS:CB	1.43	1.47
3:A:220:VAL:HG11	3:A:262:LYS:CB	1.44	1.47
3:C:220:VAL:HG11	3:C:262:LYS:CB	1.44	1.47
3:B:220:VAL:HG11	3:B:262:LYS:CB	1.43	1.47
3:E:220:VAL:HG11	3:E:262:LYS:CB	1.44	1.45
3:F:220:VAL:HG11	3:F:262:LYS:CB	1.44	1.44
5:X:149:GLY:O	5:X:158:PHE:CD2	1.72	1.42
3:D:220:VAL:CG1	3:D:262:LYS:HB3	1.50	1.40
3:E:191:ARG:NH2	3:F:243:ARG:NH2	1.69	1.40
3:A:191:ARG:NH2	3:B:243:ARG:NH2	1.69	1.40
3:C:191:ARG:NH2	3:D:243:ARG:NH2	1.69	1.40
3:C:220:VAL:CG1	3:C:262:LYS:HB3	1.51	1.39
3:A:220:VAL:CG1	3:A:262:LYS:HB3	1.51	1.39
3:B:220:VAL:CG1	3:B:262:LYS:HB3	1.51	1.39
3:F:220:VAL:CG1	3:F:262:LYS:HB3	1.51	1.39
3:G:220:VAL:CG2	3:G:261:LYS:CB	2.01	1.38
3:E:191:ARG:CZ	3:F:243:ARG:NH2	1.87	1.37
3:E:220:VAL:CG1	3:E:262:LYS:HB3	1.50	1.37
3:B:191:ARG:NH2	3:C:243:ARG:NH2	1.68	1.36
3:C:191:ARG:CZ	3:D:243:ARG:NH2	1.87	1.36
3:A:191:ARG:CZ	3:B:243:ARG:NH2	1.87	1.33
3:F:220:VAL:HG12	3:F:261:LYS:O	1.30	1.31
3:H:220:VAL:CG1	3:H:261:LYS:O	1.76	1.30
3:G:220:VAL:CB	3:G:261:LYS:O	1.78	1.29
3:J:65:GLY:CA	7:J:302:ATP:O2A	1.78	1.29
3:B:191:ARG:CZ	3:C:243:ARG:NH2	1.95	1.28
3:A:220:VAL:HG12	3:A:261:LYS:O	1.30	1.27
3:I:220:VAL:HG21	3:I:262:LYS:CA	1.63	1.27
3:C:220:VAL:HG12	3:C:261:LYS:O	1.30	1.27
3:E:220:VAL:HG12	3:E:261:LYS:O	1.30	1.27
3:B:220:VAL:HG12	3:B:261:LYS:O	1.30	1.26
3:D:220:VAL:HG12	3:D:261:LYS:O	1.30	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:220:VAL:HB	3:G:261:LYS:O	1.12	1.26
5:X:149:GLY:O	5:X:158:PHE:HD2	0.95	1.26
3:H:220:VAL:HG12	3:H:261:LYS:O	1.14	1.26
3:G:220:VAL:CG2	3:G:261:LYS:HB3	1.61	1.25
3:H:191:ARG:NH2	3:I:243:ARG:NH2	1.84	1.25
3:C:220:VAL:HG11	3:C:262:LYS:CA	1.70	1.22
3:D:220:VAL:HG11	3:D:262:LYS:CA	1.70	1.21
3:F:220:VAL:HG11	3:F:262:LYS:CA	1.70	1.21
3:B:220:VAL:HG11	3:B:262:LYS:CA	1.70	1.20
3:E:220:VAL:HG11	3:E:262:LYS:CA	1.70	1.20
3:J:65:GLY:HA2	7:J:302:ATP:O2A	1.03	1.20
3:A:220:VAL:HG11	3:A:262:LYS:CA	1.70	1.20
3:H:191:ARG:NH2	3:I:243:ARG:HH21	1.38	1.19
3:B:220:VAL:CG1	3:B:261:LYS:O	1.92	1.18
3:C:116:ARG:NE	3:H:184:GLU:OE2	1.76	1.18
3:F:220:VAL:CG1	3:F:261:LYS:O	1.92	1.18
3:D:220:VAL:CG1	3:D:261:LYS:O	1.92	1.18
3:G:65:GLY:HA2	7:G:302:ATP:O1A	1.42	1.18
3:C:220:VAL:CG1	3:C:261:LYS:O	1.92	1.17
3:H:65:GLY:HA2	7:H:302:ATP:O2A	1.44	1.17
3:J:191:ARG:NH2	3:K:243:ARG:NH2	1.92	1.17
3:I:65:GLY:HA2	7:I:302:ATP:O1A	1.42	1.17
3:E:220:VAL:CG1	3:E:261:LYS:O	1.92	1.16
3:A:220:VAL:CG1	3:A:261:LYS:O	1.92	1.16
3:D:85:ARG:HD2	3:K:273:LYS:HE2	1.22	1.15
3:G:220:VAL:HG23	3:G:261:LYS:CB	1.71	1.15
5:X:59:ASN:HB3	5:X:60:PRO:HD3	1.27	1.14
3:H:220:VAL:CG1	3:H:262:LYS:HB3	1.76	1.14
5:Y:138:ALA:HB2	5:Y:153:ARG:CZ	1.76	1.13
5:Y:138:ALA:CB	5:Y:153:ARG:HH12	1.40	1.13
3:G:220:VAL:HG11	3:G:262:LYS:CB	1.79	1.13
3:G:220:VAL:HG21	3:G:261:LYS:HB2	1.24	1.12
1:1:4:DT:OP1	3:A:121:THR:OG1	1.64	1.12
5:Y:138:ALA:HB1	5:Y:153:ARG:NH1	1.47	1.12
3:G:220:VAL:HG21	3:G:261:LYS:CB	1.71	1.11
5:Y:138:ALA:HB2	5:Y:153:ARG:NH1	1.41	1.10
5:X:150:CYS:SG	5:X:155:ARG:CZ	2.40	1.10
3:I:220:VAL:CG2	3:I:262:LYS:CB	1.81	1.09
5:Y:150:CYS:SG	5:Y:155:ARG:CZ	2.40	1.09
3:G:220:VAL:CG2	3:G:261:LYS:HB2	1.78	1.09
3:I:220:VAL:HG23	3:I:262:LYS:HB3	1.30	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:220:VAL:CG2	3:G:261:LYS:O	2.00	1.08
3:I:191:ARG:NH2	3:J:243:ARG:NH2	2.01	1.08
3:I:114:LYS:HD2	5:Y:7:VAL:HG23	1.09	1.08
3:B:185:GLN:NE2	3:C:173:THR:HG21	1.69	1.07
3:I:114:LYS:HD2	5:Y:7:VAL:CG2	1.86	1.06
3:A:191:ARG:CZ	3:B:243:ARG:HH21	1.58	1.06
3:G:191:ARG:NH2	3:H:243:ARG:NH2	2.02	1.06
3:G:220:VAL:HG11	3:G:262:LYS:HB3	1.06	1.06
3:G:114:LYS:HD2	5:X:7:VAL:CG2	1.86	1.05
3:G:220:VAL:CG1	3:G:262:LYS:CB	2.33	1.05
3:G:114:LYS:HD2	5:X:7:VAL:HG23	1.09	1.04
3:G:191:ARG:CZ	3:H:243:ARG:NH2	2.19	1.04
3:I:191:ARG:CZ	3:J:243:ARG:NH2	2.19	1.04
3:D:191:ARG:NH2	3:E:243:ARG:NH2	2.06	1.04
3:C:220:VAL:HG21	3:C:262:LYS:HD3	1.41	1.03
3:E:220:VAL:HG21	3:E:262:LYS:HD3	1.41	1.03
3:C:85:ARG:HD2	3:J:273:LYS:HE2	1.32	1.03
3:I:85:ARG:HB2	3:I:86:PRO:CD	1.89	1.02
3:G:85:ARG:HB2	3:G:86:PRO:CD	1.89	1.02
3:B:220:VAL:HG21	3:B:262:LYS:HD3	1.40	1.02
3:A:220:VAL:HG21	3:A:262:LYS:HD3	1.41	1.01
3:I:85:ARG:HB2	3:I:86:PRO:HD2	1.04	1.01
3:A:85:ARG:HD2	3:H:273:LYS:HE2	1.40	1.01
3:G:85:ARG:HB2	3:G:86:PRO:HD2	1.04	1.01
3:D:220:VAL:HG21	3:D:262:LYS:HD3	1.41	1.01
3:B:191:ARG:NH2	3:C:243:ARG:HH21	1.40	1.01
3:F:220:VAL:HG21	3:F:262:LYS:HD3	1.40	1.00
2:2:6:DA:OP1	5:Y:38:SER:OG	1.80	1.00
3:D:85:ARG:CD	3:K:273:LYS:HE2	1.90	0.99
3:E:191:ARG:CZ	3:F:243:ARG:HH21	1.58	0.99
3:H:220:VAL:HG13	3:H:262:LYS:HB3	1.41	0.98
3:D:191:ARG:NH2	3:E:243:ARG:HH21	1.60	0.98
3:B:191:ARG:CZ	3:C:243:ARG:HH21	1.64	0.98
3:E:191:ARG:NH2	3:F:243:ARG:HH22	1.48	0.98
3:C:191:ARG:CZ	3:D:243:ARG:HH21	1.58	0.97
3:B:220:VAL:CG1	3:B:262:LYS:CB	2.24	0.97
3:J:191:ARG:CZ	3:K:243:ARG:NH2	2.27	0.96
3:I:127:ASP:OD2	5:Y:34:HIS:CD2	2.18	0.96
3:G:127:ASP:OD2	5:X:34:HIS:CD2	2.18	0.96
3:H:191:ARG:HH21	3:I:243:ARG:HH21	1.06	0.96
3:E:220:VAL:CG1	3:E:262:LYS:CB	2.24	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:220:VAL:HG12	3:G:262:LYS:HB3	1.45	0.95
5:Y:138:ALA:HB1	5:Y:153:ARG:HH12	1.08	0.95
3:G:220:VAL:CG2	3:G:261:LYS:C	2.39	0.95
3:J:191:ARG:NH2	3:K:243:ARG:HH21	1.59	0.94
3:C:220:VAL:CG1	3:C:262:LYS:CB	2.24	0.94
3:G:114:LYS:NZ	5:X:3:GLU:OE2	2.01	0.94
3:G:220:VAL:HG23	3:G:261:LYS:HB3	0.94	0.94
3:H:220:VAL:HG11	3:H:262:LYS:HB3	1.47	0.94
3:A:191:ARG:NH2	3:B:243:ARG:HH22	1.48	0.94
3:I:114:LYS:NZ	5:Y:3:GLU:OE2	2.01	0.94
3:C:191:ARG:NH2	3:D:243:ARG:HH22	1.48	0.94
3:G:85:ARG:CB	3:G:86:PRO:HD2	1.93	0.93
5:X:59:ASN:HB3	5:X:60:PRO:CD	1.99	0.93
3:A:191:ARG:NH2	3:B:243:ARG:HH21	1.47	0.93
3:A:220:VAL:HG11	3:A:262:LYS:HB3	0.93	0.93
3:B:191:ARG:NH2	3:C:243:ARG:HH22	1.53	0.92
3:B:220:VAL:HG11	3:B:262:LYS:HB3	0.92	0.92
5:Y:59:ASN:HB2	5:Y:60:PRO:HD3	1.48	0.92
3:D:220:VAL:HG11	3:D:262:LYS:HB3	0.93	0.92
3:F:220:VAL:HG11	3:F:262:LYS:HB3	0.93	0.92
3:E:191:ARG:NH2	3:F:243:ARG:HH21	1.46	0.92
3:E:220:VAL:HG11	3:E:262:LYS:HB3	0.93	0.92
3:C:220:VAL:HG11	3:C:262:LYS:HB3	0.93	0.92
5:X:150:CYS:SG	5:X:155:ARG:NH1	2.44	0.91
1:I:21:DT:OP2	3:J:121:THR:OG1	1.87	0.91
3:C:191:ARG:NH2	3:D:243:ARG:HH21	1.46	0.91
3:I:85:ARG:CB	3:I:86:PRO:HD2	1.93	0.91
5:Y:150:CYS:SG	5:Y:155:ARG:NH1	2.44	0.90
3:G:220:VAL:HG21	3:G:261:LYS:C	1.95	0.90
5:X:157:PRO:O	5:X:158:PHE:CD2	2.25	0.90
5:Y:59:ASN:N	5:Y:60:PRO:HD2	1.86	0.89
5:X:59:ASN:N	5:X:60:PRO:HD2	1.86	0.89
3:E:86:PRO:HG3	3:K:195:ARG:HD2	1.53	0.89
3:G:202:GLU:OE1	3:G:202:GLU:N	2.07	0.88
3:F:125:PHE:O	3:F:127:ASP:N	2.05	0.88
3:I:202:GLU:OE1	3:I:202:GLU:N	2.07	0.87
3:D:184:GLU:OE2	3:E:62:SER:OG	1.92	0.87
3:D:220:VAL:CG1	3:D:262:LYS:CB	2.24	0.87
3:I:117:VAL:HG11	3:I:128:ARG:HD3	1.57	0.87
3:I:131:GLU:OE1	5:Y:34:HIS:ND1	2.08	0.87
3:B:26:ALA:O	3:B:29:LYS:HG2	1.75	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:26:ALA:O	3:F:29:LYS:HG2	1.75	0.86
3:A:220:VAL:CG1	3:A:262:LYS:CB	2.24	0.86
3:D:26:ALA:O	3:D:29:LYS:HG2	1.75	0.86
5:X:59:ASN:CB	5:X:60:PRO:HD3	2.05	0.86
3:C:85:ARG:CD	3:J:273:LYS:HE2	2.06	0.86
3:F:220:VAL:CG1	3:F:262:LYS:CB	2.24	0.86
3:G:131:GLU:OE1	5:X:34:HIS:ND1	2.08	0.85
3:E:191:ARG:NE	3:F:243:ARG:HH21	1.74	0.85
3:I:220:VAL:CG2	3:I:262:LYS:CA	2.36	0.85
5:X:149:GLY:C	5:X:158:PHE:CD2	2.54	0.85
3:A:191:ARG:NE	3:B:243:ARG:HH21	1.75	0.85
3:C:191:ARG:NE	3:D:243:ARG:HH21	1.74	0.84
3:G:117:VAL:HG21	3:G:128:ARG:HD3	1.59	0.84
3:G:191:ARG:NH2	3:H:243:ARG:HH22	1.73	0.84
3:D:131:GLU:OE1	3:J:181:LYS:NZ	2.09	0.84
3:A:85:ARG:CD	3:H:273:LYS:HE2	2.08	0.84
3:I:185:GLN:HE22	3:J:62:SER:HB3	1.39	0.84
3:I:191:ARG:CZ	3:J:243:ARG:HH21	1.91	0.84
3:G:185:GLN:HE22	3:H:62:SER:HB3	1.39	0.84
5:Y:59:ASN:CB	5:Y:60:PRO:HD3	2.06	0.83
3:J:202:GLU:OE1	3:J:202:GLU:N	2.09	0.83
5:X:149:GLY:HA3	5:X:158:PHE:CE2	2.13	0.83
3:G:191:ARG:CZ	3:H:243:ARG:HH21	1.91	0.82
3:K:202:GLU:OE1	3:K:202:GLU:N	2.09	0.82
3:A:220:VAL:CG1	3:A:262:LYS:CA	2.56	0.82
3:C:220:VAL:CB	3:C:262:LYS:HB3	2.10	0.82
3:I:191:ARG:NH2	3:J:243:ARG:HH22	1.73	0.82
3:C:220:VAL:CG1	3:C:262:LYS:CA	2.56	0.82
3:E:220:VAL:CG1	3:E:262:LYS:CA	2.56	0.81
5:Y:59:ASN:HB2	5:Y:60:PRO:CD	2.09	0.81
3:F:220:VAL:CG1	3:F:262:LYS:CA	2.56	0.81
3:F:220:VAL:CB	3:F:262:LYS:HB3	2.10	0.81
3:B:191:ARG:HH21	3:C:243:ARG:HH21	1.28	0.81
3:H:220:VAL:HG13	3:H:220:VAL:O	1.78	0.81
3:A:220:VAL:CB	3:A:262:LYS:HB3	2.10	0.81
3:B:220:VAL:CB	3:B:262:LYS:HB3	2.10	0.81
3:F:220:VAL:CG2	3:F:262:LYS:HD3	2.11	0.81
3:H:202:GLU:OE1	3:H:202:GLU:N	2.09	0.81
3:E:220:VAL:CB	3:E:262:LYS:HB3	2.10	0.80
3:F:184:GLU:OE2	3:G:61:GLU:OE2	2.00	0.80
3:D:220:VAL:CG2	3:D:262:LYS:HB3	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:220:VAL:CB	3:D:262:LYS:HB3	2.10	0.80
3:K:38:GLN:HA	3:K:38:GLN:NE2	1.96	0.80
3:B:220:VAL:CG2	3:B:262:LYS:HD3	2.11	0.80
3:E:220:VAL:CG2	3:E:262:LYS:HD3	2.11	0.80
3:G:220:VAL:HG11	3:G:262:LYS:CG	2.11	0.80
3:H:116:ARG:HH21	5:X:147:GLU:HG3	1.46	0.80
3:C:220:VAL:CG2	3:C:262:LYS:HD3	2.11	0.80
3:J:191:ARG:NH2	3:K:243:ARG:HH22	1.78	0.80
3:A:220:VAL:CG2	3:A:262:LYS:HB3	2.11	0.80
3:C:220:VAL:CG2	3:C:262:LYS:HB3	2.11	0.80
3:D:220:VAL:CG2	3:D:262:LYS:HD3	2.11	0.80
3:E:220:VAL:CG2	3:E:262:LYS:HB3	2.11	0.80
3:F:220:VAL:CG2	3:F:262:LYS:HB3	2.11	0.79
3:I:191:ARG:NH2	3:J:243:ARG:HH21	1.79	0.79
3:B:220:VAL:CG1	3:B:262:LYS:CA	2.56	0.79
5:X:59:ASN:CB	5:X:60:PRO:CD	2.60	0.79
3:B:220:VAL:CG2	3:B:262:LYS:HB3	2.11	0.79
3:I:65:GLY:HA2	7:I:302:ATP:PA	2.23	0.79
3:B:185:GLN:HE21	3:C:173:THR:HG21	1.42	0.79
3:H:220:VAL:HG11	3:H:261:LYS:O	1.77	0.79
3:G:114:LYS:CD	5:X:7:VAL:HG23	2.04	0.79
3:I:131:GLU:OE1	5:Y:34:HIS:CE1	2.36	0.79
1:1:10:DT:O4	2:2:19:DA:N1	2.16	0.79
3:H:119:LYS:HE2	3:H:119:LYS:HA	1.65	0.79
3:D:220:VAL:CG1	3:D:262:LYS:CA	2.56	0.78
3:F:119:LYS:HD2	3:F:120:GLY:H	1.48	0.78
3:G:220:VAL:CB	3:G:262:LYS:HB3	2.13	0.78
3:J:191:ARG:CZ	3:K:243:ARG:HH21	1.93	0.78
5:Y:59:ASN:CB	5:Y:60:PRO:CD	2.61	0.78
3:G:131:GLU:OE1	5:X:34:HIS:CE1	2.36	0.78
3:K:40:LYS:NZ	3:K:44:ASP:OD2	2.14	0.78
3:F:220:VAL:HG21	3:F:262:LYS:CD	2.14	0.78
3:A:220:VAL:CG2	3:A:262:LYS:HD3	2.11	0.78
3:C:220:VAL:HG21	3:C:262:LYS:CD	2.14	0.78
3:A:220:VAL:HG21	3:A:262:LYS:CD	2.14	0.77
3:K:224:LEU:HD23	3:K:224:LEU:N	1.98	0.77
5:X:75:GLU:HG3	5:X:75:GLU:O	1.82	0.77
5:Y:75:GLU:O	5:Y:75:GLU:HG3	1.82	0.77
3:E:220:VAL:HG21	3:E:262:LYS:CD	2.14	0.77
3:G:65:GLY:HA2	7:G:302:ATP:PA	2.23	0.77
3:B:220:VAL:HG21	3:B:262:LYS:CD	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:185:GLN:NE2	3:E:173:THR:HG21	2.00	0.77
3:D:220:VAL:HG21	3:D:262:LYS:CD	2.15	0.77
1:I:21:DT:O4	2:2:8:DA:N1	2.19	0.76
3:B:131:GLU:OE1	3:H:181:LYS:NZ	2.19	0.76
3:H:65:GLY:HA2	7:H:302:ATP:PA	2.26	0.75
5:X:156:MET:HB3	5:X:157:PRO:CD	2.17	0.75
3:I:114:LYS:CD	5:Y:7:VAL:HG23	2.04	0.75
3:I:220:VAL:HG23	3:I:262:LYS:CB	1.96	0.75
3:G:191:ARG:NH2	3:H:243:ARG:HH21	1.79	0.75
3:J:40:LYS:NZ	3:J:44:ASP:OD2	2.14	0.74
3:H:40:LYS:NZ	3:H:44:ASP:OD2	2.14	0.74
3:C:191:ARG:NE	3:D:243:ARG:NH2	2.34	0.74
3:E:191:ARG:NE	3:F:243:ARG:NH2	2.34	0.74
3:B:85:ARG:HD2	3:I:273:LYS:HE2	1.70	0.73
3:G:220:VAL:HG21	3:G:261:LYS:CA	2.17	0.73
5:Y:156:MET:HB3	5:Y:157:PRO:CD	2.16	0.73
3:A:191:ARG:HH21	3:B:243:ARG:NH2	1.82	0.73
3:B:191:ARG:HH21	3:C:243:ARG:NH2	1.79	0.73
3:E:86:PRO:HG3	3:K:195:ARG:CD	2.18	0.73
3:I:185:GLN:NE2	3:J:173:THR:HG21	2.03	0.73
5:Y:156:MET:HE3	5:Y:161:MET:SD	2.29	0.73
3:F:51:LYS:O	3:G:29:LYS:NZ	2.22	0.73
3:E:191:ARG:HH21	3:F:243:ARG:NH2	1.82	0.73
5:X:156:MET:HE3	5:X:161:MET:SD	2.29	0.73
3:G:185:GLN:NE2	3:H:173:THR:HG21	2.03	0.73
5:X:79:GLN:N	5:X:79:GLN:OE1	2.22	0.73
3:G:191:ARG:NE	3:H:243:ARG:HH21	1.87	0.73
3:E:116:ARG:HG2	3:J:184:GLU:CD	2.13	0.72
5:X:156:MET:HB2	5:X:161:MET:HE3	1.71	0.72
5:Y:79:GLN:N	5:Y:79:GLN:OE1	2.22	0.72
3:A:191:ARG:NE	3:B:243:ARG:NH2	2.34	0.72
3:C:191:ARG:HH21	3:D:243:ARG:HH21	1.36	0.72
3:G:228:GLU:OE1	3:G:228:GLU:N	2.18	0.72
3:I:220:VAL:CB	3:I:262:LYS:HB3	2.13	0.72
3:J:224:LEU:HD23	3:J:233:LEU:HD11	1.72	0.71
3:J:185:GLN:HE22	3:K:62:SER:HB3	1.55	0.71
3:I:191:ARG:NE	3:J:243:ARG:HH21	1.87	0.71
5:Y:156:MET:HB2	5:Y:161:MET:HE3	1.71	0.71
3:H:119:LYS:HA	3:H:119:LYS:CE	2.21	0.71
3:I:185:GLN:NE2	3:J:62:SER:HB3	2.05	0.71
3:J:191:ARG:HH21	3:K:243:ARG:HH21	1.34	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:185:GLN:NE2	3:H:62:SER:HB3	2.05	0.71
3:H:224:LEU:HD23	3:H:233:LEU:HD11	1.72	0.71
3:I:220:VAL:CG2	3:I:262:LYS:HB2	2.11	0.71
3:C:191:ARG:HH21	3:D:243:ARG:NH2	1.82	0.71
3:I:228:GLU:OE1	3:I:228:GLU:N	2.18	0.70
3:I:74:ARG:HD2	3:I:112:TYR:OH	1.91	0.70
3:G:65:GLY:CA	7:G:302:ATP:O1A	2.31	0.70
3:G:220:VAL:HB	3:G:261:LYS:C	2.13	0.70
3:E:115:TYR:HE2	3:K:195:ARG:NH2	1.89	0.70
3:B:85:ARG:CD	3:I:273:LYS:HE2	2.22	0.69
3:B:191:ARG:NE	3:C:243:ARG:HH21	1.88	0.69
3:C:220:VAL:HG21	3:C:262:LYS:HB3	1.75	0.69
3:I:65:GLY:CA	7:I:302:ATP:O1A	2.32	0.69
3:G:74:ARG:HD2	3:G:112:TYR:OH	1.91	0.69
3:G:220:VAL:CG1	3:G:262:LYS:HD2	2.22	0.69
5:Y:156:MET:HB3	5:Y:157:PRO:HD2	1.72	0.69
3:B:220:VAL:HG21	3:B:262:LYS:HB3	1.75	0.69
3:J:191:ARG:HH21	3:K:243:ARG:NH2	1.89	0.69
3:B:185:GLN:HE22	3:C:173:THR:HG21	1.55	0.69
3:E:220:VAL:HG21	3:E:262:LYS:HB3	1.75	0.69
3:H:119:LYS:HZ3	3:H:119:LYS:HB3	1.56	0.69
3:D:191:ARG:CZ	3:E:243:ARG:NH2	2.56	0.69
3:D:220:VAL:HG21	3:D:262:LYS:HB3	1.75	0.69
3:F:220:VAL:HG21	3:F:262:LYS:HB3	1.74	0.69
3:I:114:LYS:NZ	5:Y:3:GLU:CD	2.50	0.69
3:J:189:ARG:HH22	7:K:302:ATP:PG	2.16	0.69
5:X:156:MET:HB3	5:X:157:PRO:HD2	1.73	0.69
5:Y:138:ALA:HB2	5:Y:153:ARG:NH2	2.08	0.69
3:A:220:VAL:HG21	3:A:262:LYS:HB3	1.74	0.68
3:J:116:ARG:NH1	3:J:116:ARG:HG3	2.08	0.68
3:G:114:LYS:NZ	5:X:3:GLU:CD	2.51	0.68
3:E:220:VAL:CG1	3:E:261:LYS:C	2.67	0.68
3:H:220:VAL:HG13	3:H:262:LYS:CB	2.21	0.68
3:I:220:VAL:CG2	3:I:262:LYS:HA	2.23	0.68
3:C:220:VAL:CG1	3:C:261:LYS:C	2.67	0.67
3:B:220:VAL:CG1	3:B:261:LYS:C	2.67	0.67
3:D:191:ARG:HH21	3:E:243:ARG:HH21	1.41	0.67
3:D:220:VAL:HG11	3:D:262:LYS:HA	1.75	0.67
3:F:185:GLN:HE22	3:G:62:SER:HB3	1.60	0.67
3:G:220:VAL:CG2	3:G:261:LYS:CA	2.70	0.67
2:2:14:DA:H2''	2:2:15:DA:H2'	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:131:GLU:OE1	3:I:181:LYS:NZ	2.25	0.67
3:G:220:VAL:HG23	3:G:261:LYS:O	1.92	0.67
3:H:116:ARG:HH21	5:X:147:GLU:CG	2.07	0.67
3:D:220:VAL:CG1	3:D:261:LYS:C	2.67	0.67
5:X:55:ARG:HG2	5:X:142:MET:HG3	1.76	0.67
3:A:220:VAL:CG1	3:A:261:LYS:C	2.67	0.66
3:H:220:VAL:CG1	3:H:261:LYS:C	2.66	0.66
3:E:191:ARG:HH21	3:F:243:ARG:HH21	1.36	0.66
3:A:228:GLU:OE1	3:A:228:GLU:N	2.23	0.66
3:F:220:VAL:CG1	3:F:261:LYS:C	2.67	0.66
3:I:85:ARG:CB	3:I:86:PRO:CD	2.62	0.66
5:Y:150:CYS:HB3	5:Y:155:ARG:HD2	1.78	0.66
3:A:191:ARG:HH21	3:B:243:ARG:HH21	1.36	0.66
3:C:220:VAL:HG11	3:C:262:LYS:N	2.11	0.66
3:D:220:VAL:HG11	3:D:262:LYS:N	2.11	0.66
3:G:220:VAL:HG11	3:G:262:LYS:HD2	1.78	0.66
3:G:220:VAL:CB	3:G:261:LYS:C	2.65	0.66
3:I:191:ARG:NE	3:J:243:ARG:NH2	2.44	0.66
5:Y:156:MET:CE	5:Y:161:MET:CE	2.11	0.66
3:I:185:GLN:OE1	7:J:302:ATP:O3G	2.14	0.65
3:E:220:VAL:HG11	3:E:262:LYS:N	2.11	0.65
5:Y:150:CYS:SG	5:Y:155:ARG:NH2	2.70	0.65
3:B:220:VAL:HG11	3:B:262:LYS:HA	1.75	0.65
3:F:220:VAL:HG11	3:F:262:LYS:N	2.11	0.65
5:X:149:GLY:O	5:X:158:PHE:CE2	2.44	0.65
3:G:191:ARG:NE	3:H:243:ARG:NH2	2.44	0.65
3:H:191:ARG:CZ	3:I:243:ARG:NH2	2.57	0.65
3:B:220:VAL:HG11	3:B:262:LYS:N	2.11	0.65
3:J:220:VAL:CG2	3:J:262:LYS:HB3	2.27	0.64
3:K:40:LYS:HD2	3:K:40:LYS:O	1.97	0.64
5:X:150:CYS:HB3	5:X:155:ARG:HD2	1.77	0.64
3:A:220:VAL:HG11	3:A:262:LYS:N	2.11	0.64
3:E:220:VAL:HG11	3:E:262:LYS:HA	1.75	0.64
3:H:185:GLN:NE2	3:I:173:THR:HG21	2.11	0.64
3:K:220:VAL:CG2	3:K:262:LYS:HB3	2.27	0.64
5:X:150:CYS:SG	5:X:155:ARG:NH2	2.70	0.64
3:B:185:GLN:NE2	3:C:173:THR:CG2	2.54	0.64
3:F:228:GLU:OE1	3:F:228:GLU:N	2.24	0.64
3:H:185:GLN:HE22	3:I:62:SER:HB3	1.61	0.64
3:H:220:VAL:HG11	3:H:261:LYS:C	2.23	0.64
3:J:40:LYS:HD2	3:J:40:LYS:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:40:LYS:HD2	3:H:40:LYS:O	1.97	0.64
3:H:261:LYS:N	3:H:261:LYS:HD2	2.13	0.64
3:J:261:LYS:HD2	3:J:261:LYS:N	2.13	0.64
3:H:185:GLN:OE1	7:I:302:ATP:O3G	2.16	0.63
3:K:261:LYS:HD2	3:K:261:LYS:N	2.13	0.63
3:H:220:VAL:CG1	3:H:220:VAL:O	2.46	0.63
3:D:191:ARG:CZ	3:E:243:ARG:HH21	2.12	0.62
3:G:220:VAL:HG11	3:G:262:LYS:CD	2.30	0.62
3:J:62:SER:O	7:J:302:ATP:O1G	2.16	0.62
5:Y:152:HIS:CE1	5:Y:153:ARG:HG2	2.35	0.62
3:I:117:VAL:HG11	3:I:128:ARG:CD	2.27	0.62
5:X:152:HIS:CE1	5:X:153:ARG:HG2	2.35	0.62
3:H:110:THR:HG22	3:H:115:TYR:O	2.00	0.62
3:E:86:PRO:CG	3:K:195:ARG:HD2	2.29	0.62
3:J:218:LEU:N	3:J:218:LEU:HD23	2.15	0.62
2:2:14:DA:H1'	2:2:15:DA:H5'	1.82	0.61
3:H:218:LEU:HD23	3:H:218:LEU:N	2.15	0.61
3:I:114:LYS:HZ3	5:Y:3:GLU:CD	2.07	0.61
3:I:126:ARG:HD3	3:J:97:HIS:CE1	2.35	0.61
3:J:110:THR:HG22	3:J:115:TYR:O	2.00	0.61
3:H:51:LYS:O	3:I:29:LYS:HE2	2.00	0.61
3:C:116:ARG:CD	3:H:184:GLU:OE2	2.49	0.61
3:E:228:GLU:OE1	3:E:228:GLU:N	2.23	0.61
3:D:220:VAL:CG1	3:D:262:LYS:HA	2.30	0.61
3:D:228:GLU:OE1	3:D:228:GLU:N	2.23	0.61
3:G:85:ARG:CB	3:G:86:PRO:CD	2.62	0.61
3:C:220:VAL:HG11	3:C:262:LYS:HA	1.74	0.61
3:G:126:ARG:HD3	3:H:97:HIS:CE1	2.35	0.61
5:X:156:MET:HB2	5:X:161:MET:CE	2.31	0.61
3:F:53:ARG:HG2	3:G:29:LYS:CE	2.30	0.61
3:F:26:ALA:HA	3:F:29:LYS:HE2	1.83	0.61
3:H:220:VAL:CG1	3:H:262:LYS:CB	2.68	0.61
3:H:65:GLY:CA	7:H:302:ATP:O2A	2.36	0.60
3:I:191:ARG:HH21	3:J:243:ARG:NH2	1.98	0.60
2:2:11:DA:H2''	2:2:12:DA:C8	2.35	0.60
3:H:116:ARG:O	3:H:116:ARG:HG2	2.01	0.60
3:B:26:ALA:HA	3:B:29:LYS:HE2	1.83	0.60
5:Y:156:MET:SD	5:Y:161:MET:HE2	2.38	0.60
3:D:26:ALA:HA	3:D:29:LYS:HE2	1.83	0.60
3:K:38:GLN:HA	3:K:38:GLN:HE21	1.66	0.60
5:X:157:PRO:O	5:X:158:PHE:CG	2.54	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:156:MET:HB2	5:Y:161:MET:CE	2.31	0.60
3:G:117:VAL:HG21	3:G:128:ARG:CD	2.30	0.60
3:G:224:LEU:C	3:G:226:SER:H	2.09	0.60
3:J:62:SER:HB2	7:J:302:ATP:O3G	2.01	0.60
5:X:4:ALA:HB1	5:X:5:PRO:HD2	1.84	0.60
5:Y:4:ALA:HB1	5:Y:5:PRO:HD2	1.84	0.60
3:I:220:VAL:HG22	3:I:262:LYS:HA	1.82	0.60
3:K:218:LEU:HD23	3:K:218:LEU:N	2.15	0.60
3:C:220:VAL:CG1	3:C:262:LYS:HA	2.31	0.60
3:B:220:VAL:HG11	3:B:261:LYS:C	2.27	0.59
3:C:116:ARG:CZ	3:H:184:GLU:OE2	2.49	0.59
3:I:224:LEU:C	3:I:226:SER:H	2.09	0.59
3:C:220:VAL:HG11	3:C:261:LYS:O	1.99	0.59
3:I:187:LEU:C	3:I:187:LEU:HD23	2.28	0.59
