



Full wwPDB EM Validation Report ⓘ

Jun 10, 2026 – 01:43 pm BST

PDB ID : 30GB / pdb_000030gb
EMDB ID : EMD-57739
Title : Cryo-EM structure of the PseCascade-ThiQ-TnsC complex bound to PseTnsB-hook motifs
Authors : Finocchio, G.; Oberli, S.; Schmitz, M.; Jinek, M.
Deposited on : 2026-04-23
Resolution : 2.90 Å(reported)
Based on initial model : .

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:

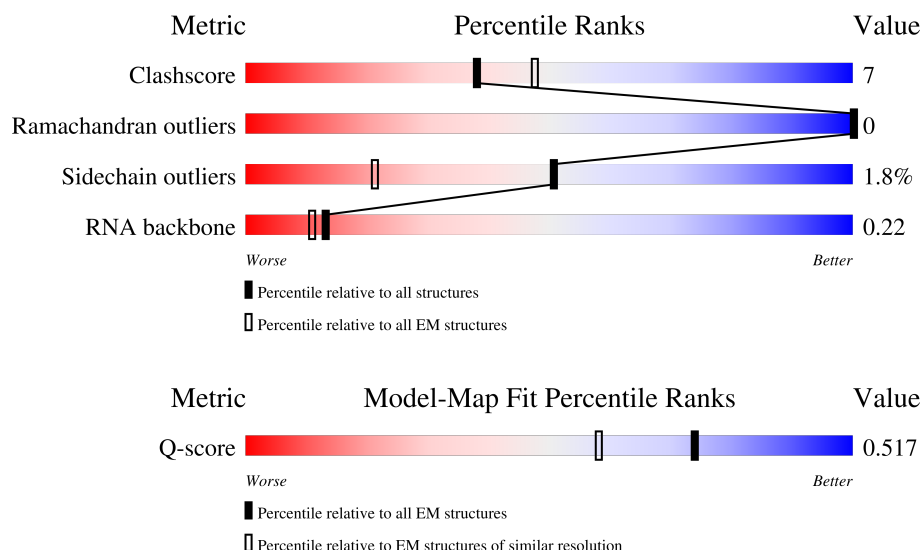
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.90 Å.

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















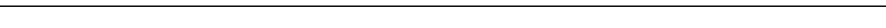
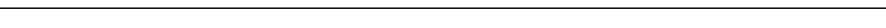




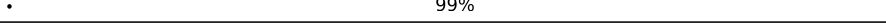
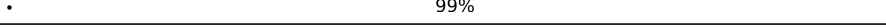
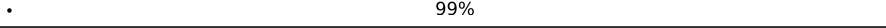
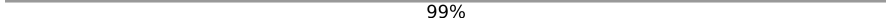
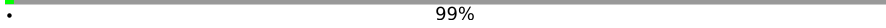
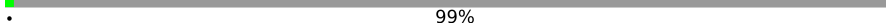
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13054 (2.40 - 3.40)

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	93	
2	2	120	
3	3	120	

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Mol	Chain	Length	Quality of chain
4	A	350	 75% 16% 8%
4	B	350	 78% 20% .
4	C	350	 84% 14% ..
4	D	350	 82% 17% .
4	E	350	 85% 13% ..
4	F	350	 82% 16% .
5	G	695	 82% 16% ..
6	H	237	 65% 19% 16%
7	I	432	 75% 18% . 6%
7	J	432	 79% 13% . 6%
8	K	333	 77% 21% ..
8	L	333	 71% 22% 6%
8	M	333	 68% 25% 7%
8	N	333	 79% 14% . 6%
8	O	333	 75% 20% . .
8	P	333	 77% 17% 6%
8	Q	333	 75% 20% .
9	R	1258	 99%
9	S	1258	 99%
9	T	1258	 99%
9	U	1258	 99%
9	V	1258	 99%
9	W	1258	 99%
9	X	1258	 99%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 52521 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 RNA chain called CRISPR RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	60	Total	C	N	O	P	0	0
			1291	577	243	412	59		

- Molecule 2 is a DNA chain called Target DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	70	Total	C	N	O	P	0	0
			1416	671	257	419	69		

- Molecule 3 is a DNA chain called Non-target DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	45	Total	C	N	O	P	0	0
			881	421	157	261	42		