3:J:185:GLN:NE2	3:K:173:THR:HG21	2.17	0.59
3:E:220:VAL:CG1	3:E:262:LYS:HA	2.31	0.59
3:H:116:ARG:HH21	5:X:147:GLU:CD	2.09	0.59
3:J:220:VAL:HG23	3:J:262:LYS:HB3	1.84	0.59
5:Y:140:PHE:CE2	5:Y:158:PHE:HZ	2.21	0.59
3:K:220:VAL:HG23	3:K:262:LYS:HB3	1.84	0.59
3:A:189:ARG:NH2	7:B:302:ATP:O3G	2.36	0.59
3:A:220:VAL:CG1	3:A:262:LYS:HA	2.31	0.59
3:C:189:ARG:NH2	7:D:302:ATP:O3G	2.36	0.59
3:D:220:VAL:HG11	3:D:261:LYS:C	2.27	0.59
3:G:187:LEU:O	3:G:187:LEU:HD23	2.03	0.59
3:J:65:GLY:C	7:J:302:ATP:O2A	2.43	0.59
3:E:220:VAL:HG11	3:E:261:LYS:C	2.27	0.59
1:I:18:DT:H2'	1:I:19:DT:H71	1.85	0.59
3:I:187:LEU:HD23	3:I:187:LEU:O	2.03	0.58
5:X:59:ASN:H	5:X:60:PRO:HD2	1.68	0.58
5:X:156:MET:CE	5:X:161:MET:CE	2.11	0.58
3:C:220:VAL:HG11	3:C:261:LYS:C	2.27	0.58
3:C:228:GLU:OE1	3:C:228:GLU:N	2.23	0.58
3:F:220:VAL:CG1	3:F:262:LYS:HA	2.30	0.58
3:G:187:LEU:HD23	3:G:187:LEU:C	2.28	0.58
5:X:149:GLY:CA	5:X:158:PHE:CE2	2.85	0.58
3:E:189:ARG:NH2	7:F:302:ATP:O3G	2.36	0.58
3:A:220:VAL:HG11	3:A:262:LYS:HA	1.74	0.58
3:A:220:VAL:HG11	3:A:261:LYS:C	2.27	0.58
5:Y:147:GLU:HG2	5:Y:148:ASP:N	2.19	0.58
3:B:220:VAL:CG1	3:B:262:LYS:HA	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:X:75:GLU:O	5:X:75:GLU:CG	2.52	0.58
5:X:147:GLU:HG2	5:X:148:ASP:N	2.19	0.58
2:2:26:DA:H2"	2:2:27:DA:H5"	1.86	0.57
3:F:220:VAL:HG11	3:F:261:LYS:C	2.27	0.57
5:Y:59:ASN:H	5:Y:60:PRO:HD2	1.68	0.57
5:Y:138:ALA:HB1	5:Y:153:ARG:HH11	1.57	0.57
3:H:185:GLN:NE2	3:I:62:SER:HB3	2.19	0.57
1:1:13:DT:H2"	1:1:14:DT:C6	2.39	0.57
3:B:189:ARG:NH1	7:C:302:ATP:O3G	2.38	0.57
3:F:185:GLN:NE2	3:G:173:THR:HG21	2.20	0.57
3:B:26:ALA:C	3:B:29:LYS:HG2	2.30	0.57
3:B:228:GLU:OE1	3:B:228:GLU:N	2.23	0.56
3:J:21:LEU:HD13	3:J:21:LEU:C	2.30	0.56
3:D:26:ALA:C	3:D:29:LYS:HG2	2.30	0.56
3:H:21:LEU:C	3:H:21:LEU:HD13	2.30	0.56
3:F:26:ALA:C	3:F:29:LYS:HG2	2.30	0.56
5:X:156:MET:SD	5:X:161:MET:HE2	2.38	0.56
3:J:35:PRO:CG	4:j:570:ILE:HD12	2.35	0.56
3:K:21:LEU:C	3:K:21:LEU:HD13	2.30	0.56
3:K:187:LEU:C	3:K:187:LEU:HD23	2.30	0.56
3:H:187:LEU:HD23	3:H:187:LEU:C	2.30	0.56
3:H:222:SER:HA	3:H:262:LYS:HE3	1.88	0.56
3:J:53:ARG:HG2	3:K:29:LYS:HD2	1.87	0.56
3:C:222:SER:OG	3:C:263:ILE:N	2.38	0.56
3:D:222:SER:OG	3:D:263:ILE:N	2.38	0.56
3:E:103:LYS:CG	3:E:125:PHE:CE2	2.89	0.56
3:H:187:LEU:HD23	3:H:187:LEU:O	2.06	0.56
3:J:187:LEU:HD23	3:J:187:LEU:C	2.30	0.56
3:K:35:PRO:CG	4:k:570:ILE:HD12	2.35	0.56
3:C:228:GLU:H	3:C:228:GLU:CD	2.12	0.56
3:H:35:PRO:CG	4:h:570:ILE:HD12	2.35	0.56
3:E:189:ARG:NH1	7:F:302:ATP:O3G	2.39	0.55
3:K:187:LEU:HD23	3:K:187:LEU:O	2.06	0.55
5:Y:99:LEU:HD23	5:Y:99:LEU:N	2.21	0.55
3:A:189:ARG:NH1	7:B:302:ATP:O3G	2.39	0.55
3:G:114:LYS:HZ3	5:X:3:GLU:CD	2.11	0.55
3:J:187:LEU:HD23	3:J:187:LEU:O	2.06	0.55
3:J:222:SER:HA	3:J:262:LYS:HE3	1.88	0.55
3:F:26:ALA:CA	3:F:29:LYS:HE2	2.37	0.55
3:D:26:ALA:CA	3:D:29:LYS:HE2	2.37	0.55
5:Y:75:GLU:O	5:Y:75:GLU:CG	2.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:185:GLN:NE2	3:K:62:SER:HB3	2.21	0.55
5:X:99:LEU:N	5:X:99:LEU:HD23	2.21	0.55
3:C:189:ARG:NH1	7:D:302:ATP:O3G	2.39	0.55
3:K:222:SER:HA	3:K:262:LYS:HE3	1.88	0.55
3:F:119:LYS:HG3	3:F:120:GLY:N	2.21	0.55
3:G:127:ASP:OD2	5:X:34:HIS:NE2	2.40	0.55
3:I:191:ARG:HH21	3:J:243:ARG:HH21	1.55	0.55
3:B:191:ARG:NE	3:C:243:ARG:NH2	2.48	0.54
3:J:189:ARG:NH2	7:K:302:ATP:PG	2.79	0.54
3:A:264:ASP:OD1	3:A:264:ASP:C	2.51	0.54
3:E:264:ASP:C	3:E:264:ASP:OD1	2.51	0.54
3:G:220:VAL:HG12	3:G:262:LYS:CB	2.21	0.54
3:E:83:ALA:HB1	3:K:41:THR:OG1	2.08	0.54
3:I:127:ASP:OD2	5:Y:34:HIS:NE2	2.40	0.54
3:I:264:ASP:OD1	3:I:264:ASP:C	2.51	0.54
3:G:264:ASP:OD1	3:G:264:ASP:C	2.51	0.54
3:G:191:ARG:HH21	3:H:243:ARG:NH2	1.98	0.54
5:Y:22:LEU:C	5:Y:22:LEU:HD23	2.32	0.54
3:B:222:SER:OG	3:B:263:ILE:N	2.38	0.54
3:E:103:LYS:HG3	3:E:125:PHE:CD2	2.43	0.54
3:J:65:GLY:N	7:J:302:ATP:O2A	2.38	0.54
5:X:22:LEU:HD23	5:X:22:LEU:C	2.32	0.54
3:B:26:ALA:CA	3:B:29:LYS:HE2	2.37	0.53
3:F:264:ASP:OD1	3:F:264:ASP:C	2.51	0.53
3:E:86:PRO:HG3	3:K:195:ARG:NE	2.23	0.53
3:F:51:LYS:C	3:G:29:LYS:NZ	2.63	0.53
3:B:264:ASP:OD1	3:B:264:ASP:C	2.51	0.53
3:J:116:ARG:NH1	3:J:116:ARG:CG	2.72	0.53
5:X:149:GLY:CA	5:X:158:PHE:CD2	2.92	0.53
2:2:23:DA:H2''	2:2:24:DA:H5'	1.91	0.53
3:A:220:VAL:HG21	3:A:262:LYS:CG	2.39	0.53
3:E:222:SER:OG	3:E:263:ILE:N	2.38	0.53
3:F:53:ARG:HG2	3:G:29:LYS:HE2	1.89	0.53
3:B:189:ARG:NH2	7:C:302:ATP:O3G	2.42	0.53
3:D:264:ASP:OD1	3:D:264:ASP:C	2.51	0.53
3:A:222:SER:OG	3:A:263:ILE:N	2.38	0.53
3:F:220:VAL:HG21	3:F:262:LYS:CG	2.39	0.53
3:G:53:ARG:HG2	3:H:29:LYS:HD2	1.90	0.53
3:C:220:VAL:HG21	3:C:262:LYS:CG	2.39	0.53
3:C:264:ASP:C	3:C:264:ASP:OD1	2.51	0.53
3:I:53:ARG:HG2	3:J:29:LYS:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:220:VAL:HG21	3:E:262:LYS:CG	2.39	0.52
3:B:220:VAL:HG21	3:B:262:LYS:CB	2.39	0.52
3:D:185:GLN:HE21	3:E:173:THR:HG21	1.74	0.52
3:D:220:VAL:HG21	3:D:262:LYS:CG	2.39	0.52
3:I:220:VAL:HG21	3:I:262:LYS:N	2.12	0.52
3:H:35:PRO:HG2	4:h:570:ILE:HD12	1.92	0.52
3:K:63:ARG:NH2	7:K:302:ATP:O1G	2.40	0.52
3:A:189:ARG:CZ	7:B:302:ATP:O3G	2.58	0.52
3:B:220:VAL:HG21	3:B:262:LYS:CG	2.39	0.52
3:F:228:GLU:H	3:F:228:GLU:CD	2.12	0.52
3:H:116:ARG:NH2	5:X:147:GLU:HG3	2.22	0.52
1:1:24:DT:H2''	1:1:25:DT:C6	2.45	0.52
3:C:189:ARG:CZ	7:D:302:ATP:O3G	2.58	0.52
3:J:35:PRO:HG2	4:j:570:ILE:HD12	1.92	0.52
3:J:112:TYR:C	3:J:112:TYR:CD2	2.88	0.52
3:K:35:PRO:HG2	4:k:570:ILE:HD12	1.92	0.51
3:C:220:VAL:HG21	3:C:262:LYS:CB	2.39	0.51
2:2:6:DA:OP1	5:Y:38:SER:CB	2.57	0.51
3:G:224:LEU:C	3:G:226:SER:N	2.67	0.51
3:G:224:LEU:O	3:G:226:SER:N	2.44	0.51
3:I:224:LEU:C	3:I:226:SER:N	2.67	0.51
3:A:220:VAL:HG21	3:A:262:LYS:CB	2.39	0.51
3:E:220:VAL:HG21	3:E:262:LYS:CB	2.39	0.51
3:E:83:ALA:CB	3:K:41:THR:OG1	2.58	0.51
3:F:119:LYS:CG	3:F:120:GLY:N	2.74	0.51
3:F:119:LYS:CD	3:F:120:GLY:H	2.19	0.51
3:H:112:TYR:C	3:H:112:TYR:CD2	2.88	0.51
3:F:220:VAL:HG21	3:F:262:LYS:CB	2.39	0.51
3:J:126:ARG:HD3	3:K:97:HIS:CE1	2.45	0.51
3:B:184:GLU:OE2	3:C:62:SER:OG	2.20	0.51
3:E:189:ARG:CZ	7:F:302:ATP:O3G	2.58	0.51
3:D:47:ASP:OD2	3:D:51:LYS:NZ	2.44	0.51
3:K:38:GLN:NE2	3:K:38:GLN:CA	2.72	0.51
3:H:119:LYS:HB3	3:H:119:LYS:NZ	2.24	0.51
3:K:37:GLN:OE1	3:K:37:GLN:HA	2.11	0.51
3:D:220:VAL:HG21	3:D:262:LYS:CB	2.40	0.50
3:J:37:GLN:HA	3:J:37:GLN:OE1	2.11	0.50
1:1:26:DT:OP1	5:X:57:HIS:CD2	2.64	0.50
3:F:187:LEU:C	3:F:187:LEU:HD23	2.37	0.50
1:1:11:DT:H2''	1:1:12:DT:O5'	2.11	0.50
1:1:25:DT:H5'	5:X:52:ARG:HH11	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:4:DA:H2''	2:2:5:DA:C8	2.47	0.50
3:A:47:ASP:OD2	3:A:51:LYS:NZ	2.44	0.50
3:C:187:LEU:HD23	3:C:187:LEU:C	2.36	0.50
3:D:112:TYR:C	3:D:112:TYR:CD2	2.89	0.50
3:F:222:SER:OG	3:F:263:ILE:N	2.38	0.50
3:H:37:GLN:HA	3:H:37:GLN:OE1	2.11	0.50
5:X:46:ILE:C	5:X:46:ILE:HD12	2.37	0.50
5:Y:46:ILE:HD12	5:Y:46:ILE:C	2.37	0.50
3:F:112:TYR:C	3:F:112:TYR:CD2	2.89	0.50
3:G:218:LEU:N	3:G:218:LEU:HD23	2.26	0.50
3:I:224:LEU:O	3:I:226:SER:N	2.44	0.50
3:B:112:TYR:C	3:B:112:TYR:CD2	2.89	0.50
3:D:26:ALA:CB	3:D:29:LYS:HE2	2.42	0.50
3:E:222:SER:OG	3:E:262:LYS:HB2	2.12	0.50
3:B:47:ASP:OD2	3:B:51:LYS:NZ	2.44	0.50
3:C:47:ASP:OD2	3:C:51:LYS:NZ	2.44	0.50
3:K:112:TYR:C	3:K:112:TYR:CD2	2.88	0.50
3:A:112:TYR:C	3:A:112:TYR:CD2	2.89	0.50
3:E:47:ASP:OD2	3:E:51:LYS:NZ	2.44	0.50
3:F:47:ASP:OD2	3:F:51:LYS:NZ	2.44	0.50
3:D:187:LEU:C	3:D:187:LEU:HD23	2.37	0.50
3:E:112:TYR:C	3:E:112:TYR:CD2	2.89	0.50
3:H:47:ASP:OD2	3:H:51:LYS:NZ	2.45	0.50
3:A:187:LEU:C	3:A:187:LEU:HD23	2.36	0.49
3:C:222:SER:OG	3:C:262:LYS:HB2	2.12	0.49
3:H:264:ASP:C	3:H:264:ASP:OD1	2.54	0.49
3:E:187:LEU:HD23	3:E:187:LEU:C	2.36	0.49
3:F:222:SER:OG	3:F:262:LYS:HB2	2.12	0.49
3:G:191:ARG:HH21	3:H:243:ARG:HH21	1.55	0.49
3:K:67:THR:CB	7:K:302:ATP:O2B	2.60	0.49
3:B:222:SER:OG	3:B:262:LYS:HB2	2.12	0.49
3:D:222:SER:OG	3:D:262:LYS:HB2	2.12	0.49
3:A:222:SER:OG	3:A:262:LYS:HB2	2.12	0.49
3:F:26:ALA:CB	3:F:29:LYS:HE2	2.42	0.49
3:J:47:ASP:OD2	3:J:51:LYS:NZ	2.45	0.49
3:J:264:ASP:C	3:J:264:ASP:OD1	2.54	0.49
2:2:23:DA:H2''	2:2:24:DA:C8	2.47	0.49
3:K:47:ASP:OD2	3:K:51:LYS:NZ	2.45	0.49
3:B:187:LEU:C	3:B:187:LEU:HD23	2.37	0.49
3:H:119:LYS:CE	3:H:119:LYS:CA	2.85	0.49
3:B:26:ALA:CB	3:B:29:LYS:HE2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:7:DT:H2'	1:1:8:DT:H71	1.95	0.49
3:J:222:SER:OG	3:J:263:ILE:N	2.46	0.49
3:H:222:SER:OG	3:H:263:ILE:N	2.46	0.48
3:I:212:GLU:OE1	3:I:224:LEU:HB2	2.13	0.48
5:X:156:MET:CE	5:X:161:MET:SD	2.95	0.48
2:2:27:DA:H2''	2:2:28:DA:C8	2.48	0.48
3:G:21:LEU:HD13	3:G:21:LEU:C	2.38	0.48
3:G:212:GLU:OE1	3:G:224:LEU:HB2	2.13	0.48
3:H:119:LYS:NZ	3:H:119:LYS:CB	2.72	0.48
1:1:16:DT:H2''	1:1:17:DT:H71	1.94	0.48
3:H:224:LEU:C	3:H:226:SER:H	2.21	0.48
3:J:224:LEU:C	3:J:226:SER:H	2.21	0.48
3:K:264:ASP:OD1	3:K:264:ASP:C	2.54	0.48
1:1:11:DT:H2'	1:1:12:DT:C6	2.47	0.48
5:Y:156:MET:CE	5:Y:161:MET:SD	2.95	0.48
3:K:224:LEU:C	3:K:226:SER:H	2.21	0.48
3:F:222:SER:HG	3:F:263:ILE:H	1.60	0.48
3:H:119:LYS:HZ3	3:H:119:LYS:CB	2.24	0.48
2:2:12:DA:H2''	2:2:13:DA:H5'	1.94	0.48
3:B:189:ARG:CZ	7:C:302:ATP:O3G	2.62	0.48
3:I:21:LEU:HD13	3:I:21:LEU:C	2.38	0.48
3:I:115:TYR:CD1	3:I:117:VAL:HG13	2.49	0.48
3:C:112:TYR:C	3:C:112:TYR:CD2	2.89	0.48
3:G:115:TYR:CD1	3:G:117:VAL:HG23	2.48	0.48
1:1:13:DT:H2''	1:1:14:DT:C5	2.48	0.48
3:A:222:SER:HG	3:A:263:ILE:H	1.61	0.48
3:I:218:LEU:N	3:I:218:LEU:HD23	2.26	0.48
5:Y:140:PHE:CE2	5:Y:158:PHE:CZ	3.01	0.47
3:D:224:LEU:HA	3:D:224:LEU:HD23	1.58	0.47
3:G:117:VAL:CG1	3:G:118:THR:N	2.77	0.47
3:J:191:ARG:NE	3:K:243:ARG:HH21	2.11	0.47
3:E:220:VAL:CB	3:E:261:LYS:O	2.62	0.47
3:F:53:ARG:CG	3:G:29:LYS:CE	2.91	0.47
3:G:47:ASP:OD2	3:G:51:LYS:NZ	2.47	0.47
3:J:152:GLU:OE1	3:J:152:GLU:N	2.33	0.47
1:1:25:DT:H5'	5:X:52:ARG:NH1	2.29	0.47
5:X:157:PRO:C	5:X:159:ALA:N	2.72	0.47
5:Y:65:GLN:OE1	5:Y:65:GLN:N	2.48	0.47
3:I:47:ASP:OD2	3:I:51:LYS:NZ	2.47	0.47
3:K:222:SER:OG	3:K:263:ILE:N	2.46	0.47
5:Y:154:CYS:SG	5:Y:156:MET:HE2	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:125:PHE:C	3:F:127:ASP:N	2.71	0.47
3:G:131:GLU:OE2	5:X:32:ALA:O	2.32	0.47
3:H:191:ARG:HH22	3:I:243:ARG:NH2	2.00	0.47
3:I:152:GLU:OE1	3:I:152:GLU:N	2.32	0.47
5:X:65:GLN:N	5:X:65:GLN:OE1	2.48	0.47
1:I:6:DT:OP1	3:B:122:VAL:HG23	2.15	0.47
3:D:228:GLU:H	3:D:228:GLU:CD	2.12	0.47
5:X:136:CYS:SG	5:X:153:ARG:HB3	2.55	0.47
3:B:261:LYS:HD2	3:B:261:LYS:N	2.30	0.47
3:I:131:GLU:OE2	5:Y:32:ALA:O	2.32	0.47
5:X:154:CYS:SG	5:X:156:MET:HE2	2.54	0.47
3:F:121:THR:H	3:F:124:ASP:HB2	1.79	0.46
3:G:112:TYR:O	3:G:112:TYR:CD2	2.68	0.46
3:I:112:TYR:CD2	3:I:112:TYR:O	2.68	0.46
5:Y:59:ASN:HB2	5:Y:60:PRO:HD2	1.95	0.46
5:Y:136:CYS:SG	5:Y:153:ARG:HB3	2.56	0.46
3:C:261:LYS:N	3:C:261:LYS:HD2	2.30	0.46
3:E:261:LYS:HD2	3:E:261:LYS:N	2.30	0.46
3:B:26:ALA:HB1	3:B:29:LYS:HE2	1.98	0.46
3:E:103:LYS:HG2	3:E:125:PHE:CE2	2.50	0.46
3:F:261:LYS:N	3:F:261:LYS:HD2	2.30	0.46
2:2:6:DA:H2"	2:2:7:DA:C8	2.50	0.46
3:C:220:VAL:CB	3:C:261:LYS:O	2.62	0.46
3:E:152:GLU:OE1	3:E:152:GLU:N	2.33	0.46
3:E:228:GLU:H	3:E:228:GLU:CD	2.12	0.46
3:G:116:ARG:C	3:G:117:VAL:HG23	2.40	0.46
3:G:88:THR:HG22	3:G:90:PRO:HD3	1.97	0.46
3:G:220:VAL:HG23	3:G:261:LYS:CA	2.42	0.46
5:Y:157:PRO:C	5:Y:159:ALA:N	2.72	0.46
3:B:220:VAL:CB	3:B:261:LYS:O	2.62	0.46
3:I:191:ARG:HE	3:J:243:ARG:HH21	1.62	0.46
5:X:157:PRO:C	5:X:159:ALA:H	2.24	0.46
3:A:261:LYS:N	3:A:261:LYS:HD2	2.30	0.46
3:G:117:VAL:HG12	3:G:118:THR:N	2.30	0.46
3:I:88:THR:HG22	3:I:90:PRO:HD3	1.97	0.46
3:G:116:ARG:O	3:G:117:VAL:CG2	2.64	0.45
2:2:17:DA:H2"	2:2:18:DA:C8	2.51	0.45
3:D:26:ALA:HA	3:D:29:LYS:CD	2.47	0.45
3:D:261:LYS:HD2	3:D:261:LYS:N	2.30	0.45
5:X:61:ARG:O	5:X:63:SER:N	2.49	0.45
3:J:62:SER:O	7:J:302:ATP:O3B	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:26:ALA:HA	3:F:29:LYS:CD	2.47	0.45
5:X:2:ILE:HG22	5:X:3:GLU:N	2.32	0.45
3:B:185:GLN:HE22	3:C:173:THR:CG2	2.22	0.45
3:D:26:ALA:HB1	3:D:29:LYS:HE2	1.97	0.45
5:Y:138:ALA:CB	5:Y:153:ARG:HH11	2.07	0.45
3:E:103:LYS:CG	3:E:125:PHE:CD2	2.99	0.45
3:F:220:VAL:CB	3:F:261:LYS:O	2.62	0.45
1:I:26:DT:OP1	5:X:57:HIS:HD2	2.00	0.45
2:2:12:DA:H2''	2:2:13:DA:H8	1.82	0.45
3:F:26:ALA:HB1	3:F:29:LYS:HE2	1.97	0.45
3:G:86:PRO:HA	3:G:87:PRO:HD3	1.71	0.45
3:A:83:ALA:HB1	3:G:41:THR:CG2	2.47	0.45
3:E:116:ARG:CG	3:J:184:GLU:CD	2.76	0.45
3:F:119:LYS:HD2	3:F:120:GLY:N	2.26	0.45
3:B:26:ALA:HA	3:B:29:LYS:CD	2.46	0.44
3:J:62:SER:O	7:J:302:ATP:PG	2.75	0.44
5:Y:157:PRO:C	5:Y:159:ALA:H	2.24	0.44
5:X:35:LEU:HD23	5:X:35:LEU:H	1.82	0.44
3:A:224:LEU:HD23	3:A:224:LEU:HA	1.58	0.44
3:D:85:ARG:HD2	3:K:273:LYS:CE	2.15	0.44
5:Y:35:LEU:HD23	5:Y:35:LEU:H	1.83	0.44
3:C:40:LYS:NZ	3:C:44:ASP:OD2	2.50	0.44
3:G:112:TYR:O	3:G:112:TYR:CG	2.71	0.44
2:2:12:DA:H2''	2:2:13:DA:C8	2.53	0.44
3:A:220:VAL:CB	3:A:261:LYS:O	2.62	0.44
3:B:152:GLU:OE1	3:B:152:GLU:N	2.33	0.44
3:E:115:TYR:CE2	3:K:195:ARG:NH2	2.78	0.44
3:H:116:ARG:NH2	5:X:147:GLU:OE2	2.51	0.44
3:H:224:LEU:C	3:H:226:SER:N	2.75	0.44
3:I:21:LEU:HD22	3:I:21:LEU:O	2.18	0.44
3:I:112:TYR:O	3:I:112:TYR:CG	2.71	0.44
1:I:14:DT:H2'	1:I:15:DT:H71	1.99	0.44
3:G:117:VAL:HG11	3:G:128:ARG:NH1	2.33	0.44
3:G:144:ASP:O	3:G:145:GLU:C	2.61	0.44
3:G:224:LEU:HA	3:G:224:LEU:HD23	1.59	0.44
1:I:22:DT:H2'	1:I:23:DT:C6	2.52	0.44
3:D:26:ALA:HA	3:D:29:LYS:CE	2.47	0.44
3:D:152:GLU:OE1	3:D:152:GLU:N	2.33	0.44
3:G:21:LEU:HD22	3:G:21:LEU:O	2.18	0.44
3:I:114:LYS:O	5:Y:10:TRP:CD1	2.70	0.44
3:I:116:ARG:C	3:I:117:VAL:HG13	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:14:DT:H2''	1:1:15:DT:O5'	2.16	0.43
3:C:152:GLU:OE1	3:C:152:GLU:N	2.33	0.43
3:I:185:GLN:HE22	3:J:173:THR:HG21	1.83	0.43
3:J:224:LEU:C	3:J:226:SER:N	2.75	0.43
5:Y:61:ARG:O	5:Y:63:SER:N	2.50	0.43
3:G:114:LYS:HZ1	5:X:3:GLU:CD	2.19	0.43
3:I:144:ASP:O	3:I:145:GLU:C	2.61	0.43
1:1:22:DT:H2''	1:1:23:DT:O5'	2.19	0.43
3:G:114:LYS:O	5:X:10:TRP:CD1	2.70	0.43
3:B:85:ARG:HD3	3:I:273:LYS:HE2	1.97	0.43
3:C:224:LEU:HD23	3:C:224:LEU:HA	1.58	0.43
3:E:40:LYS:NZ	3:E:44:ASP:OD2	2.50	0.43
3:G:185:GLN:HE22	3:H:173:THR:HG21	1.83	0.43
3:B:40:LYS:NZ	3:B:44:ASP:OD2	2.50	0.43
3:D:220:VAL:CB	3:D:261:LYS:O	2.62	0.43
3:I:116:ARG:O	3:I:117:VAL:CG1	2.66	0.43
3:K:152:GLU:OE1	3:K:152:GLU:N	2.33	0.43
3:B:228:GLU:H	3:B:228:GLU:CD	2.12	0.43
3:E:224:LEU:HD23	3:E:224:LEU:HA	1.58	0.43
3:A:152:GLU:OE1	3:A:152:GLU:N	2.33	0.43
3:F:26:ALA:HA	3:F:29:LYS:CE	2.47	0.43
3:I:220:VAL:HG23	3:I:262:LYS:HB2	1.90	0.43
3:I:224:LEU:HA	3:I:224:LEU:HD23	1.59	0.43
5:Y:156:MET:CB	5:Y:157:PRO:CD	2.92	0.43
3:B:224:LEU:HA	3:B:224:LEU:HD23	1.58	0.42
3:J:220:VAL:HG23	3:J:220:VAL:O	2.20	0.42
3:C:86:PRO:HA	3:C:87:PRO:HD3	1.88	0.42
3:D:40:LYS:NZ	3:D:44:ASP:OD2	2.50	0.42
3:D:128:ARG:HH11	3:J:181:LYS:NZ	2.17	0.42
3:F:185:GLN:HE22	3:G:173:THR:HG21	1.83	0.42
3:G:116:ARG:O	3:G:117:VAL:HG23	2.20	0.42
1:1:2:DT:H2'	1:1:3:DT:C6	2.54	0.42
3:A:187:LEU:HD23	3:A:187:LEU:O	2.20	0.42
3:F:26:ALA:O	3:F:29:LYS:CG	2.59	0.42
3:A:131:GLU:OE1	3:G:181:LYS:NZ	2.34	0.42
3:D:187:LEU:HD23	3:D:187:LEU:O	2.20	0.42
3:F:224:LEU:HD23	3:F:224:LEU:HA	1.58	0.42
5:X:53:TRP:CD1	5:X:53:TRP:N	2.87	0.42
5:X:158:PHE:CD1	5:X:159:ALA:N	2.88	0.42
3:C:187:LEU:HD23	3:C:187:LEU:O	2.20	0.42
3:E:187:LEU:HD23	3:E:187:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:187:LEU:HD23	3:F:187:LEU:O	2.20	0.42
3:B:26:ALA:HA	3:B:29:LYS:CE	2.47	0.42
3:B:187:LEU:HD23	3:B:187:LEU:O	2.20	0.42
3:C:220:VAL:HG13	3:C:262:LYS:CB	2.39	0.42
5:X:4:ALA:CB	5:X:5:PRO:HD2	2.48	0.42
5:Y:135:ASN:HD22	5:Y:156:MET:CE	2.33	0.42
2:2:1:DA:H2''	2:2:2:DA:H5'	2.00	0.42
3:G:53:ARG:CG	3:H:29:LYS:HD2	2.50	0.42
5:X:147:GLU:CG	5:X:148:ASP:N	2.81	0.42
3:G:117:VAL:HG11	3:G:128:ARG:CZ	2.50	0.42
3:I:110:THR:HG21	3:I:117:VAL:HG21	2.02	0.42
3:D:185:GLN:HE22	3:E:173:THR:HG21	1.80	0.41
3:I:53:ARG:CG	3:J:29:LYS:HD2	2.50	0.41
3:J:53:ARG:CG	3:K:29:LYS:HD2	2.48	0.41
3:K:224:LEU:C	3:K:226:SER:N	2.75	0.41
5:X:135:ASN:ND2	5:X:156:MET:CE	2.83	0.41
5:Y:135:ASN:ND2	5:Y:156:MET:CE	2.83	0.41
3:G:152:GLU:OE1	3:G:152:GLU:N	2.32	0.41
5:Y:53:TRP:N	5:Y:53:TRP:CD1	2.87	0.41
5:Y:4:ALA:HA	5:Y:5:PRO:HD3	1.86	0.41
3:D:189:ARG:NH1	7:E:302:ATP:O3G	2.54	0.41
5:Y:35:LEU:HD23	5:Y:35:LEU:N	2.35	0.41
5:X:35:LEU:HD23	5:X:35:LEU:N	2.35	0.41
3:F:40:LYS:NZ	3:F:44:ASP:OD2	2.50	0.41
3:K:220:VAL:HG23	3:K:220:VAL:O	2.20	0.41
3:E:86:PRO:HA	3:E:87:PRO:HD3	1.88	0.41
5:Y:11:LEU:C	5:Y:11:LEU:HD12	2.45	0.41
3:E:220:VAL:HG13	3:E:262:LYS:CB	2.39	0.41
3:H:191:ARG:CZ	3:I:243:ARG:HH21	2.20	0.41
3:I:116:ARG:O	3:I:117:VAL:HG13	2.20	0.41
5:X:135:ASN:HD22	5:X:156:MET:CE	2.33	0.41
1:1:11:DT:H2'	1:1:12:DT:C5	2.55	0.41
5:X:11:LEU:HD12	5:X:11:LEU:C	2.45	0.41
3:B:220:VAL:HG13	3:B:262:LYS:CB	2.39	0.40
3:F:86:PRO:HA	3:F:87:PRO:HD3	1.88	0.40
3:A:86:PRO:HA	3:A:87:PRO:HD3	1.88	0.40
3:F:53:ARG:HB2	3:G:29:LYS:HE3	2.02	0.40
5:X:135:ASN:ND2	5:X:156:MET:HE1	2.36	0.40
5:Y:135:ASN:ND2	5:Y:156:MET:HE1	2.36	0.40
3:E:83:ALA:HB1	3:K:41:THR:CB	2.51	0.40
3:G:113:LEU:HD23	3:G:113:LEU:HA	1.67	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:185:GLN:HE21	3:I:173:THR:HG21	1.83	0.40
3:H:126:ARG:HD3	3:I:97:HIS:CE1	2.56	0.40
5:Y:127:LEU:C	5:Y:127:LEU:HD12	2.47	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	
3	A	255/276 (92%)	251 (98%)	4 (2%)	0	100	100
3	B	255/276 (92%)	251 (98%)	4 (2%)	0	100	100
3	C	255/276 (92%)	251 (98%)	4 (2%)	0	100	100
3	D	255/276 (92%)	251 (98%)	4 (2%)	0	100	100
3	E	255/276 (92%)	251 (98%)	4 (2%)	0	100	100
3	F	255/276 (92%)	249 (98%)	4 (2%)	2 (1%)	16	49
3	G	255/276 (92%)	251 (98%)	3 (1%)	1 (0%)	30	62
3	H	255/276 (92%)	247 (97%)	7 (3%)	1 (0%)	30	62
3	I	255/276 (92%)	251 (98%)	3 (1%)	1 (0%)	30	62
3	J	255/276 (92%)	248 (97%)	7 (3%)	0	100	100
3	K	255/276 (92%)	249 (98%)	6 (2%)	0	100	100
4	a	12/15 (80%)	12 (100%)	0	0	100	100
4	b	12/15 (80%)	12 (100%)	0	0	100	100
4	c	12/15 (80%)	12 (100%)	0	0	100	100
4	d	12/15 (80%)	12 (100%)	0	0	100	100
4	e	12/15 (80%)	12 (100%)	0	0	100	100
4	f	12/15 (80%)	12 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	h	12/15 (80%)	12 (100%)	0	0	100	100
4	j	12/15 (80%)	12 (100%)	0	0	100	100
4	k	12/15 (80%)	12 (100%)	0	0	100	100
5	X	163/167 (98%)	151 (93%)	12 (7%)	0	100	100
5	Y	163/167 (98%)	151 (93%)	12 (7%)	0	100	100
All	All	3239/3505 (92%)	3160 (98%)	74 (2%)	5 (0%)	44	74

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	126	ARG
3	G	225	LYS
3	I	225	LYS
3	F	125	PHE
3	H	119	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	224/238 (94%)	224 (100%)	0	100	100
3	B	224/238 (94%)	224 (100%)	0	100	100
3	C	224/238 (94%)	224 (100%)	0	100	100
3	D	224/238 (94%)	224 (100%)	0	100	100
3	E	224/238 (94%)	224 (100%)	0	100	100
3	F	224/238 (94%)	224 (100%)	0	100	100
3	G	224/238 (94%)	224 (100%)	0	100	100
3	H	224/238 (94%)	220 (98%)	4 (2%)	51	69
3	I	224/238 (94%)	223 (100%)	1 (0%)	84	81
3	J	224/238 (94%)	221 (99%)	3 (1%)	61	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	224/238 (94%)	221 (99%)	3 (1%)	61	72
4	a	13/14 (93%)	13 (100%)	0	100	100
4	b	13/14 (93%)	13 (100%)	0	100	100
4	c	13/14 (93%)	13 (100%)	0	100	100
4	d	13/14 (93%)	13 (100%)	0	100	100
4	e	13/14 (93%)	13 (100%)	0	100	100
4	f	13/14 (93%)	13 (100%)	0	100	100
4	h	13/14 (93%)	13 (100%)	0	100	100
4	j	13/14 (93%)	13 (100%)	0	100	100
4	k	13/14 (93%)	13 (100%)	0	100	100
5	X	137/139 (99%)	137 (100%)	0	100	100
5	Y	137/139 (99%)	136 (99%)	1 (1%)	76	78
All	All	2855/3022 (94%)	2843 (100%)	12 (0%)	81	81