- Molecule 4 is a protein called Cas7.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	321	Total	C	N	O	S	0	0
			2580	1649	429	490	12		
4	B	346	Total	C	N	O	S	0	0
			2777	1774	462	529	12		
4	C	346	Total	C	N	O	S	0	0
			2777	1774	462	529	12		
4	D	346	Total	C	N	O	S	0	0
			2777	1774	462	529	12		
4	E	346	Total	C	N	O	S	0	0
			2777	1774	462	529	12		
4	F	344	Total	C	N	O	S	0	0
			2763	1766	460	525	12		

- Molecule 5 is a protein called Cas8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	684	Total	C	N	O	S	0	0
			5489	3525	945	994	25		

- Molecule 6 is a protein called Cas6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	198	Total	C	N	O	S	0	0
			1599	1019	278	293	9		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	204	SER	-	expression tag	UNP A0ABF7PQC0
H	205	ALA	-	expression tag	UNP A0ABF7PQC0
H	206	TRP	-	expression tag	UNP A0ABF7PQC0
H	207	SER	-	expression tag	UNP A0ABF7PQC0
H	208	HIS	-	expression tag	UNP A0ABF7PQC0
H	209	PRO	-	expression tag	UNP A0ABF7PQC0
H	210	GLN	-	expression tag	UNP A0ABF7PQC0
H	211	PHE	-	expression tag	UNP A0ABF7PQC0
H	212	GLU	-	expression tag	UNP A0ABF7PQC0
H	213	LYS	-	expression tag	UNP A0ABF7PQC0
H	214	GLY	-	expression tag	UNP A0ABF7PQC0
H	215	GLY	-	expression tag	UNP A0ABF7PQC0
H	216	GLY	-	expression tag	UNP A0ABF7PQC0
H	217	SER	-	expression tag	UNP A0ABF7PQC0
H	218	GLY	-	expression tag	UNP A0ABF7PQC0
H	219	GLY	-	expression tag	UNP A0ABF7PQC0
H	220	GLY	-	expression tag	UNP A0ABF7PQC0
H	221	SER	-	expression tag	UNP A0ABF7PQC0
H	222	GLY	-	expression tag	UNP A0ABF7PQC0
H	223	GLY	-	expression tag	UNP A0ABF7PQC0
H	224	SER	-	expression tag	UNP A0ABF7PQC0
H	225	ALA	-	expression tag	UNP A0ABF7PQC0
H	226	TRP	-	expression tag	UNP A0ABF7PQC0
H	227	SER	-	expression tag	UNP A0ABF7PQC0
H	228	HIS	-	expression tag	UNP A0ABF7PQC0
H	229	PRO	-	expression tag	UNP A0ABF7PQC0
H	230	GLN	-	expression tag	UNP A0ABF7PQC0
H	231	PHE	-	expression tag	UNP A0ABF7PQC0
H	232	GLU	-	expression tag	UNP A0ABF7PQC0
H	233	LYS	-	expression tag	UNP A0ABF7PQC0
H	234	SER	-	expression tag	UNP A0ABF7PQC0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	235	GLY	-	expression tag	UNP A0ABF7PQC0
H	236	GLY	-	expression tag	UNP A0ABF7PQC0
H	237	GLY	-	expression tag	UNP A0ABF7PQC0

- Molecule 7 is a protein called TniQ.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	408	Total	C	N	O	S	0	0
			3311	2120	561	614	16		
7	J	404	Total	C	N	O	S	0	0
			3271	2094	556	604	17		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-22	MET	-	initiating methionine	UNP A0ABF7PQC1
I	-21	GLY	-	expression tag	UNP A0ABF7PQC1
I	-20	HIS	-	expression tag	UNP A0ABF7PQC1
I	-19	HIS	-	expression tag	UNP A0ABF7PQC1
I	-18	HIS	-	expression tag	UNP A0ABF7PQC1
I	-17	HIS	-	expression tag	UNP A0ABF7PQC1
I	-16	HIS	-	expression tag	UNP A0ABF7PQC1
I	-15	HIS	-	expression tag	UNP A0ABF7PQC1
I	-14	HIS	-	expression tag	UNP A0ABF7PQC1
I	-13	HIS	-	expression tag	UNP A0ABF7PQC1
I	-12	HIS	-	expression tag	UNP A0ABF7PQC1
I	-11	HIS	-	expression tag	UNP A0ABF7PQC1
I	-10	GLY	-	expression tag	UNP A0ABF7PQC1
I	-9	GLY	-	expression tag	UNP A0ABF7PQC1
I	-8	SER	-	expression tag	UNP A0ABF7PQC1
I	-7	GLU	-	expression tag	UNP A0ABF7PQC1
I	-6	ASN	-	expression tag	UNP A0ABF7PQC1
I	-5	LEU	-	expression tag	UNP A0ABF7PQC1
I	-4	TYR	-	expression tag	UNP A0ABF7PQC1
I	-3	PHE	-	expression tag	UNP A0ABF7PQC1
I	-2	GLN	-	expression tag	UNP A0ABF7PQC1
I	-1	SER	-	expression tag	UNP A0ABF7PQC1
I	0	GLY	-	expression tag	UNP A0ABF7PQC1
J	-22	MET	-	initiating methionine	UNP A0ABF7PQC1
J	-21	GLY	-	expression tag	UNP A0ABF7PQC1
J	-20	HIS	-	expression tag	UNP A0ABF7PQC1
J	-19	HIS	-	expression tag	UNP A0ABF7PQC1