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	114	LYS
3	H	116	ARG
3	H	117	VAL
3	H	119	LYS
3	I	220	VAL
3	J	116	ARG
3	J	117	VAL
3	J	220	VAL
3	K	38	GLN
3	K	220	VAL
3	K	224	LEU
5	Y	158	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	77	HIS
3	B	77	HIS
3	C	77	HIS
3	D	77	HIS

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Mol	Chain	Res	Type
3	E	77	HIS
3	F	77	HIS
3	H	38	GLN
3	H	185	GLN
3	H	269	GLN
3	J	38	GLN
3	J	185	GLN
3	J	269	GLN
3	K	38	GLN
3	K	269	GLN
5	X	24	HIS
5	X	135	ASN
5	Y	24	HIS
5	Y	135	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 11 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ATP	H	302	6	32,33,33	1.41	4 (12%)	48,52,52	1.77	9 (18%)
7	ATP	K	302	6	32,33,33	1.44	5 (15%)	48,52,52	1.76	9 (18%)
7	ATP	I	302	6	32,33,33	1.40	4 (12%)	48,52,52	1.83	11 (22%)
7	ATP	D	302	6	32,33,33	1.40	4 (12%)	48,52,52	1.77	9 (18%)
7	ATP	B	302	6	32,33,33	1.40	4 (12%)	48,52,52	1.77	9 (18%)
7	ATP	F	302	6	32,33,33	1.41	4 (12%)	48,52,52	1.77	9 (18%)
7	ATP	C	302	6	32,33,33	1.41	4 (12%)	48,52,52	1.77	9 (18%)
7	ATP	E	302	6	32,33,33	1.41	4 (12%)	48,52,52	1.77	9 (18%)
7	ATP	J	302	6	32,33,33	2.15	8 (25%)	48,52,52	2.11	17 (35%)
7	ATP	G	302	6	32,33,33	1.42	4 (12%)	48,52,52	1.77	10 (20%)
7	ATP	A	302	6	32,33,33	1.41	4 (12%)	48,52,52	1.78	9 (18%)

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
7	ATP	H	302	6	-	7/22/38/38	0/3/3/3
7	ATP	K	302	6	-	8/22/38/38	0/3/3/3
7	ATP	I	302	6	-	2/22/38/38	0/3/3/3
7	ATP	D	302	6	-	3/22/38/38	0/3/3/3
7	ATP	B	302	6	-	3/22/38/38	0/3/3/3
7	ATP	F	302	6	-	3/22/38/38	0/3/3/3
7	ATP	C	302	6	-	3/22/38/38	0/3/3/3
7	ATP	E	302	6	-	3/22/38/38	0/3/3/3
7	ATP	J	302	6	-	2/22/38/38	0/3/3/3
7	ATP	G	302	6	-	2/22/38/38	0/3/3/3
7	ATP	A	302	6	-	3/22/38/38	0/3/3/3

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	J	302	ATP	C5-N7	-5.49	1.29	1.39
7	A	302	ATP	C5-C4	4.80	1.47	1.39
7	D	302	ATP	C5-C4	4.77	1.47	1.39
7	G	302	ATP	C5-C4	4.76	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	302	ATP	C5-C4	4.76	1.47	1.39
7	C	302	ATP	C5-C4	4.74	1.47	1.39
7	F	302	ATP	C5-C4	4.74	1.47	1.39
7	H	302	ATP	C5-C4	4.73	1.47	1.39
7	K	302	ATP	C5-C4	4.72	1.47	1.39
7	B	302	ATP	C5-C4	4.69	1.47	1.39
7	I	302	ATP	C5-C4	4.62	1.47	1.39
7	J	302	ATP	PB-O3A	-4.61	1.54	1.59
7	J	302	ATP	C4-N9	-4.53	1.28	1.37
7	J	302	ATP	C8-N9	-4.17	1.30	1.37
7	G	302	ATP	C5-C6	2.77	1.48	1.41
7	K	302	ATP	C5-C6	2.77	1.48	1.41
7	C	302	ATP	C5-C6	2.77	1.48	1.41
7	B	302	ATP	C5-C6	2.76	1.48	1.41
7	H	302	ATP	C5-C6	2.76	1.48	1.41
7	E	302	ATP	C5-C6	2.76	1.48	1.41
7	F	302	ATP	C5-C6	2.76	1.48	1.41
7	D	302	ATP	C5-C6	2.75	1.48	1.41
7	A	302	ATP	C5-C6	2.74	1.48	1.41
7	I	302	ATP	C5-C6	2.74	1.48	1.41
7	K	302	ATP	PB-O3B	2.60	1.62	1.59
7	J	302	ATP	PB-O3B	-2.43	1.56	1.59
7	I	302	ATP	C8-N7	2.42	1.36	1.31
7	J	302	ATP	PA-O3A	-2.39	1.56	1.59
7	G	302	ATP	C8-N7	2.37	1.36	1.31
7	C	302	ATP	C8-N7	2.37	1.36	1.31
7	K	302	ATP	C8-N7	2.37	1.36	1.31
7	A	302	ATP	C8-N7	2.36	1.36	1.31
7	F	302	ATP	C8-N7	2.35	1.36	1.31
7	H	302	ATP	C8-N7	2.33	1.36	1.31
7	D	302	ATP	C8-N7	2.32	1.36	1.31
7	B	302	ATP	C8-N7	2.32	1.36	1.31
7	E	302	ATP	C8-N7	2.31	1.36	1.31
7	J	302	ATP	C5-C4	2.30	1.43	1.39
7	F	302	ATP	C5-N7	-2.26	1.35	1.39
7	I	302	ATP	C5-N7	-2.25	1.35	1.39
7	A	302	ATP	C5-N7	-2.25	1.35	1.39
7	E	302	ATP	C5-N7	-2.25	1.35	1.39
7	J	302	ATP	O4'-C4'	-2.24	1.40	1.45
7	C	302	ATP	C5-N7	-2.24	1.35	1.39
7	G	302	ATP	C5-N7	-2.23	1.35	1.39
7	K	302	ATP	C5-N7	-2.21	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	302	ATP	C5-N7	-2.21	1.35	1.39
7	B	302	ATP	C5-N7	-2.21	1.35	1.39
7	H	302	ATP	C5-N7	-2.20	1.35	1.39

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	302	ATP	C5-C4-N3	-5.87	118.64	126.72
7	H	302	ATP	C5-C4-N3	-5.85	118.67	126.72
7	B	302	ATP	C5-C4-N3	-5.83	118.69	126.72
7	D	302	ATP	C5-C4-N3	-5.83	118.69	126.72
7	F	302	ATP	C5-C4-N3	-5.82	118.70	126.72
7	C	302	ATP	C5-C4-N3	-5.82	118.70	126.72
7	I	302	ATP	C5-C4-N3	-5.82	118.70	126.72
7	E	302	ATP	C5-C4-N3	-5.81	118.71	126.72
7	G	302	ATP	C5-C4-N3	-5.81	118.72	126.72
7	K	302	ATP	C5-C4-N3	-5.81	118.72	126.72
7	A	302	ATP	N3-C4-N9	4.64	135.06	127.17
7	I	302	ATP	N3-C4-N9	4.63	135.04	127.17
7	D	302	ATP	N3-C4-N9	4.61	135.01	127.17
7	J	302	ATP	C5-C4-N3	-4.61	120.38	126.72
7	K	302	ATP	N3-C4-N9	4.61	135.00	127.17
7	E	302	ATP	N3-C4-N9	4.60	135.00	127.17
7	B	302	ATP	N3-C4-N9	4.60	134.99	127.17
7	C	302	ATP	N3-C4-N9	4.59	134.98	127.17
7	G	302	ATP	N3-C4-N9	4.59	134.97	127.17
7	F	302	ATP	N3-C4-N9	4.58	134.96	127.17
7	H	302	ATP	N3-C4-N9	4.57	134.94	127.17
7	J	302	ATP	C2'-C1'-N9	-4.46	102.21	113.30
7	J	302	ATP	O3A-PB-O1B	-4.23	97.97	110.70
7	J	302	ATP	N3-C4-N9	3.99	133.95	127.17
7	J	302	ATP	C4-N9-C8	3.90	109.83	105.74
7	I	302	ATP	C2-N3-C4	3.89	121.33	111.83
7	I	302	ATP	N3-C2-N1	-3.73	122.93	128.58
7	A	302	ATP	C2-N3-C4	3.73	120.93	111.83
7	D	302	ATP	C2-N3-C4	3.70	120.87	111.83
7	K	302	ATP	C2-N3-C4	3.70	120.87	111.83
7	C	302	ATP	C2-N3-C4	3.70	120.86	111.83
7	F	302	ATP	C2-N3-C4	3.69	120.85	111.83
7	H	302	ATP	C2-N3-C4	3.69	120.84	111.83
7	B	302	ATP	C2-N3-C4	3.69	120.84	111.83
7	E	302	ATP	C2-N3-C4	3.68	120.82	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	302	ATP	C2-N3-C4	3.68	120.81	111.83
7	H	302	ATP	C4-C5-N7	-3.54	106.53	110.58
7	A	302	ATP	C4-C5-N7	-3.51	106.56	110.58
7	I	302	ATP	C4-C5-N7	-3.51	106.56	110.58
7	F	302	ATP	C4-C5-N7	-3.51	106.57	110.58
7	G	302	ATP	C4-C5-N7	-3.49	106.59	110.58
7	D	302	ATP	C4-C5-N7	-3.49	106.59	110.58
7	C	302	ATP	C4-C5-N7	-3.47	106.61	110.58
7	B	302	ATP	C4-C5-N7	-3.47	106.61	110.58
7	E	302	ATP	C4-C5-N7	-3.47	106.61	110.58
7	K	302	ATP	C4-C5-N7	-3.44	106.65	110.58
7	J	302	ATP	O3'-C3'-C4'	-3.38	101.38	111.08
7	J	302	ATP	N3-C2-N1	-3.30	123.59	128.58
7	C	302	ATP	N3-C2-N1	-3.25	123.66	128.58
7	A	302	ATP	N3-C2-N1	-3.25	123.67	128.58
7	D	302	ATP	N3-C2-N1	-3.23	123.69	128.58
7	K	302	ATP	N3-C2-N1	-3.22	123.70	128.58
7	E	302	ATP	N3-C2-N1	-3.21	123.72	128.58
7	B	302	ATP	N3-C2-N1	-3.21	123.73	128.58
7	F	302	ATP	N3-C2-N1	-3.20	123.73	128.58
7	H	302	ATP	N3-C2-N1	-3.19	123.75	128.58
7	G	302	ATP	N3-C2-N1	-3.17	123.78	128.58
7	J	302	ATP	C4-C5-N7	-2.93	107.23	110.58
7	J	302	ATP	N9-C8-N7	-2.90	109.83	113.94
7	I	302	ATP	C4-N9-C8	2.89	108.78	105.74
7	J	302	ATP	C2-N1-C6	2.76	123.26	118.73
7	I	302	ATP	C5-N7-C8	2.74	107.75	103.45
7	J	302	ATP	O3G-PG-O2G	2.65	117.74	107.80
7	G	302	ATP	C4-N9-C8	2.64	108.51	105.74
7	J	302	ATP	C2'-C3'-C4'	2.63	107.69	102.61
7	A	302	ATP	C4-N9-C8	2.63	108.50	105.74
7	K	302	ATP	C4-N9-C8	2.62	108.49	105.74
7	F	302	ATP	C4-N9-C8	2.60	108.47	105.74
7	E	302	ATP	C4-N9-C8	2.59	108.46	105.74
7	B	302	ATP	C4-N9-C8	2.59	108.45	105.74
7	D	302	ATP	C4-N9-C8	2.59	108.45	105.74
7	J	302	ATP	C2-N3-C4	2.58	118.13	111.83
7	G	302	ATP	C5-N7-C8	2.58	107.50	103.45
7	C	302	ATP	C4-N9-C8	2.58	108.44	105.74
7	A	302	ATP	C5-N7-C8	2.57	107.49	103.45
7	H	302	ATP	C5-N7-C8	2.56	107.48	103.45
7	F	302	ATP	C5-N7-C8	2.56	107.48	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	302	ATP	C4-N9-C8	2.56	108.43	105.74
7	E	302	ATP	C5-N7-C8	2.55	107.45	103.45
7	D	302	ATP	C5-N7-C8	2.55	107.45	103.45
7	B	302	ATP	C5-N7-C8	2.53	107.43	103.45
7	J	302	ATP	C5-N7-C8	2.53	107.43	103.45
7	C	302	ATP	C5-N7-C8	2.53	107.43	103.45
7	K	302	ATP	C5-N7-C8	2.52	107.41	103.45
7	J	302	ATP	O3B-PG-O1G	-2.50	97.86	111.04
7	E	302	ATP	C3'-C2'-C1'	2.48	106.15	101.46
7	G	302	ATP	C3'-C2'-C1'	2.48	106.15	101.46
7	D	302	ATP	C3'-C2'-C1'	2.47	106.14	101.46
7	A	302	ATP	C3'-C2'-C1'	2.46	106.11	101.46
7	I	302	ATP	C3'-C2'-C1'	2.45	106.11	101.46
7	B	302	ATP	C3'-C2'-C1'	2.45	106.10	101.46
7	F	302	ATP	C3'-C2'-C1'	2.45	106.09	101.46
7	K	302	ATP	C3'-C2'-C1'	2.44	106.09	101.46
7	C	302	ATP	C3'-C2'-C1'	2.44	106.08	101.46
7	H	302	ATP	C3'-C2'-C1'	2.44	106.08	101.46
7	I	302	ATP	N9-C8-N7	-2.32	110.65	113.94
7	I	302	ATP	C6-C5-N7	2.18	136.29	132.09
7	J	302	ATP	O3B-PB-O1B	-2.13	104.31	110.70
7	F	302	ATP	C6-C5-N7	2.12	136.17	132.09
7	H	302	ATP	C6-C5-N7	2.11	136.16	132.09
7	A	302	ATP	C6-C5-N7	2.11	136.15	132.09
7	G	302	ATP	C6-C5-N7	2.10	136.15	132.09
7	D	302	ATP	C6-C5-N7	2.10	136.13	132.09
7	I	302	ATP	C2-N1-C6	2.10	122.17	118.73
7	E	302	ATP	C6-C5-N7	2.09	136.13	132.09
7	C	302	ATP	C6-C5-N7	2.09	136.11	132.09
7	B	302	ATP	C6-C5-N7	2.07	136.07	132.09
7	J	302	ATP	O2A-PA-O3A	2.06	112.85	107.27
7	K	302	ATP	C6-C5-N7	2.06	136.07	132.09
7	G	302	ATP	N9-C8-N7	-2.00	111.09	113.94

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	302	ATP	C5'-O5'-PA-O3A
7	B	302	ATP	C5'-O5'-PA-O3A
7	C	302	ATP	C5'-O5'-PA-O3A
7	D	302	ATP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
7	E	302	ATP	C5'-O5'-PA-O3A
7	F	302	ATP	C5'-O5'-PA-O3A
7	H	302	ATP	C5'-O5'-PA-O1A
7	H	302	ATP	C5'-O5'-PA-O2A
7	H	302	ATP	C5'-O5'-PA-O3A
7	K	302	ATP	C5'-O5'-PA-O1A
7	K	302	ATP	C5'-O5'-PA-O2A
7	K	302	ATP	C5'-O5'-PA-O3A
7	K	302	ATP	C3'-C4'-C5'-O5'
7	J	302	ATP	C3'-C4'-C5'-O5'
7	K	302	ATP	O4'-C4'-C5'-O5'
7	J	302	ATP	O4'-C4'-C5'-O5'
7	H	302	ATP	C4'-C5'-O5'-PA
7	E	302	ATP	C3'-C4'-C5'-O5'
7	A	302	ATP	C3'-C4'-C5'-O5'
7	B	302	ATP	C3'-C4'-C5'-O5'
7	C	302	ATP	C3'-C4'-C5'-O5'
7	D	302	ATP	C3'-C4'-C5'-O5'
7	F	302	ATP	C3'-C4'-C5'-O5'
7	I	302	ATP	C3'-C4'-C5'-O5'
7	G	302	ATP	C3'-C4'-C5'-O5'
7	K	302	ATP	PG-O3B-PB-O1B
7	G	302	ATP	C4'-C5'-O5'-PA
7	I	302	ATP	C4'-C5'-O5'-PA
7	A	302	ATP	C5'-O5'-PA-O1A
7	B	302	ATP	C5'-O5'-PA-O1A
7	C	302	ATP	C5'-O5'-PA-O1A
7	D	302	ATP	C5'-O5'-PA-O1A
7	E	302	ATP	C5'-O5'-PA-O1A
7	F	302	ATP	C5'-O5'-PA-O1A
7	K	302	ATP	PA-O3A-PB-O1B
7	K	302	ATP	PA-O3A-PB-O2B
7	H	302	ATP	C3'-C4'-C5'-O5'
7	H	302	ATP	C2'-C1'-N9-C8
7	H	302	ATP	PB-O3A-PA-O2A

There are no ring outliers.