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-18	HIS	-	expression tag	UNP A0ABF7PQC1
J	-17	HIS	-	expression tag	UNP A0ABF7PQC1
J	-16	HIS	-	expression tag	UNP A0ABF7PQC1
J	-15	HIS	-	expression tag	UNP A0ABF7PQC1
J	-14	HIS	-	expression tag	UNP A0ABF7PQC1
J	-13	HIS	-	expression tag	UNP A0ABF7PQC1
J	-12	HIS	-	expression tag	UNP A0ABF7PQC1
J	-11	HIS	-	expression tag	UNP A0ABF7PQC1
J	-10	GLY	-	expression tag	UNP A0ABF7PQC1
J	-9	GLY	-	expression tag	UNP A0ABF7PQC1
J	-8	SER	-	expression tag	UNP A0ABF7PQC1
J	-7	GLU	-	expression tag	UNP A0ABF7PQC1
J	-6	ASN	-	expression tag	UNP A0ABF7PQC1
J	-5	LEU	-	expression tag	UNP A0ABF7PQC1
J	-4	TYR	-	expression tag	UNP A0ABF7PQC1
J	-3	PHE	-	expression tag	UNP A0ABF7PQC1
J	-2	GLN	-	expression tag	UNP A0ABF7PQC1
J	-1	SER	-	expression tag	UNP A0ABF7PQC1
J	0	GLY	-	expression tag	UNP A0ABF7PQC1

- Molecule 8 is a protein called AAA+ ATPase domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	327	Total	C	N	O	S	0	0
			2658	1704	455	486	13		
8	L	313	Total	C	N	O	S	0	0
			2545	1631	434	467	13		
8	M	311	Total	C	N	O	S	0	0
			2529	1622	432	463	12		
8	N	313	Total	C	N	O	S	0	0
			2547	1635	435	465	12		
8	O	319	Total	C	N	O	S	0	0
			2592	1664	443	473	12		
8	P	314	Total	C	N	O	S	0	0
			2559	1644	436	467	12		
8	Q	319	Total	C	N	O	S	0	0
			2598	1669	445	472	12		

There are 161 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	11	LYS	GLN	conflict	UNP A0A290S0Z4

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Chain	Residue	Modelled	Actual	Comment	Reference
K	27	THR	ALA	conflict	UNP A0A290S0Z4
K	47	CYS	GLY	conflict	UNP A0A290S0Z4
K	84	VAL	ILE	conflict	UNP A0A290S0Z4
K	98	VAL	ILE	conflict	UNP A0A290S0Z4
K	112	ILE	MET	conflict	UNP A0A290S0Z4
K	120	ASP	GLU	conflict	UNP A0A290S0Z4
K	219	ALA	VAL	conflict	UNP A0A290S0Z4
K	221	LYS	GLN	conflict	UNP A0A290S0Z4
K	226	VAL	GLU	conflict	UNP A0A290S0Z4
K	234	ASN	HIS	conflict	UNP A0A290S0Z4
K	237	ILE	MET	conflict	UNP A0A290S0Z4
K	255	LEU	MET	conflict	UNP A0A290S0Z4
K	275	THR	ALA	conflict	UNP A0A290S0Z4
K	276	ALA	VAL	conflict	UNP A0A290S0Z4
K	278	ASP	GLU	conflict	UNP A0A290S0Z4
K	287	GLU	ASP	conflict	UNP A0A290S0Z4
K	288	LYS	SER	conflict	UNP A0A290S0Z4
K	291	SER	LEU	conflict	UNP A0A290S0Z4
K	303	GLU	ILE	conflict	UNP A0A290S0Z4
K	308	ILE	THR	conflict	UNP A0A290S0Z4
K	326	ASP	GLY	conflict	UNP A0A290S0Z4
K	328	VAL	LYS	conflict	UNP A0A290S0Z4
L	11	LYS	GLN	conflict	UNP A0A290S0Z4
L	27	THR	ALA	conflict	UNP A0A290S0Z4
L	47	CYS	GLY	conflict	UNP A0A290S0Z4
L	84	VAL	ILE	conflict	UNP A0A290S0Z4
L	98	VAL	ILE	conflict	UNP A0A290S0Z4
L	112	ILE	MET	conflict	UNP A0A290S0Z4
L	120	ASP	GLU	conflict	UNP A0A290S0Z4
L	219	ALA	VAL	conflict	UNP A0A290S0Z4
L	221	LYS	GLN	conflict	UNP A0A290S0Z4
L	226	VAL	GLU	conflict	UNP A0A290S0Z4
L	234	ASN	HIS	conflict	UNP A0A290S0Z4
L	237	ILE	MET	conflict	UNP A0A290S0Z4
L	255	LEU	MET	conflict	UNP A0A290S0Z4
L	275	THR	ALA	conflict	UNP A0A290S0Z4
L	276	ALA	VAL	conflict	UNP A0A290S0Z4
L	278	ASP	GLU	conflict	UNP A0A290S0Z4
L	287	GLU	ASP	conflict	UNP A0A290S0Z4
L	288	LYS	SER	conflict	UNP A0A290S0Z4
L	291	SER	LEU	conflict	UNP A0A290S0Z4
L	303	GLU	ILE	conflict	UNP A0A290S0Z4

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Chain	Residue	Modelled	Actual	Comment	Reference
L	308	ILE	THR	conflict	UNP A0A290S0Z4
L	326	ASP	GLY	conflict	UNP A0A290S0Z4
L	328	VAL	LYS	conflict	UNP A0A290S0Z4
M	11	LYS	GLN	conflict	UNP A0A290S0Z4
M	27	THR	ALA	conflict	UNP A0A290S0Z4
M	47	CYS	GLY	conflict	UNP A0A290S0Z4
M	84	VAL	ILE	conflict	UNP A0A290S0Z4
M	98	VAL	ILE	conflict	UNP A0A290S0Z4
M	112	ILE	MET	conflict	UNP A0A290S0Z4
M	120	ASP	GLU	conflict	UNP A0A290S0Z4
M	219	ALA	VAL	conflict	UNP A0A290S0Z4
M	221	LYS	GLN	conflict	UNP A0A290S0Z4
M	226	VAL	GLU	conflict	UNP A0A290S0Z4
M	234	ASN	HIS	conflict	UNP A0A290S0Z4
M	237	ILE	MET	conflict	UNP A0A290S0Z4
M	255	LEU	MET	conflict	UNP A0A290S0Z4
M	275	THR	ALA	conflict	UNP A0A290S0Z4
M	276	ALA	VAL	conflict	UNP A0A290S0Z4
M	278	ASP	GLU	conflict	UNP A0A290S0Z4
M	287	GLU	ASP	conflict	UNP A0A290S0Z4
M	288	LYS	SER	conflict	UNP A0A290S0Z4
M	291	SER	LEU	conflict	UNP A0A290S0Z4
M	303	GLU	ILE	conflict	UNP A0A290S0Z4
M	308	ILE	THR	conflict	UNP A0A290S0Z4
M	326	ASP	GLY	conflict	UNP A0A290S0Z4
M	328	VAL	LYS	conflict	UNP A0A290S0Z4
N	11	LYS	GLN	conflict	UNP A0A290S0Z4
N	27	THR	ALA	conflict	UNP A0A290S0Z4
N	47	CYS	GLY	conflict	UNP A0A290S0Z4
N	84	VAL	ILE	conflict	UNP A0A290S0Z4
N	98	VAL	ILE	conflict	UNP A0A290S0Z4
N	112	ILE	MET	conflict	UNP A0A290S0Z4
N	120	ASP	GLU	conflict	UNP A0A290S0Z4
N	219	ALA	VAL	conflict	UNP A0A290S0Z4
N	221	LYS	GLN	conflict	UNP A0A290S0Z4
N	226	VAL	GLU	conflict	UNP A0A290S0Z4
N	234	ASN	HIS	conflict	UNP A0A290S0Z4
N	237	ILE	MET	conflict	UNP A0A290S0Z4
N	255	LEU	MET	conflict	UNP A0A290S0Z4
N	275	THR	ALA	conflict	UNP A0A290S0Z4
N	276	ALA	VAL	conflict	UNP A0A290S0Z4
N	278	ASP	GLU	conflict	UNP A0A290S0Z4