10 monomers are involved in 36 short contacts:

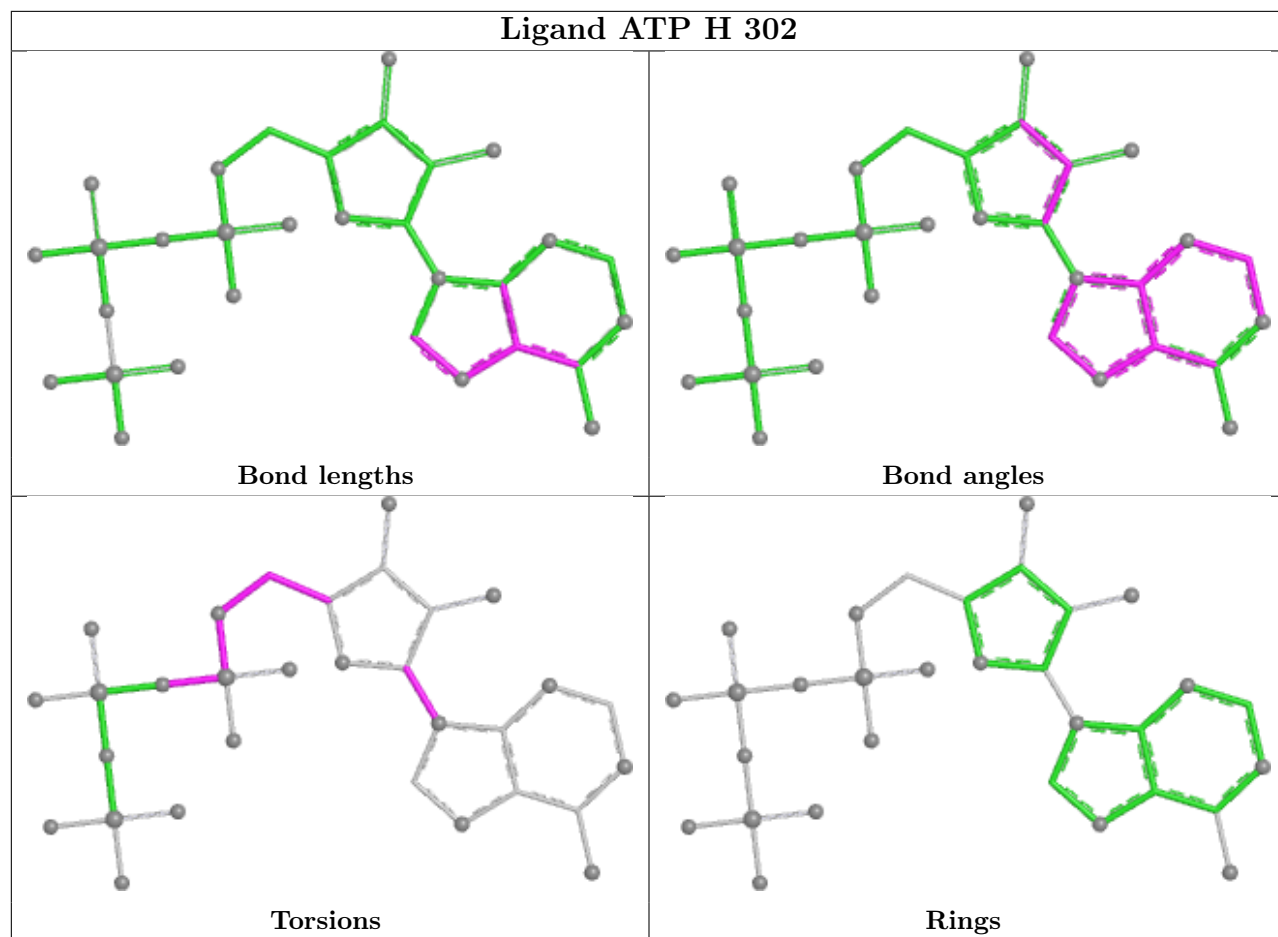
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	302	ATP	3	0
7	K	302	ATP	4	0

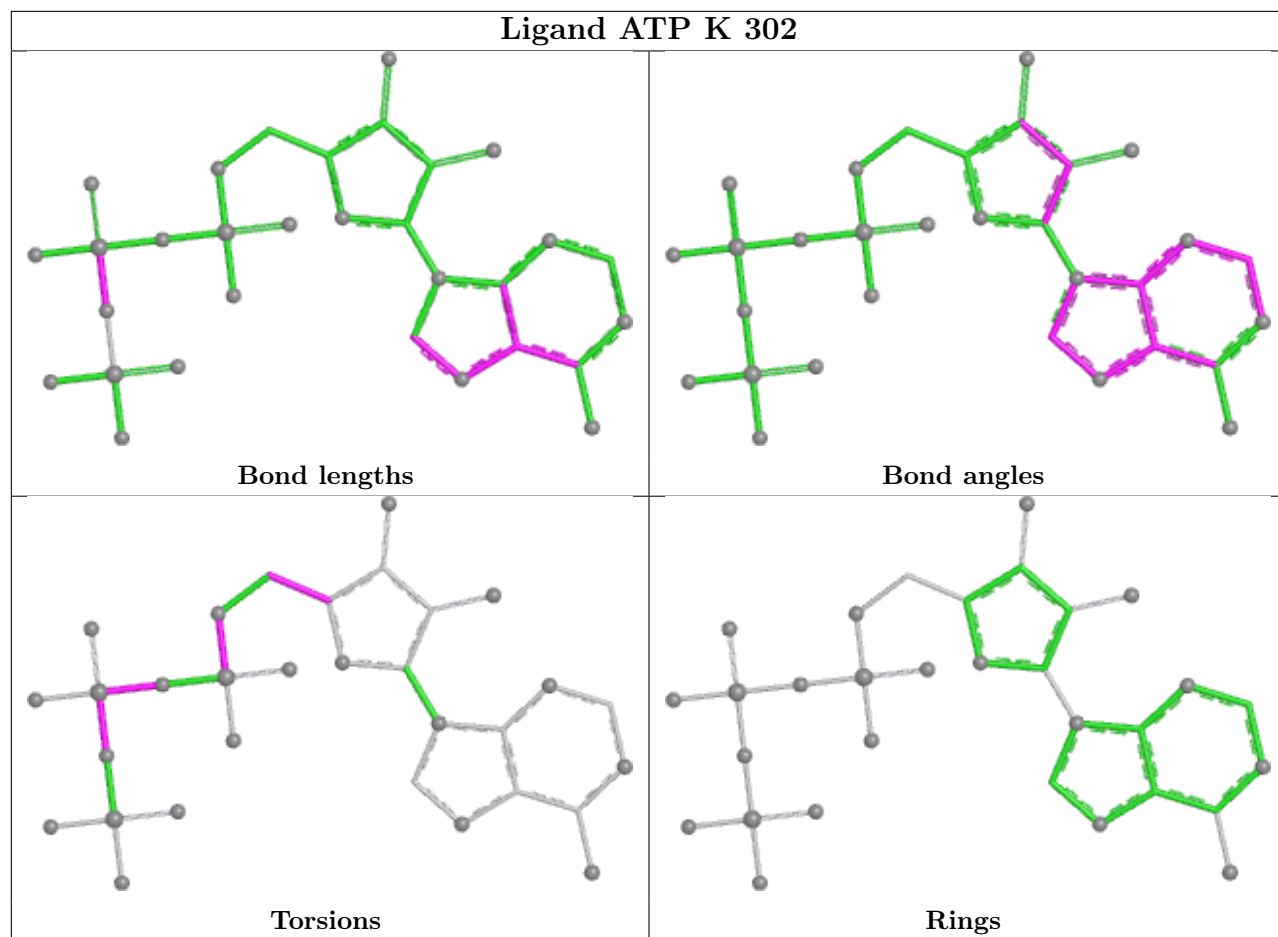
Continued on next page...

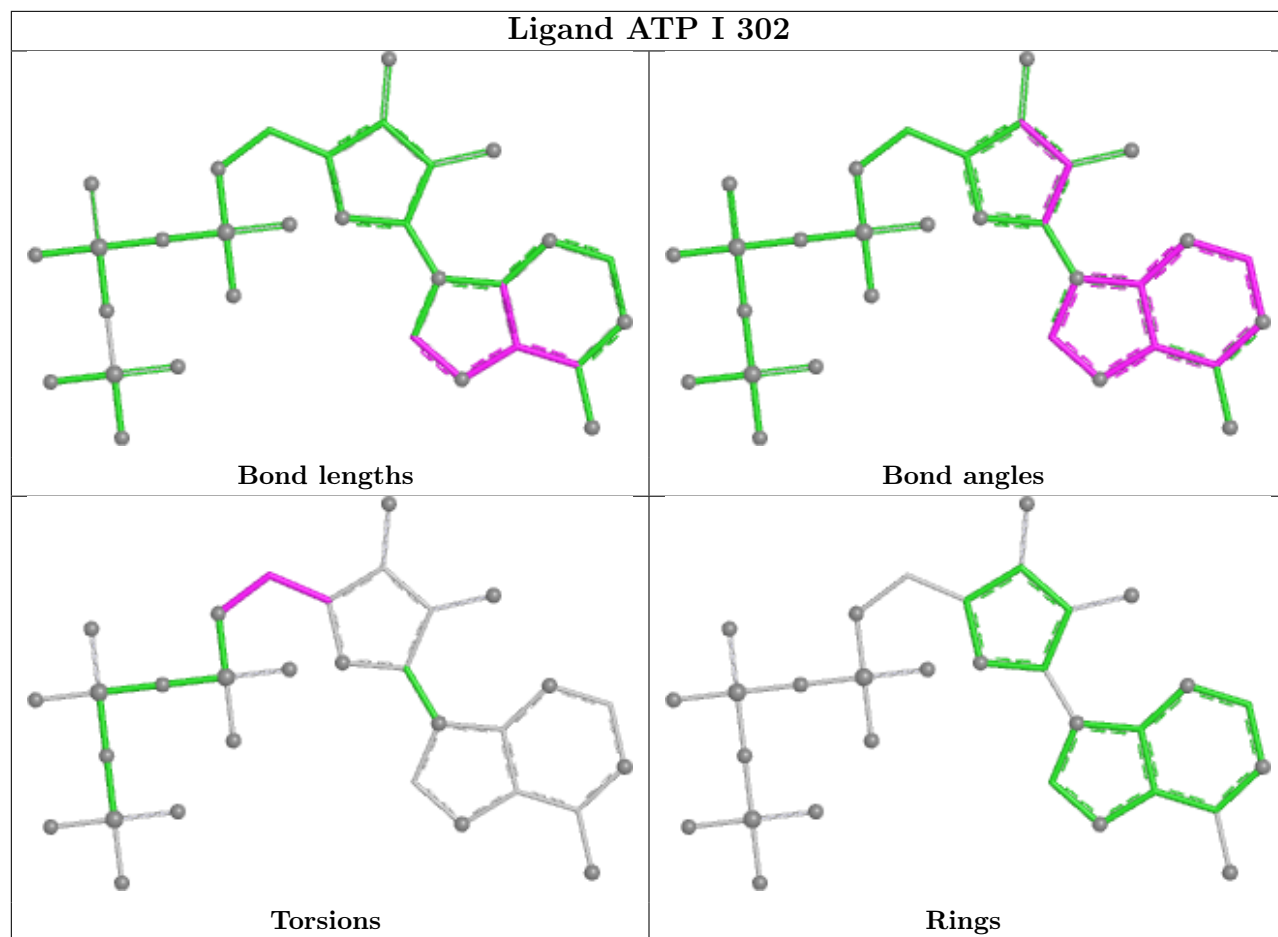
Continued from previous page...

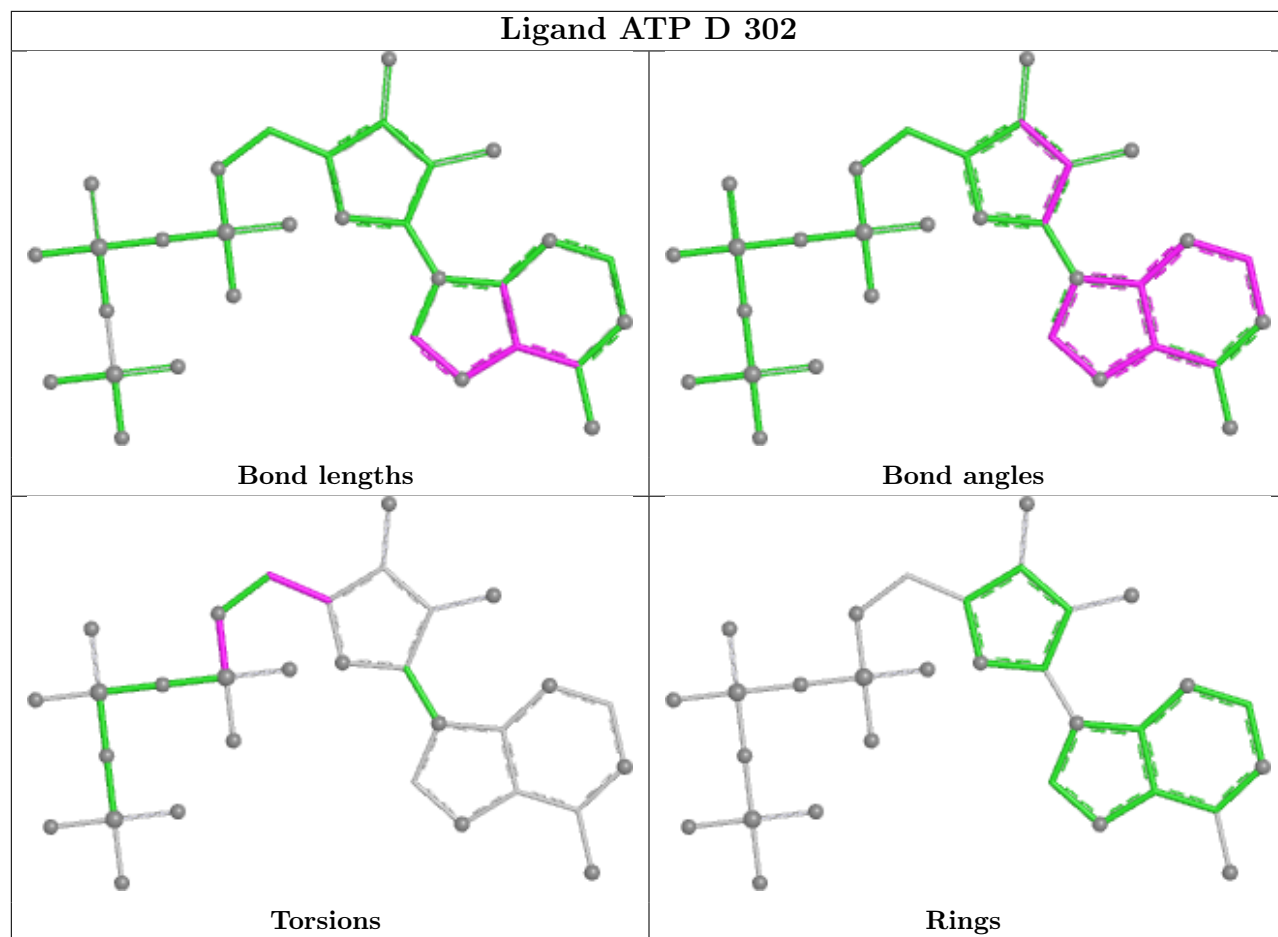
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	I	302	ATP	4	0
7	D	302	ATP	3	0
7	B	302	ATP	3	0
7	F	302	ATP	3	0
7	C	302	ATP	3	0
7	E	302	ATP	1	0
7	J	302	ATP	9	0
7	G	302	ATP	3	0

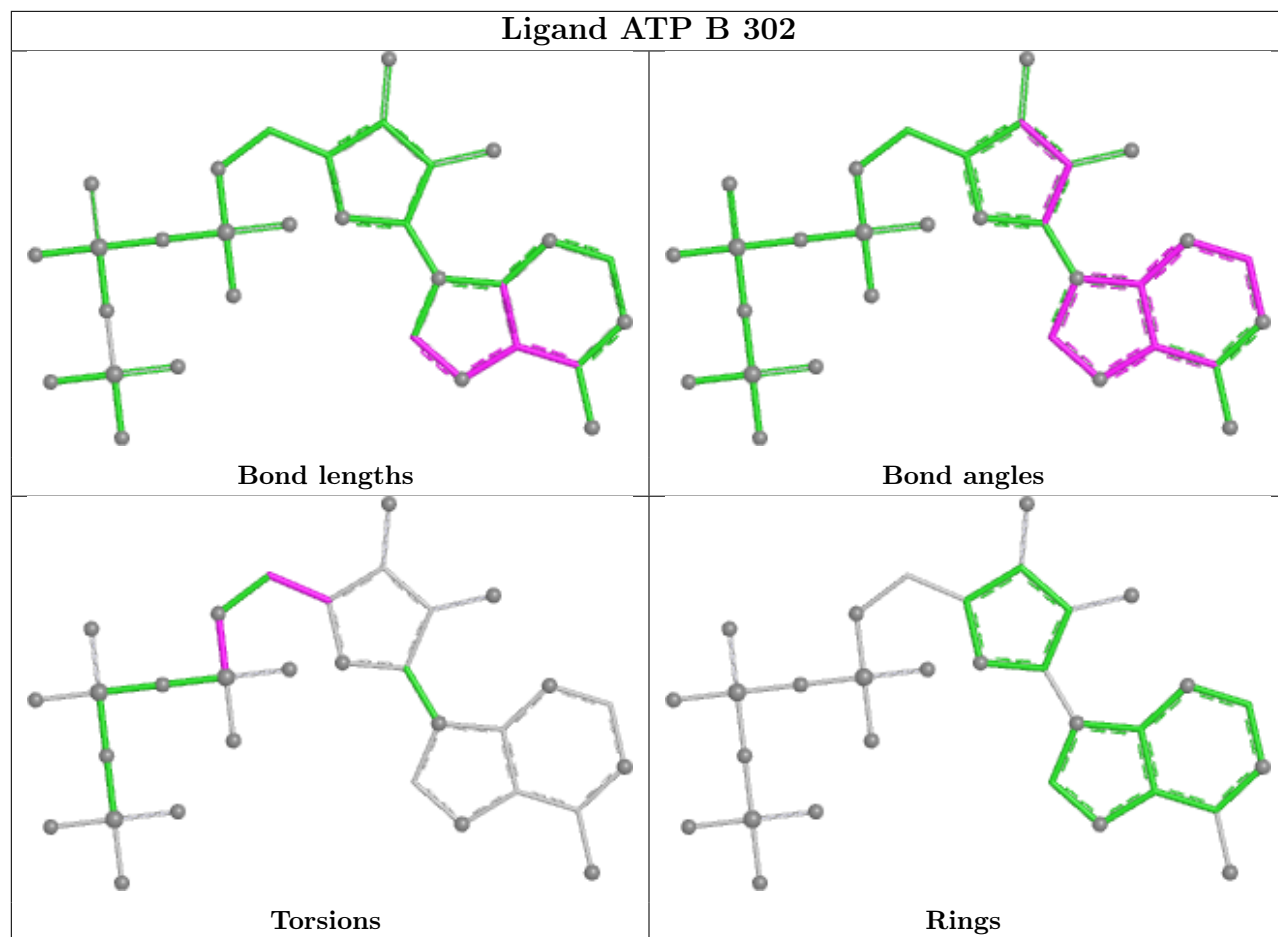
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

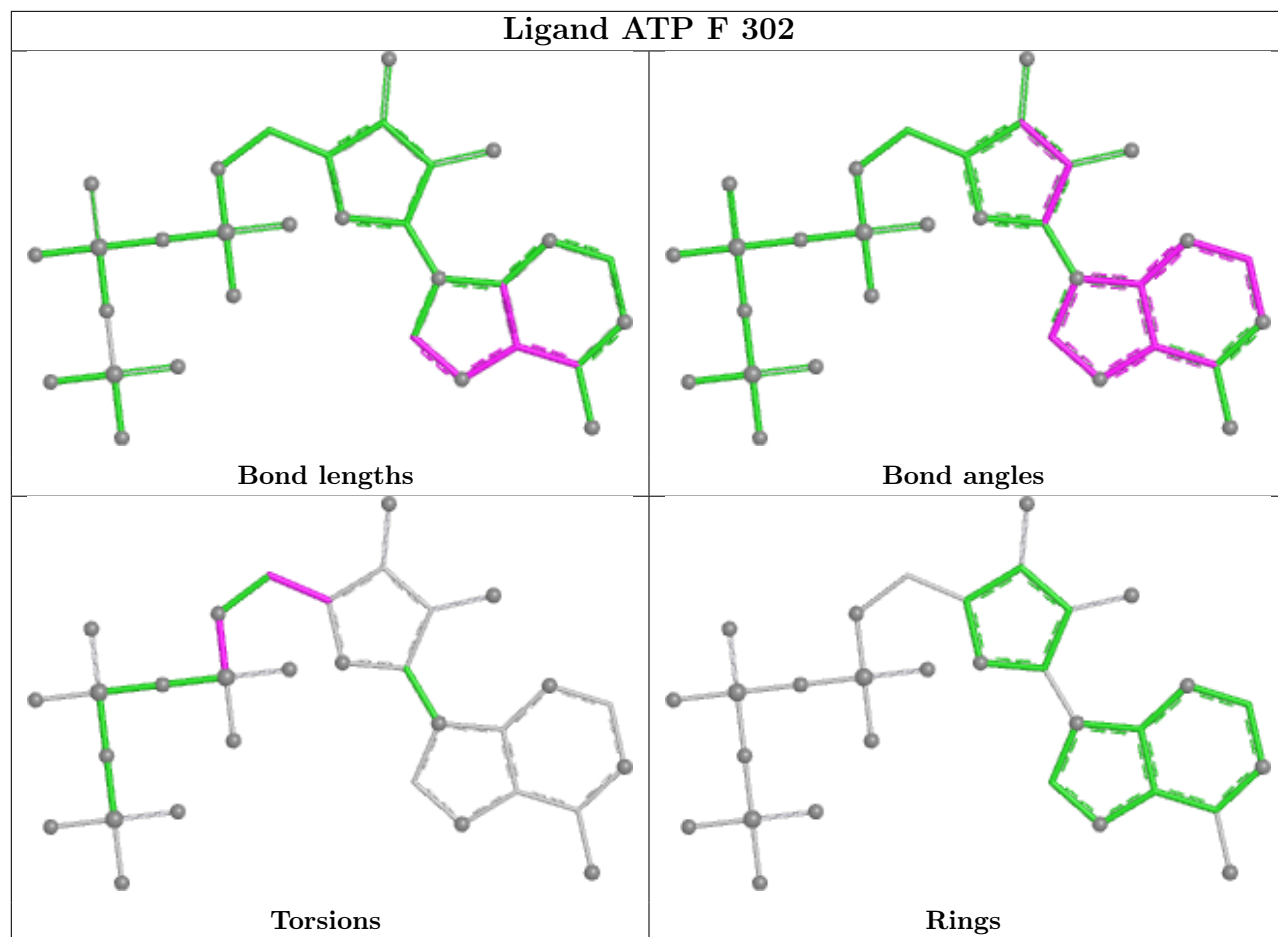


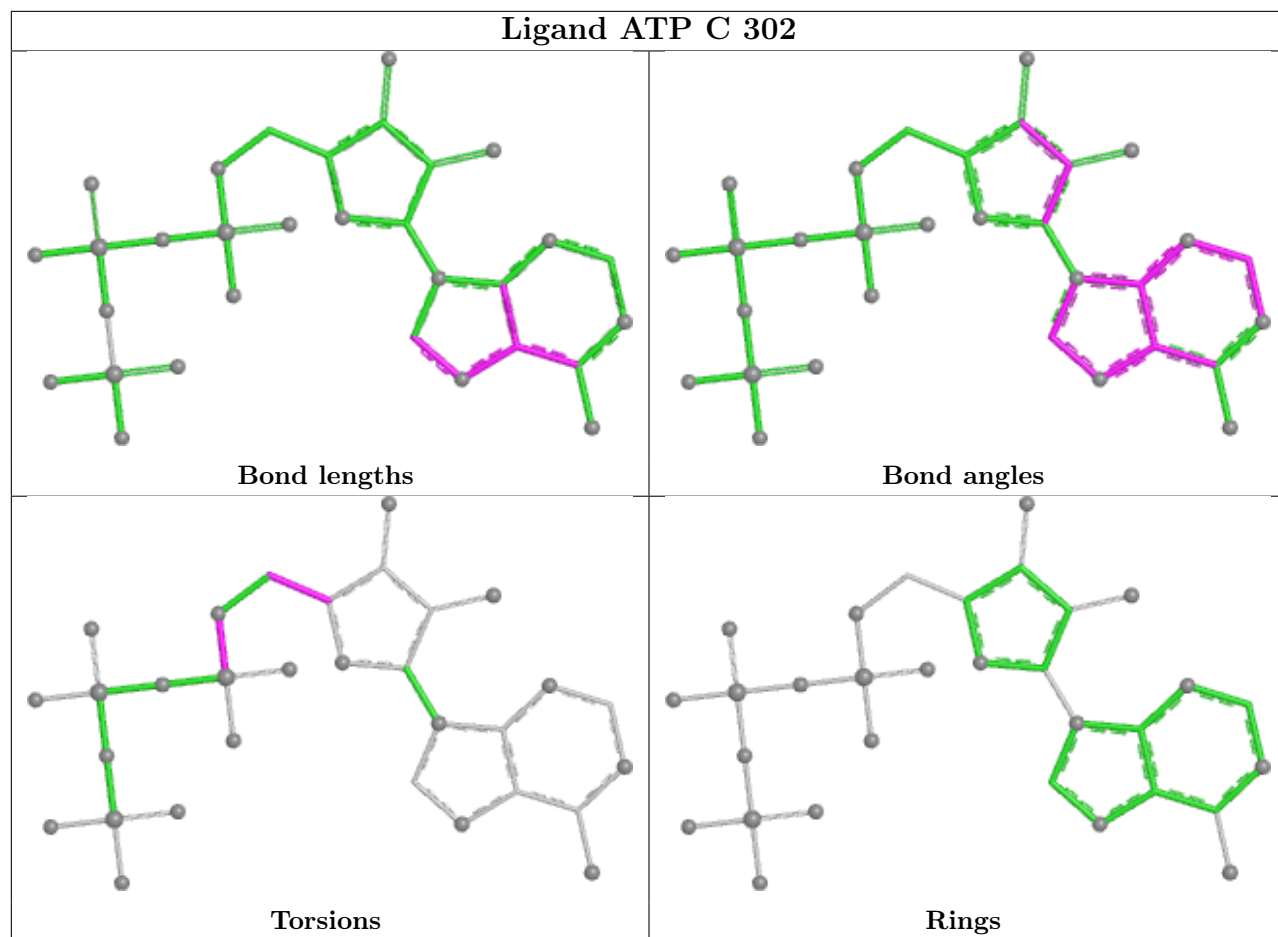


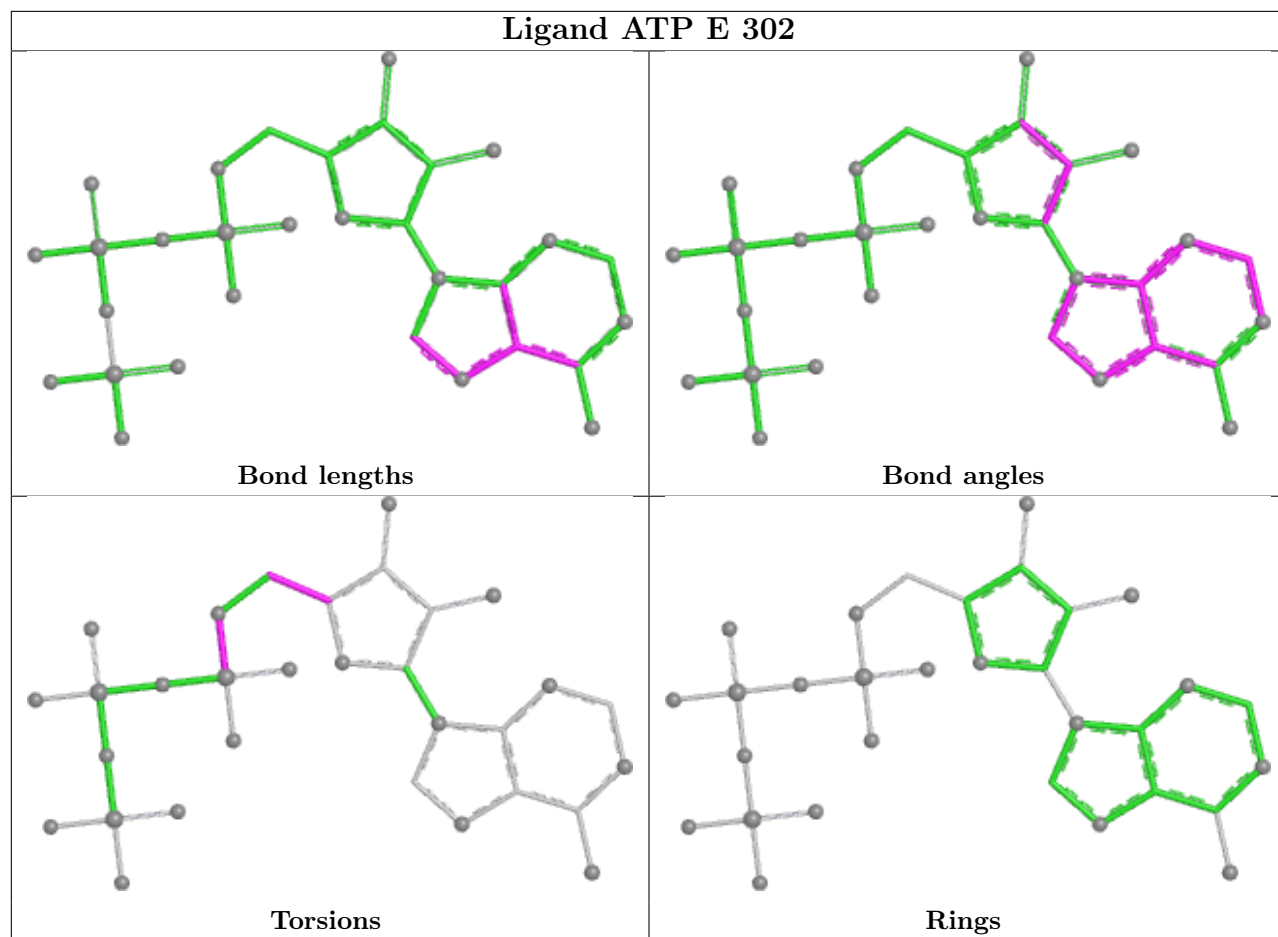




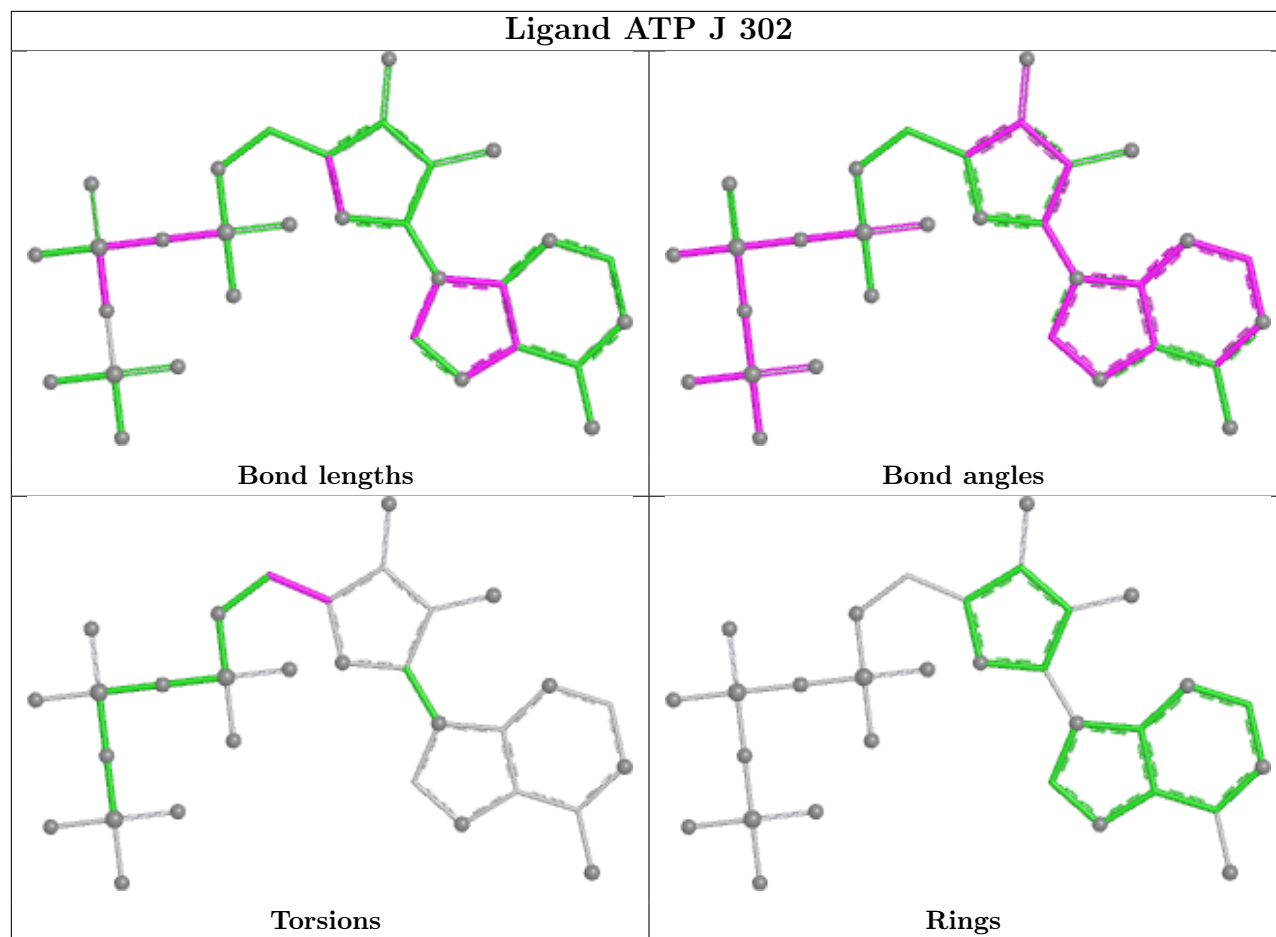


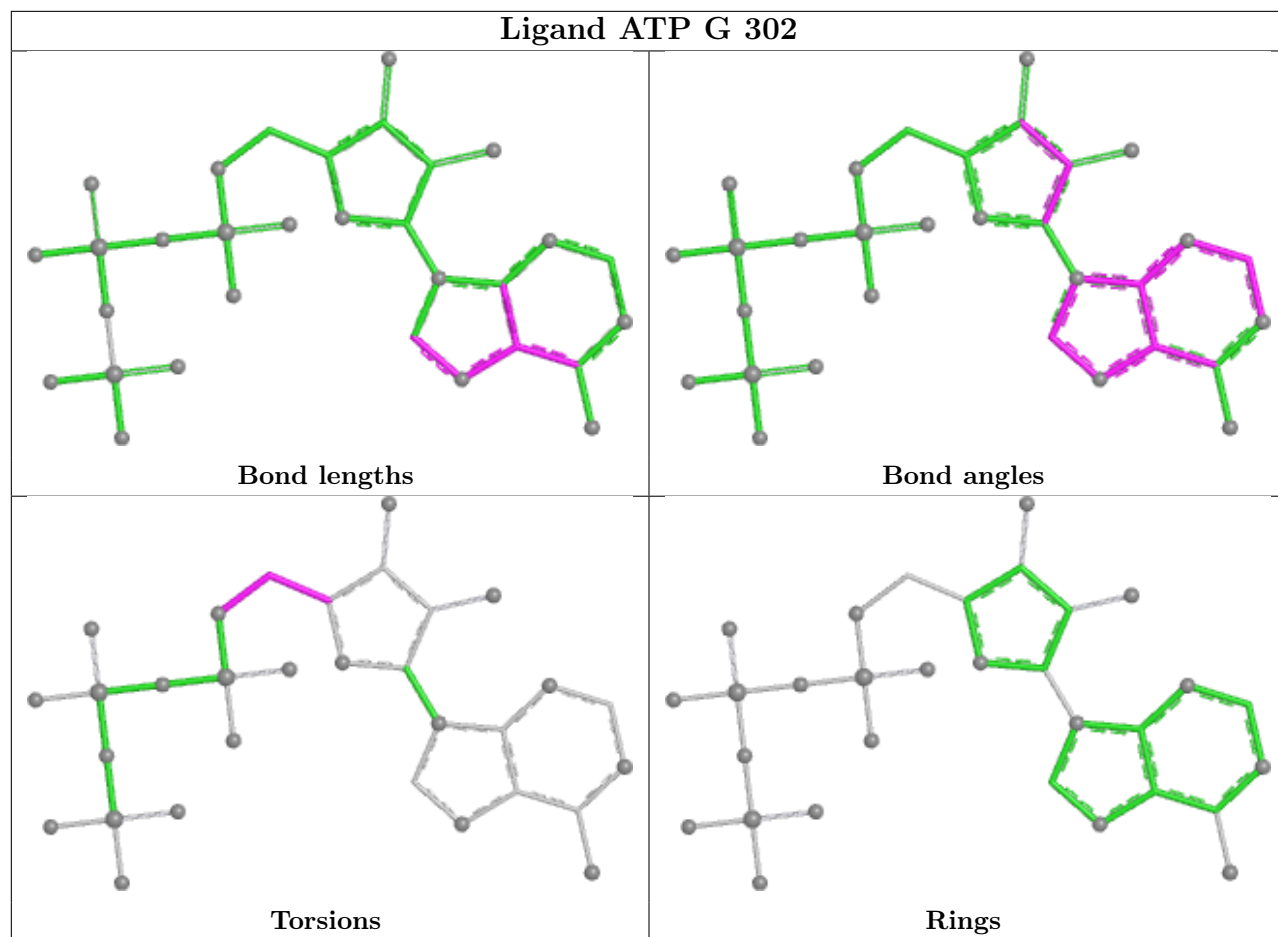


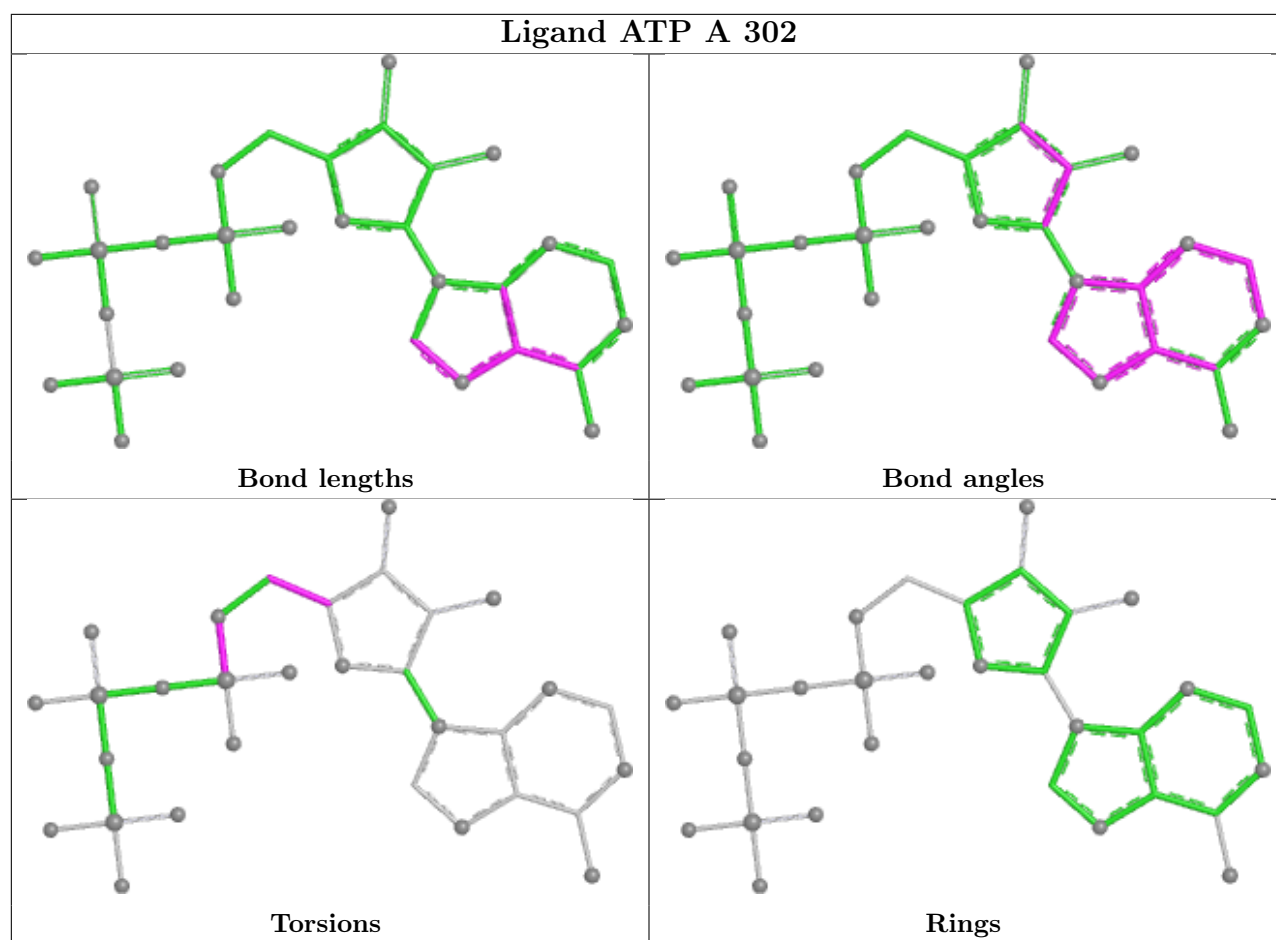




Ligand ATP J 302







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.