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Chain	Residue	Modelled	Actual	Comment	Reference
N	287	GLU	ASP	conflict	UNP A0A290S0Z4
N	288	LYS	SER	conflict	UNP A0A290S0Z4
N	291	SER	LEU	conflict	UNP A0A290S0Z4
N	303	GLU	ILE	conflict	UNP A0A290S0Z4
N	308	ILE	THR	conflict	UNP A0A290S0Z4
N	326	ASP	GLY	conflict	UNP A0A290S0Z4
N	328	VAL	LYS	conflict	UNP A0A290S0Z4
O	11	LYS	GLN	conflict	UNP A0A290S0Z4
O	27	THR	ALA	conflict	UNP A0A290S0Z4
O	47	CYS	GLY	conflict	UNP A0A290S0Z4
O	84	VAL	ILE	conflict	UNP A0A290S0Z4
O	98	VAL	ILE	conflict	UNP A0A290S0Z4
O	112	ILE	MET	conflict	UNP A0A290S0Z4
O	120	ASP	GLU	conflict	UNP A0A290S0Z4
O	219	ALA	VAL	conflict	UNP A0A290S0Z4
O	221	LYS	GLN	conflict	UNP A0A290S0Z4
O	226	VAL	GLU	conflict	UNP A0A290S0Z4
O	234	ASN	HIS	conflict	UNP A0A290S0Z4
O	237	ILE	MET	conflict	UNP A0A290S0Z4
O	255	LEU	MET	conflict	UNP A0A290S0Z4
O	275	THR	ALA	conflict	UNP A0A290S0Z4
O	276	ALA	VAL	conflict	UNP A0A290S0Z4
O	278	ASP	GLU	conflict	UNP A0A290S0Z4
O	287	GLU	ASP	conflict	UNP A0A290S0Z4
O	288	LYS	SER	conflict	UNP A0A290S0Z4
O	291	SER	LEU	conflict	UNP A0A290S0Z4
O	303	GLU	ILE	conflict	UNP A0A290S0Z4
O	308	ILE	THR	conflict	UNP A0A290S0Z4
O	326	ASP	GLY	conflict	UNP A0A290S0Z4
O	328	VAL	LYS	conflict	UNP A0A290S0Z4
P	11	LYS	GLN	conflict	UNP A0A290S0Z4
P	27	THR	ALA	conflict	UNP A0A290S0Z4
P	47	CYS	GLY	conflict	UNP A0A290S0Z4
P	84	VAL	ILE	conflict	UNP A0A290S0Z4
P	98	VAL	ILE	conflict	UNP A0A290S0Z4
P	112	ILE	MET	conflict	UNP A0A290S0Z4
P	120	ASP	GLU	conflict	UNP A0A290S0Z4
P	219	ALA	VAL	conflict	UNP A0A290S0Z4
P	221	LYS	GLN	conflict	UNP A0A290S0Z4
P	226	VAL	GLU	conflict	UNP A0A290S0Z4
P	234	ASN	HIS	conflict	UNP A0A290S0Z4
P	237	ILE	MET	conflict	UNP A0A290S0Z4