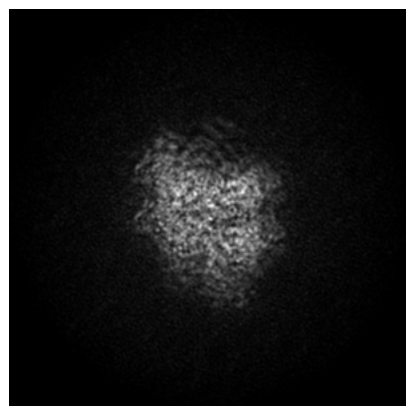
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25453. These allow visual inspection of the internal detail of the map and identification of artifacts.

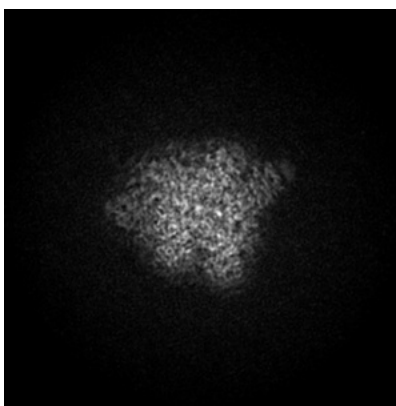
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

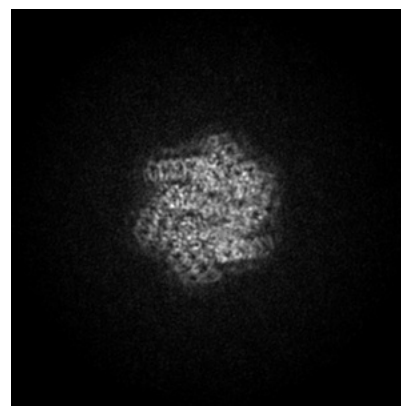
6.1.1 Primary map



X

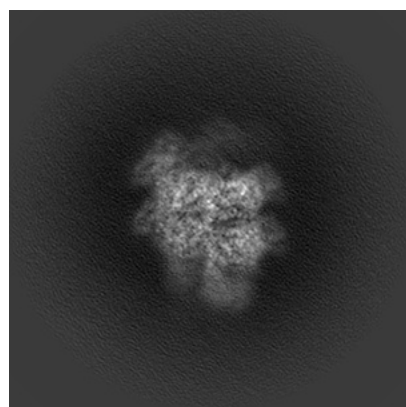


Y

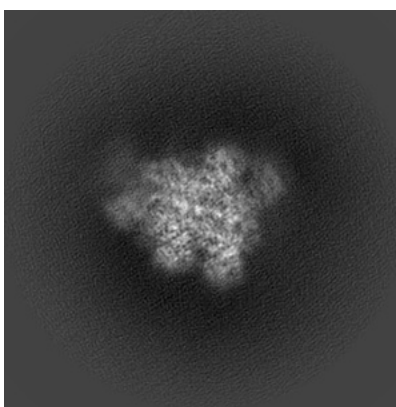


Z

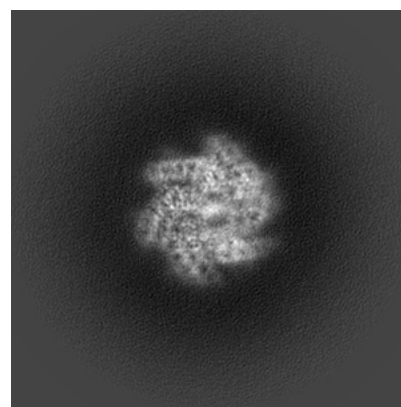
6.1.2 Raw map



X



Y

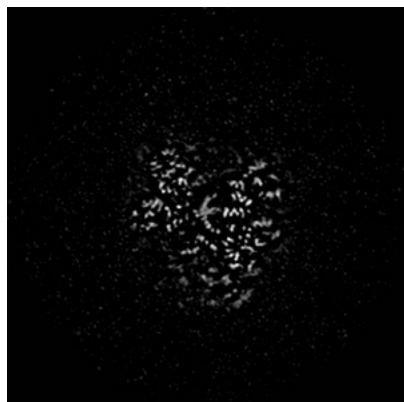


Z

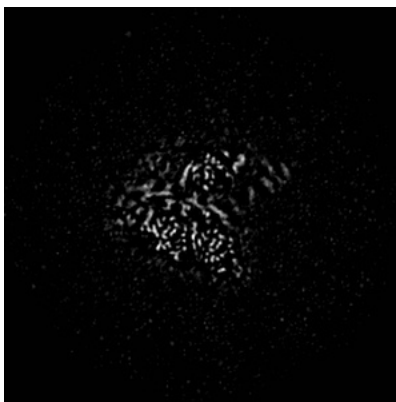
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

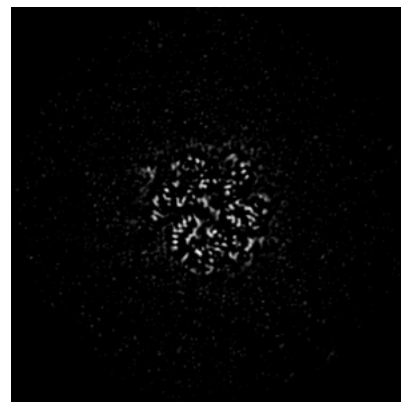
6.2.1 Primary map



X Index: 128

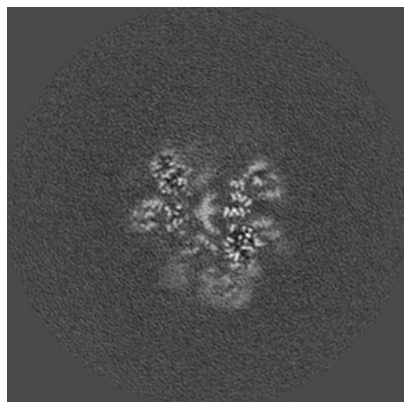


Y Index: 128

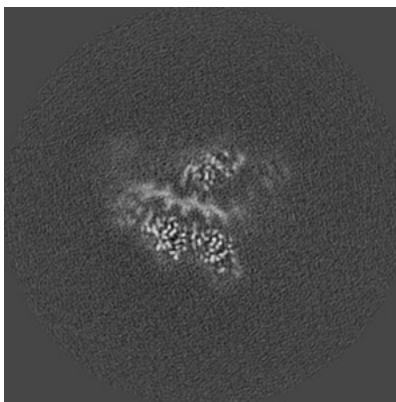


Z Index: 128

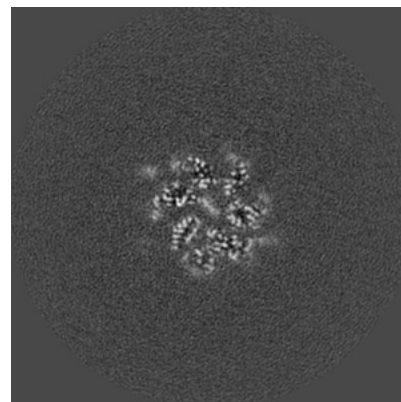
6.2.2 Raw map



X Index: 128



Y Index: 128

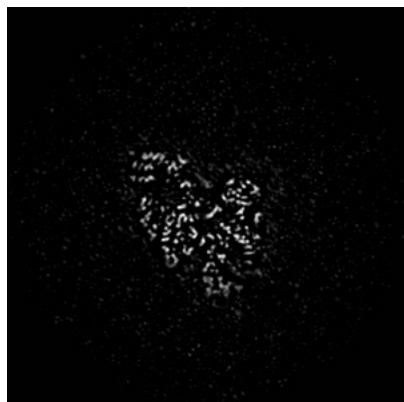


Z Index: 128

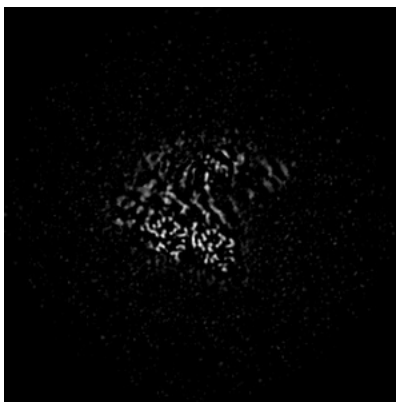
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

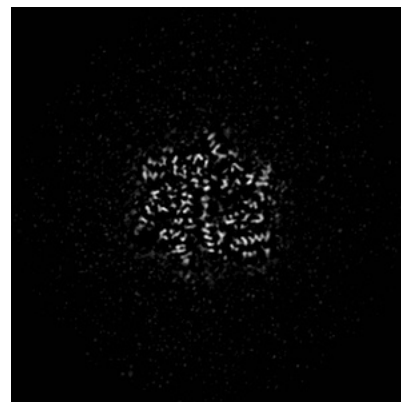
6.3.1 Primary map



X Index: 117

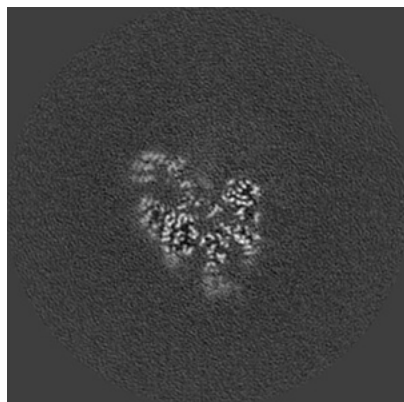


Y Index: 129

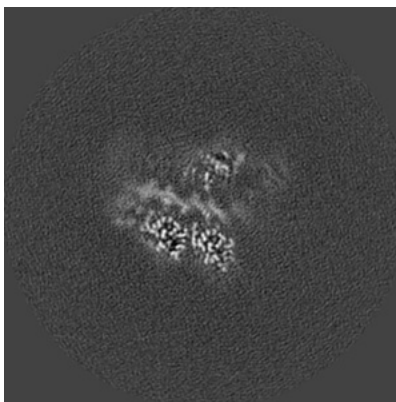


Z Index: 137

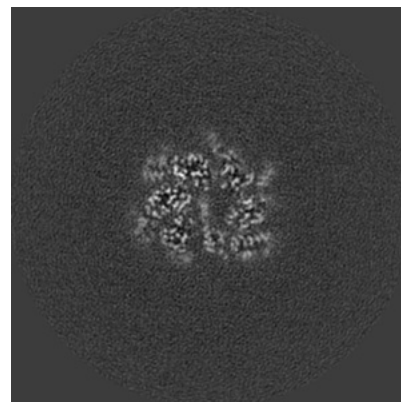
6.3.2 Raw map



X Index: 117



Y Index: 129

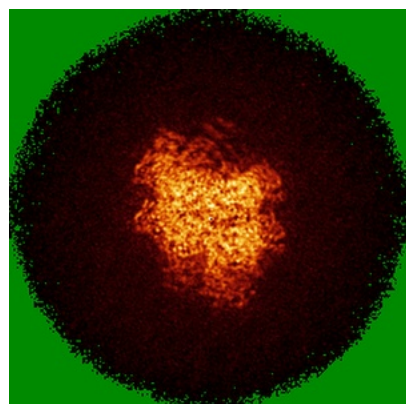


Z Index: 138

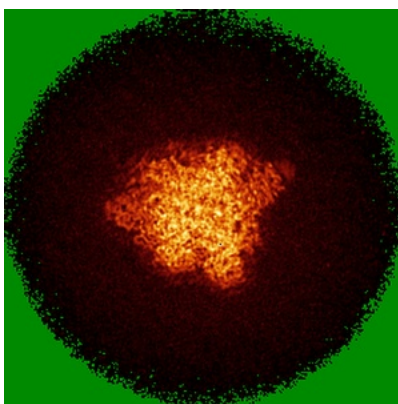
The images above show the largest variance slices of the map in three orthogonal directions.

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

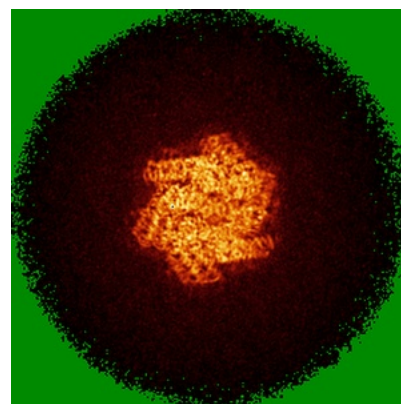
6.4.1 Primary map



X

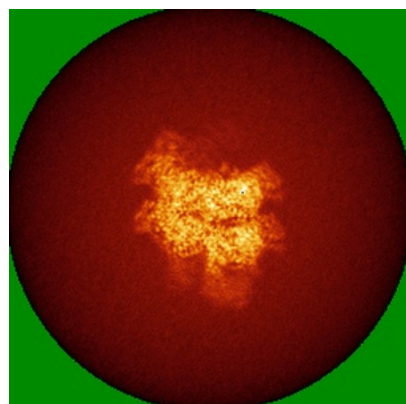


Y

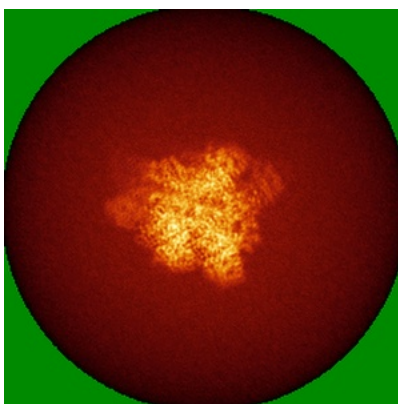


Z

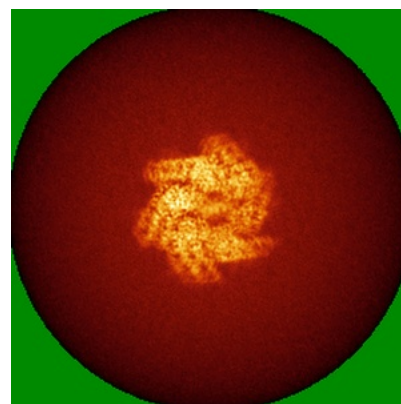
6.4.2 Raw map



X



Y

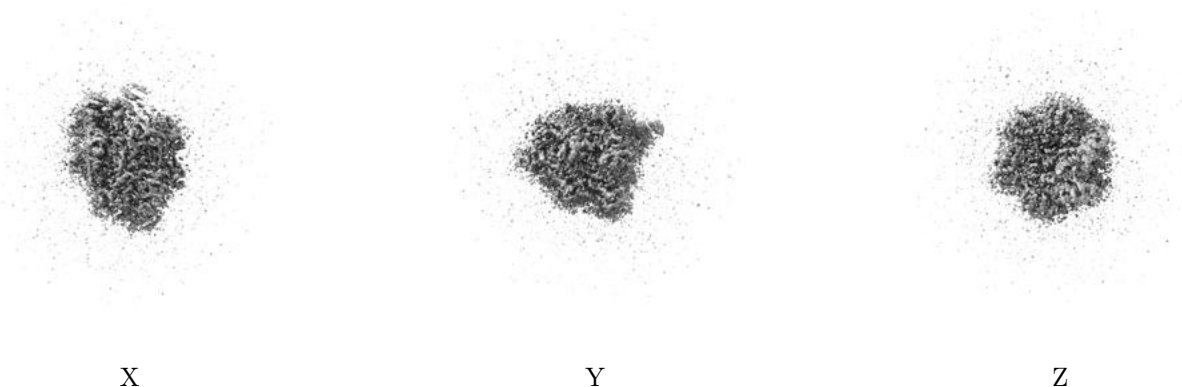


Z

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.

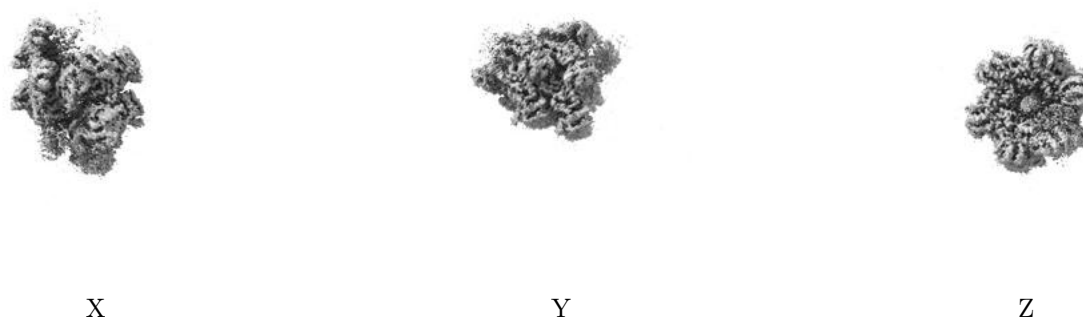
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 3.5. 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.

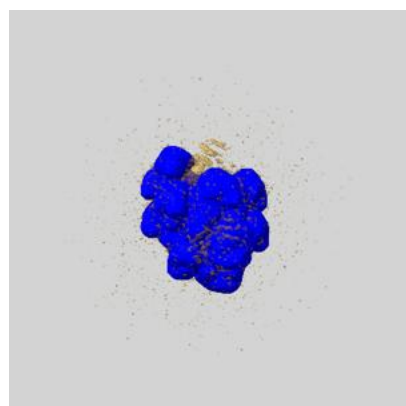
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

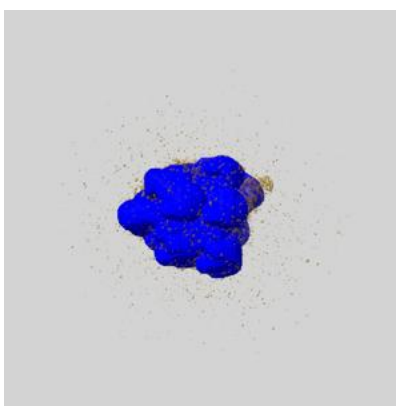
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

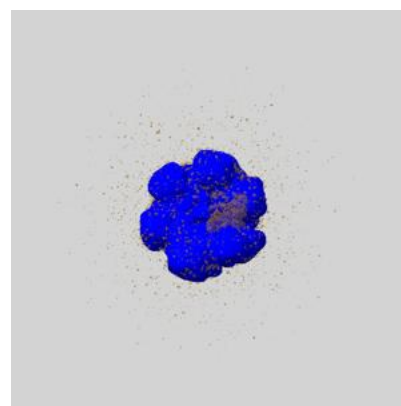
6.6.1 emd_25453_msk_1.map [i](#)