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Chain	Residue	Modelled	Actual	Comment	Reference
P	255	LEU	MET	conflict	UNP A0A290S0Z4
P	275	THR	ALA	conflict	UNP A0A290S0Z4
P	276	ALA	VAL	conflict	UNP A0A290S0Z4
P	278	ASP	GLU	conflict	UNP A0A290S0Z4
P	287	GLU	ASP	conflict	UNP A0A290S0Z4
P	288	LYS	SER	conflict	UNP A0A290S0Z4
P	291	SER	LEU	conflict	UNP A0A290S0Z4
P	303	GLU	ILE	conflict	UNP A0A290S0Z4
P	308	ILE	THR	conflict	UNP A0A290S0Z4
P	326	ASP	GLY	conflict	UNP A0A290S0Z4
P	328	VAL	LYS	conflict	UNP A0A290S0Z4
Q	11	LYS	GLN	conflict	UNP A0A290S0Z4
Q	27	THR	ALA	conflict	UNP A0A290S0Z4
Q	47	CYS	GLY	conflict	UNP A0A290S0Z4
Q	84	VAL	ILE	conflict	UNP A0A290S0Z4
Q	98	VAL	ILE	conflict	UNP A0A290S0Z4
Q	112	ILE	MET	conflict	UNP A0A290S0Z4
Q	120	ASP	GLU	conflict	UNP A0A290S0Z4
Q	219	ALA	VAL	conflict	UNP A0A290S0Z4
Q	221	LYS	GLN	conflict	UNP A0A290S0Z4
Q	226	VAL	GLU	conflict	UNP A0A290S0Z4
Q	234	ASN	HIS	conflict	UNP A0A290S0Z4
Q	237	ILE	MET	conflict	UNP A0A290S0Z4
Q	255	LEU	MET	conflict	UNP A0A290S0Z4
Q	275	THR	ALA	conflict	UNP A0A290S0Z4
Q	276	ALA	VAL	conflict	UNP A0A290S0Z4
Q	278	ASP	GLU	conflict	UNP A0A290S0Z4
Q	287	GLU	ASP	conflict	UNP A0A290S0Z4
Q	288	LYS	SER	conflict	UNP A0A290S0Z4
Q	291	SER	LEU	conflict	UNP A0A290S0Z4
Q	303	GLU	ILE	conflict	UNP A0A290S0Z4
Q	308	ILE	THR	conflict	UNP A0A290S0Z4
Q	326	ASP	GLY	conflict	UNP A0A290S0Z4
Q	328	VAL	LYS	conflict	UNP A0A290S0Z4

- Molecule 9 is a protein called Maltose/maltodextrin-binding periplasmic protein,TnsA endonuclease N-terminal domain-containing protein,TnsB transposase.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	R	9	Total	C	N	O	0	0
			80	51	10	19		
9	S	9	Total	C	N	O	0	0
			80	51	10	19		

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Mol	Chain	Residues	Atoms				AltConf	Trace
9	T	9	Total	C	N	O	0	0
			80	51	10	19		
9	U	9	Total	C	N	O	0	0
			80	51	10	19		
9	V	9	Total	C	N	O	0	0
			80	51	10	19		
9	W	9	Total	C	N	O	0	0
			80	51	10	19		
9	X	9	Total	C	N	O	0	0
			80	51	10	19		

There are 287 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-406	MET	-	initiating methionine	UNP P0AEX9
R	-405	GLY	-	expression tag	UNP P0AEX9
R	-404	SER	-	expression tag	UNP P0AEX9
R	-403	SER	-	expression tag	UNP P0AEX9
R	-402	HIS	-	expression tag	UNP P0AEX9
R	-401	HIS	-	expression tag	UNP P0AEX9
R	-400	HIS	-	expression tag	UNP P0AEX9
R	-399	HIS	-	expression tag	UNP P0AEX9
R	-398	HIS	-	expression tag	UNP P0AEX9
R	-397	HIS	-	expression tag	UNP P0AEX9
R	-396	GLY	-	expression tag	UNP P0AEX9
R	-395	SER	-	expression tag	UNP P0AEX9
R	-394	SER	-	expression tag	UNP P0AEX9
R	-393	MET	-	expression tag	UNP P0AEX9
R	-26	ASN	-	linker	UNP P0AEX9
R	-25	SER	-	linker	UNP P0AEX9
R	-24	SER	-	linker	UNP P0AEX9
R	-23	SER	-	linker	UNP P0AEX9
R	-22	ASN	-	linker	UNP P0AEX9
R	-21	ASN	-	linker	UNP P0AEX9
R	-20	ASN	-	linker	UNP P0AEX9
R	-19	ASN	-	linker	UNP P0AEX9
R	-18	ASN	-	linker	UNP P0AEX9
R	-17	ASN	-	linker	UNP P0AEX9
R	-16	ASN	-	linker	UNP P0AEX9
R	-15	ASN	-	linker	UNP P0AEX9
R	-14	ASN	-	linker	UNP P0AEX9
R	-13	ASN	-	linker	UNP P0AEX9
R	-12	LEU	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-11	GLY	-	linker	UNP P0AEX9
R	-10	ILE	-	linker	UNP P0AEX9
R	-9	GLU	-	linker	UNP P0AEX9
R	-8	GLU	-	linker	UNP P0AEX9
R	-7	ASN	-	linker	UNP P0AEX9
R	-6	LEU	-	linker	UNP P0AEX9
R	-5	TYR	-	linker	UNP P0AEX9
R	-4	PHE	-	linker	UNP P0AEX9
R	-3	GLN	-	linker	UNP P0AEX9
R	-2	SER	-	linker	UNP P0AEX9
R	-1	ASN	-	linker	UNP P0AEX9
R	0	ALA	-	linker	UNP P0AEX9
S	-406	MET	-	initiating methionine	UNP P0AEX9
S	-405	GLY	-	expression tag	UNP P0AEX9
S	-404	SER	-	expression tag	UNP P0AEX9
S	-403	SER	-	expression tag	UNP P0AEX9
S	-402	HIS	-	expression tag	UNP P0AEX9
S	-401	HIS	-	expression tag	UNP P0AEX9
S	-400	HIS	-	expression tag	UNP P0AEX9
S	-399	HIS	-	expression tag	UNP P0AEX9
S	-398	HIS	-	expression tag	UNP P0AEX9
S	-397	HIS	-	expression tag	UNP P0AEX9
S	-396	GLY	-	expression tag	UNP P0AEX9
S	-395	SER	-	expression tag	UNP P0AEX9
S	-394	SER	-	expression tag	UNP P0AEX9
S	-393	MET	-	expression tag	UNP P0AEX9
S	-26	ASN	-	linker	UNP P0AEX9
S	-25	SER	-	linker	UNP P0AEX9
S	-24	SER	-	linker	UNP P0AEX9
S	-23	SER	-	linker	UNP P0AEX9
S	-22	ASN	-	linker	UNP P0AEX9
S	-21	ASN	-	linker	UNP P0AEX9
S	-20	ASN	-	linker	UNP P0AEX9
S	-19	ASN	-	linker	UNP P0AEX9
S	-18	ASN	-	linker	UNP P0AEX9
S	-17	ASN	-	linker	UNP P0AEX9
S	-16	ASN	-	linker	UNP P0AEX9
S	-15	ASN	-	linker	UNP P0AEX9
S	-14	ASN	-	linker	UNP P0AEX9
S	-13	ASN	-	linker	UNP P0AEX9
S	-12	LEU	-	linker	UNP P0AEX9
S	-11	GLY	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
S	-10	ILE	-	linker	UNP P0AEX9
S	-9	GLU	-	linker	UNP P0AEX9
S	-8	GLU	-	linker	UNP P0AEX9
S	-7	ASN	-	linker	UNP P0AEX9
S	-6	LEU	-	linker	UNP P0AEX9
S	-5	TYR	-	linker	UNP P0AEX9
S	-4	PHE	-	linker	UNP P0AEX9
S	-3	GLN	-	linker	UNP P0AEX9
S	-2	SER	-	linker	UNP P0AEX9
S	-1	ASN	-	linker	UNP P0AEX9
S	0	ALA	-	linker	UNP P0AEX9
T	-406	MET	-	initiating methionine	UNP P0AEX9
T	-405	GLY	-	expression tag	UNP P0AEX9