X



Y

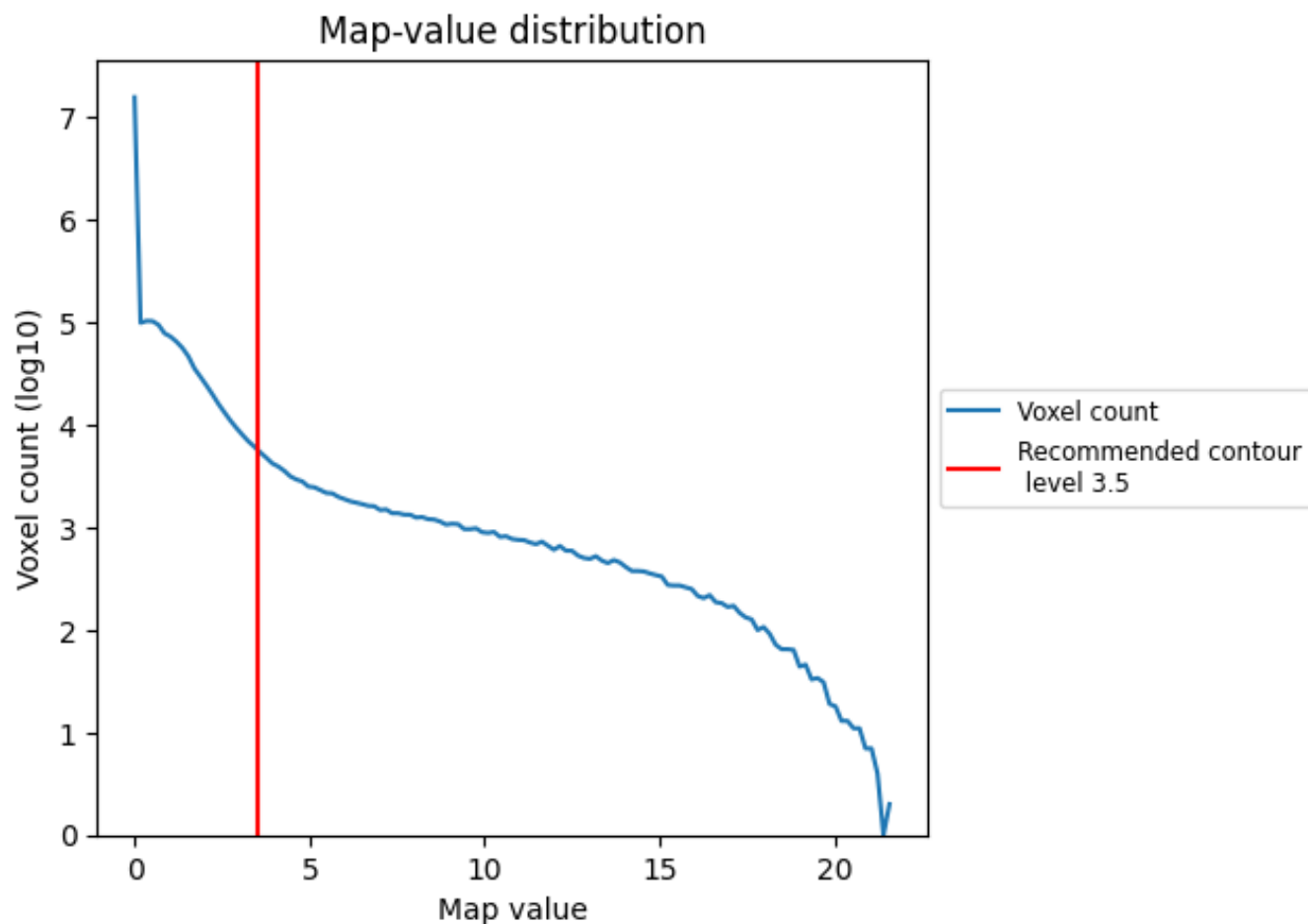


Z

7 Map analysis [i](#)

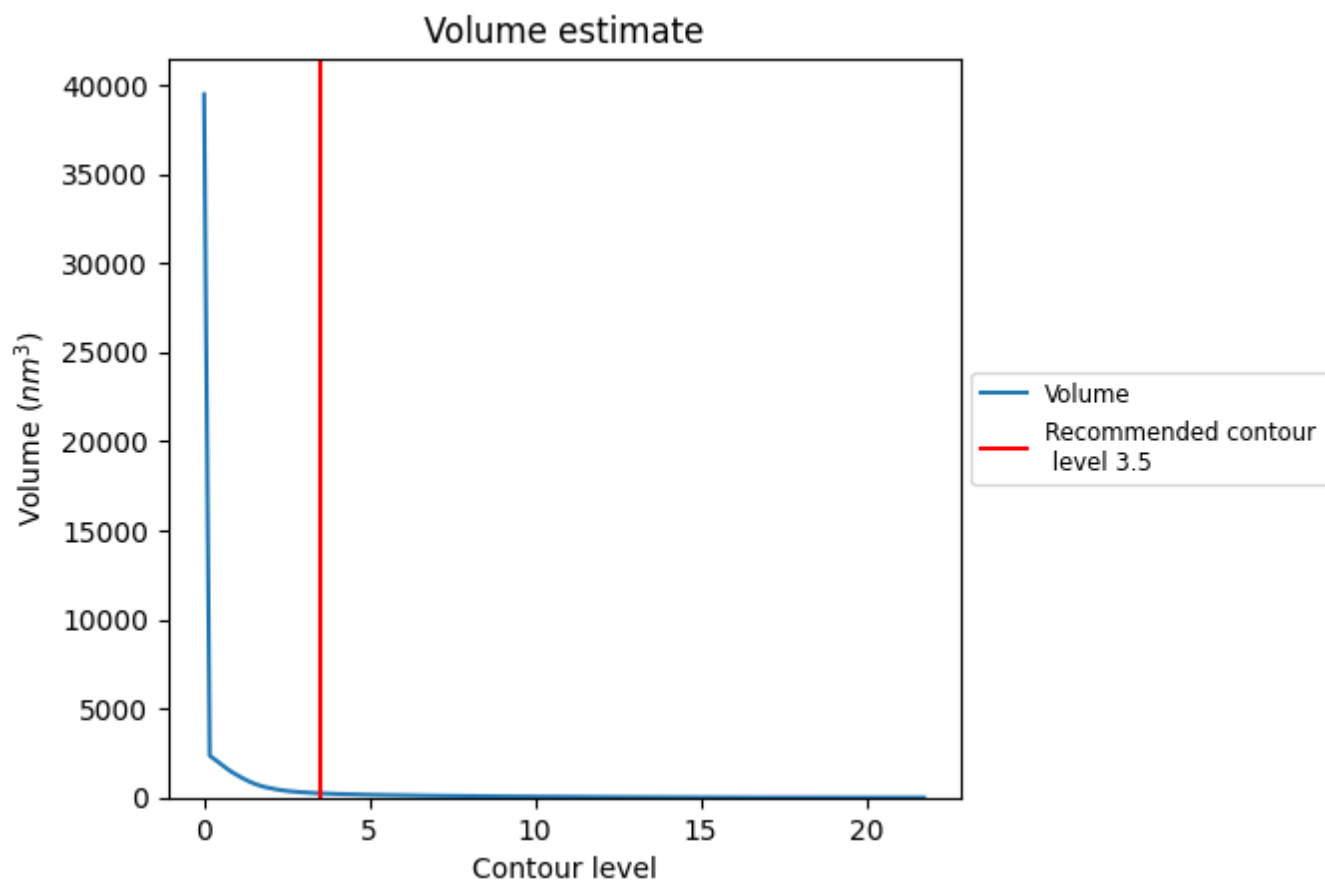
This section contains the results of statistical analysis of the map.

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.

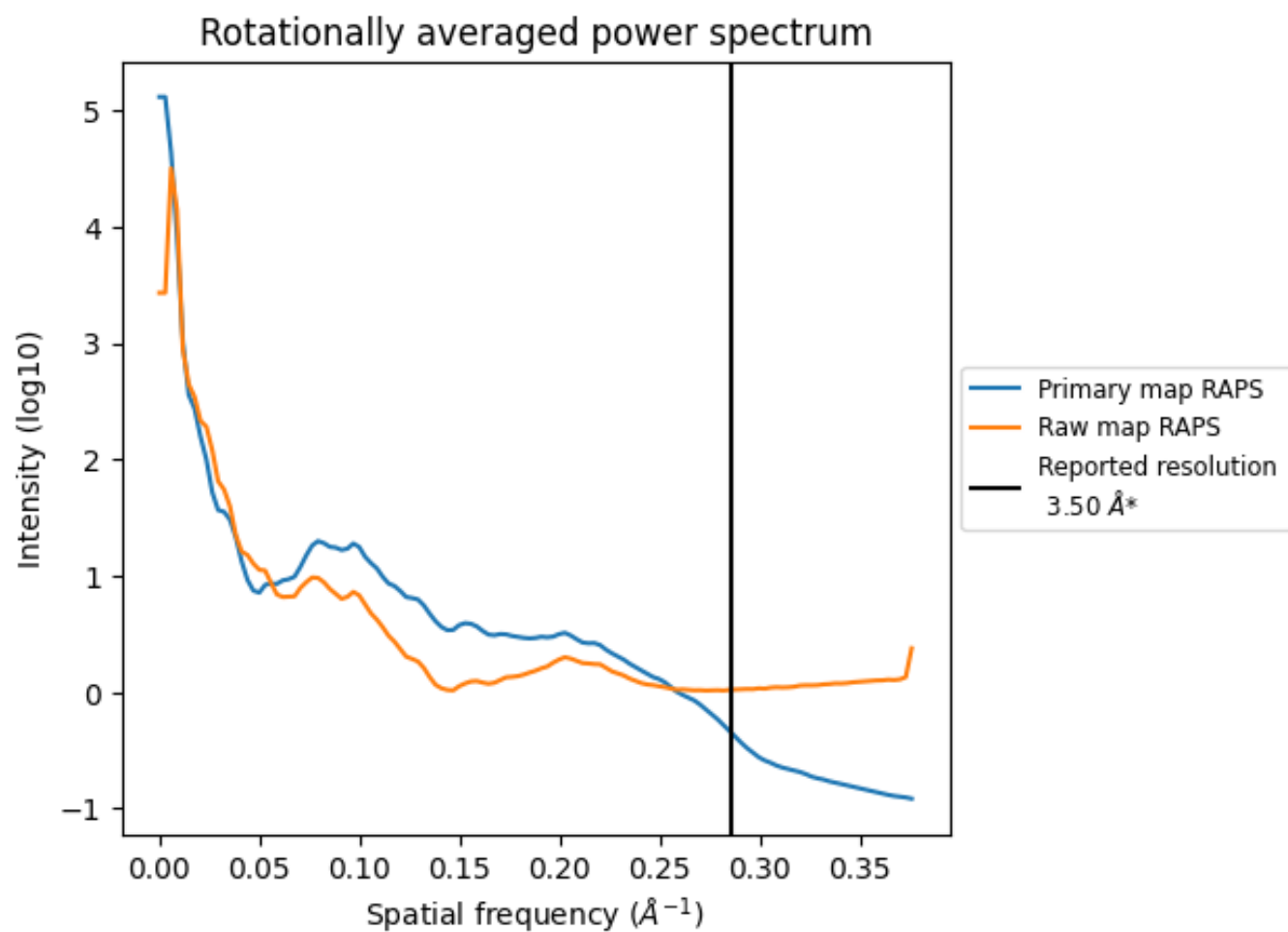
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 238 nm³; this corresponds to an approximate mass of 215 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

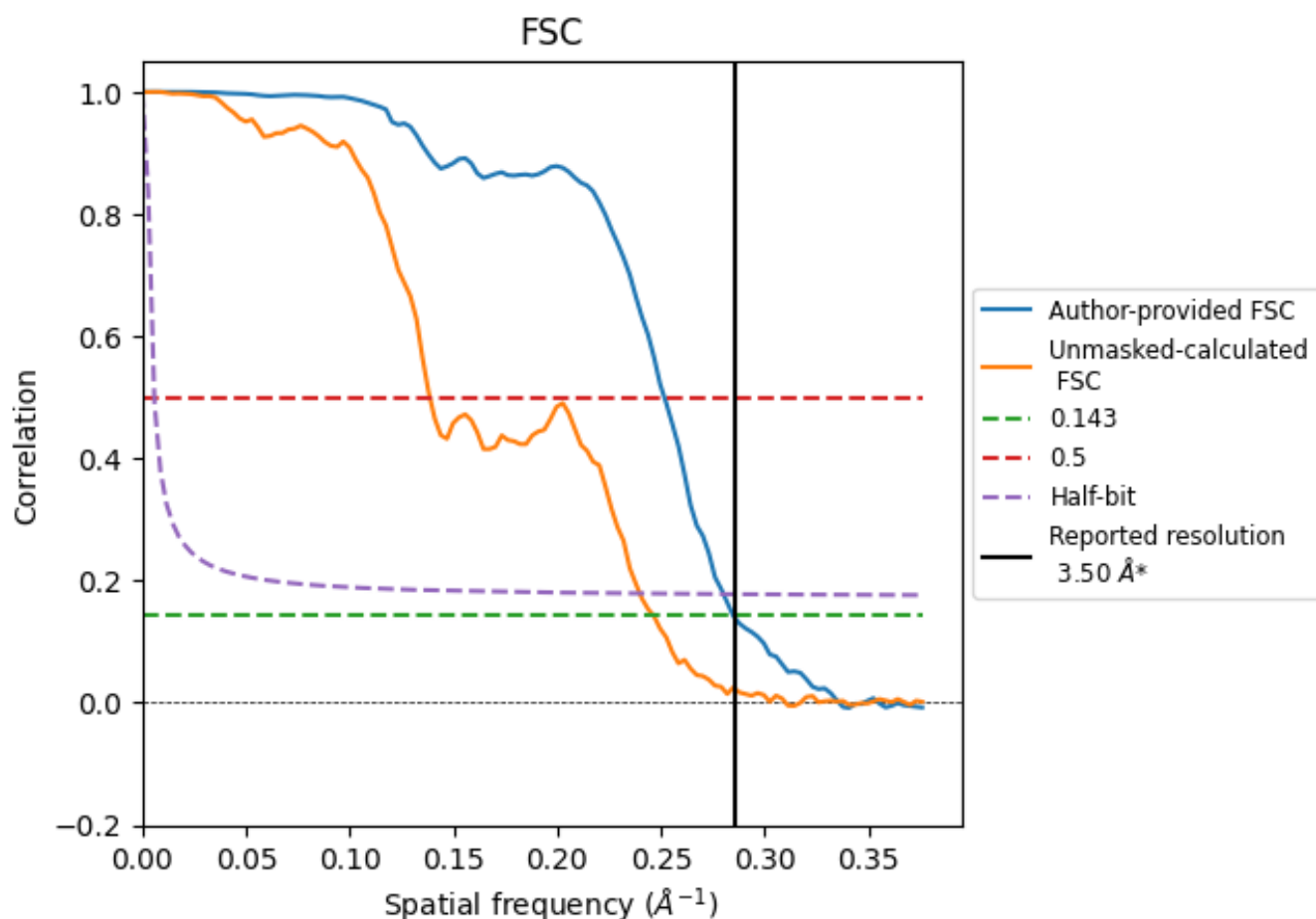


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

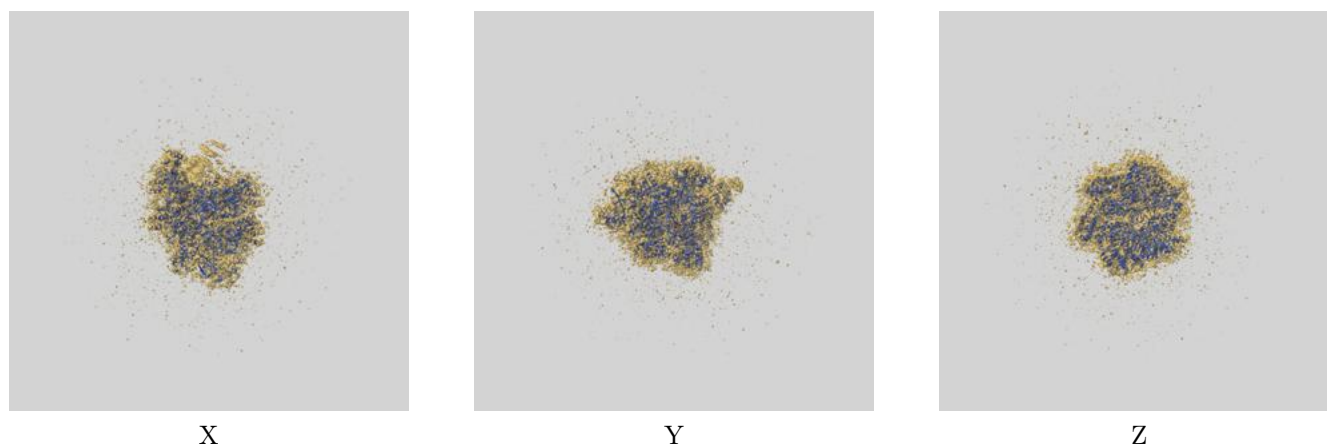
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.51	3.97	3.57
Unmasked-calculated*	4.06	7.22	4.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.06 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

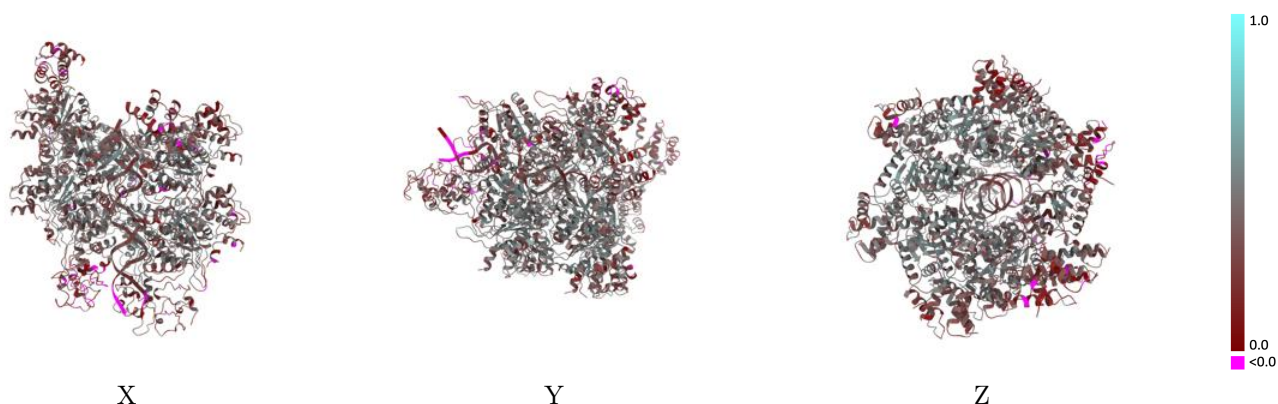
This section contains information regarding the fit between EMDB map EMD-25453 and PDB model 7SVU. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



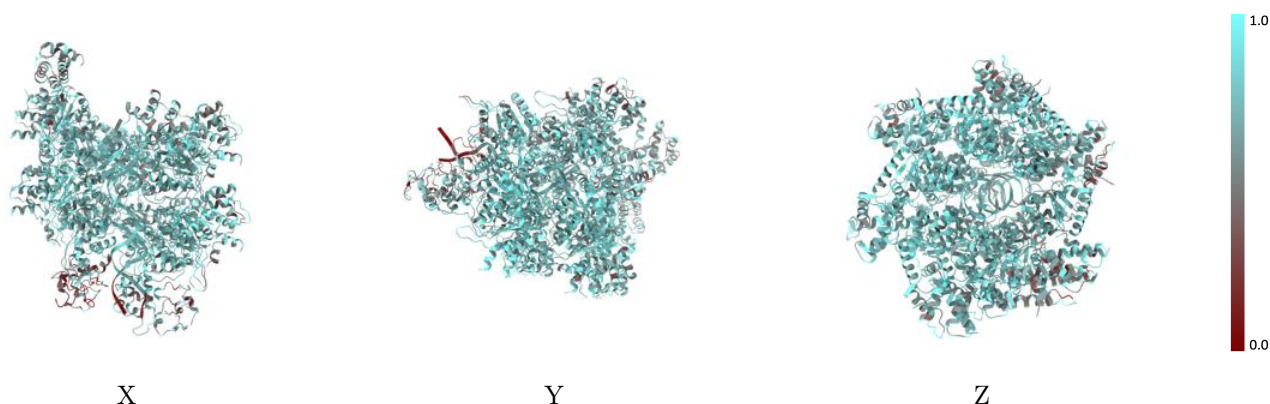
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



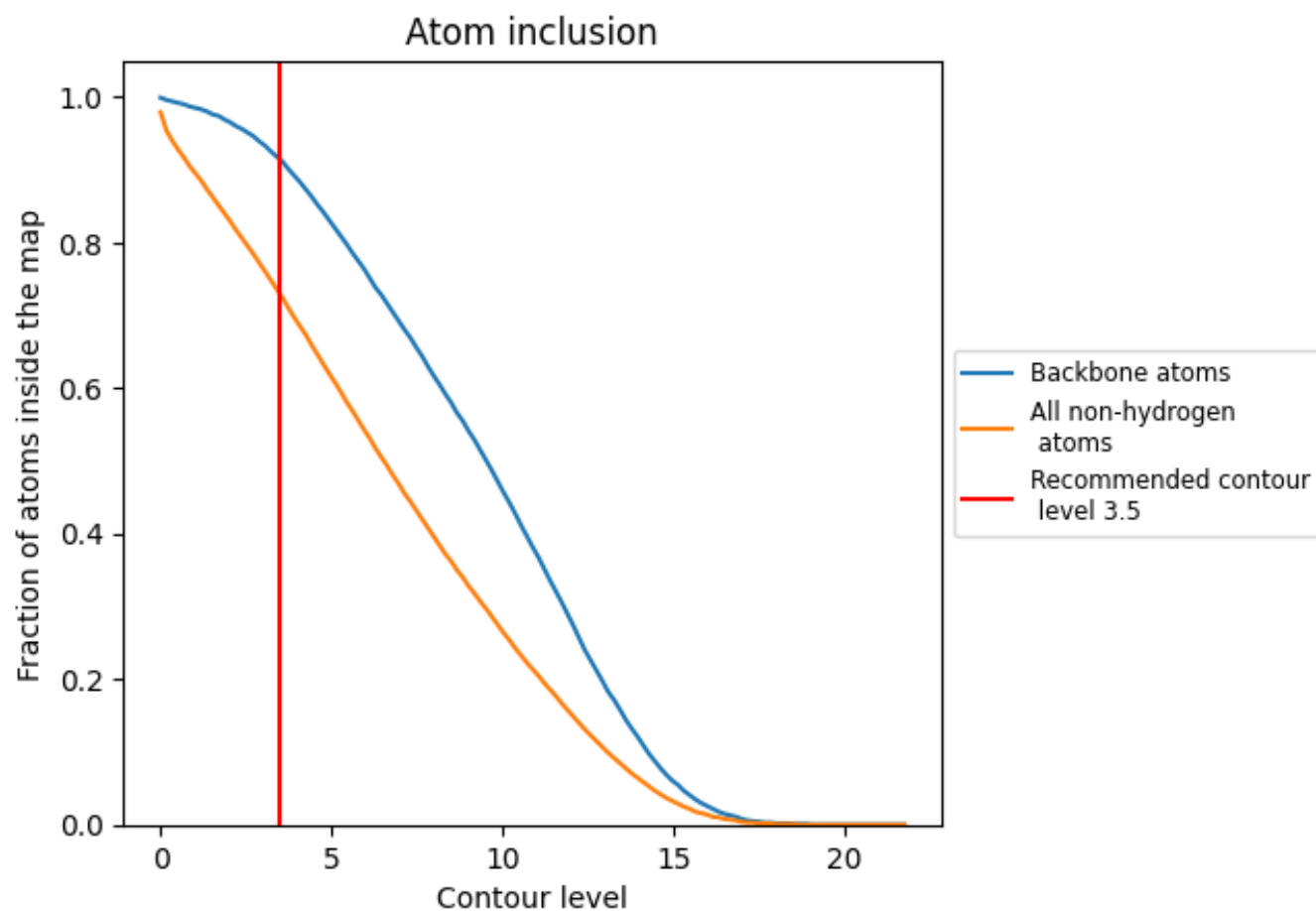
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.5).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 73% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7280	 0.3790
1	 0.6820	 0.2630
2	 0.7360	 0.2690
A	 0.6900	 0.3500
B	 0.7640	 0.4140
C	 0.7900	 0.4470
D	 0.7750	 0.4200
E	 0.7250	 0.3590
F	 0.7020	 0.3320
G	 0.7740	 0.4170
H	 0.7790	 0.4280
I	 0.8050	 0.4520
J	 0.8050	 0.4470
K	 0.7250	 0.3700
X	 0.4150	 0.1770
Y	 0.6260	 0.3080
a	 0.5890	 0.3080
b	 0.6690	 0.3250
c	 0.6850	 0.4020
d	 0.6690	 0.3600
e	 0.6530	 0.3330
f	 0.5560	 0.1960
h	 0.6370	 0.2780
j	 0.6690	 0.3400
k	 0.5650	 0.2400