T	-404	SER	-	expression tag	UNP P0AEX9
T	-403	SER	-	expression tag	UNP P0AEX9
T	-402	HIS	-	expression tag	UNP P0AEX9
T	-401	HIS	-	expression tag	UNP P0AEX9
T	-400	HIS	-	expression tag	UNP P0AEX9
T	-399	HIS	-	expression tag	UNP P0AEX9
T	-398	HIS	-	expression tag	UNP P0AEX9
T	-397	HIS	-	expression tag	UNP P0AEX9
T	-396	GLY	-	expression tag	UNP P0AEX9
T	-395	SER	-	expression tag	UNP P0AEX9
T	-394	SER	-	expression tag	UNP P0AEX9
T	-393	MET	-	expression tag	UNP P0AEX9
T	-26	ASN	-	linker	UNP P0AEX9
T	-25	SER	-	linker	UNP P0AEX9
T	-24	SER	-	linker	UNP P0AEX9
T	-23	SER	-	linker	UNP P0AEX9
T	-22	ASN	-	linker	UNP P0AEX9
T	-21	ASN	-	linker	UNP P0AEX9
T	-20	ASN	-	linker	UNP P0AEX9
T	-19	ASN	-	linker	UNP P0AEX9
T	-18	ASN	-	linker	UNP P0AEX9
T	-17	ASN	-	linker	UNP P0AEX9
T	-16	ASN	-	linker	UNP P0AEX9
T	-15	ASN	-	linker	UNP P0AEX9
T	-14	ASN	-	linker	UNP P0AEX9
T	-13	ASN	-	linker	UNP P0AEX9
T	-12	LEU	-	linker	UNP P0AEX9
T	-11	GLY	-	linker	UNP P0AEX9
T	-10	ILE	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-9	GLU	-	linker	UNP P0AEX9
T	-8	GLU	-	linker	UNP P0AEX9
T	-7	ASN	-	linker	UNP P0AEX9
T	-6	LEU	-	linker	UNP P0AEX9
T	-5	TYR	-	linker	UNP P0AEX9
T	-4	PHE	-	linker	UNP P0AEX9
T	-3	GLN	-	linker	UNP P0AEX9
T	-2	SER	-	linker	UNP P0AEX9
T	-1	ASN	-	linker	UNP P0AEX9
T	0	ALA	-	linker	UNP P0AEX9
U	-406	MET	-	initiating methionine	UNP P0AEX9
U	-405	GLY	-	expression tag	UNP P0AEX9
U	-404	SER	-	expression tag	UNP P0AEX9
U	-403	SER	-	expression tag	UNP P0AEX9
U	-402	HIS	-	expression tag	UNP P0AEX9
U	-401	HIS	-	expression tag	UNP P0AEX9
U	-400	HIS	-	expression tag	UNP P0AEX9
U	-399	HIS	-	expression tag	UNP P0AEX9
U	-398	HIS	-	expression tag	UNP P0AEX9
U	-397	HIS	-	expression tag	UNP P0AEX9
U	-396	GLY	-	expression tag	UNP P0AEX9
U	-395	SER	-	expression tag	UNP P0AEX9
U	-394	SER	-	expression tag	UNP P0AEX9
U	-393	MET	-	expression tag	UNP P0AEX9
U	-26	ASN	-	linker	UNP P0AEX9
U	-25	SER	-	linker	UNP P0AEX9
U	-24	SER	-	linker	UNP P0AEX9
U	-23	SER	-	linker	UNP P0AEX9
U	-22	ASN	-	linker	UNP P0AEX9
U	-21	ASN	-	linker	UNP P0AEX9
U	-20	ASN	-	linker	UNP P0AEX9
U	-19	ASN	-	linker	UNP P0AEX9
U	-18	ASN	-	linker	UNP P0AEX9
U	-17	ASN	-	linker	UNP P0AEX9
U	-16	ASN	-	linker	UNP P0AEX9
U	-15	ASN	-	linker	UNP P0AEX9
U	-14	ASN	-	linker	UNP P0AEX9
U	-13	ASN	-	linker	UNP P0AEX9
U	-12	LEU	-	linker	UNP P0AEX9
U	-11	GLY	-	linker	UNP P0AEX9
U	-10	ILE	-	linker	UNP P0AEX9
U	-9	GLU	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
U	-8	GLU	-	linker	UNP P0AEX9
U	-7	ASN	-	linker	UNP P0AEX9
U	-6	LEU	-	linker	UNP P0AEX9
U	-5	TYR	-	linker	UNP P0AEX9
U	-4	PHE	-	linker	UNP P0AEX9
U	-3	GLN	-	linker	UNP P0AEX9
U	-2	SER	-	linker	UNP P0AEX9
U	-1	ASN	-	linker	UNP P0AEX9
U	0	ALA	-	linker	UNP P0AEX9
V	-406	MET	-	initiating methionine	UNP P0AEX9
V	-405	GLY	-	expression tag	UNP P0AEX9
V	-404	SER	-	expression tag	UNP P0AEX9
V	-403	SER	-	expression tag	UNP P0AEX9
V	-402	HIS	-	expression tag	UNP P0AEX9
V	-401	HIS	-	expression tag	UNP P0AEX9
V	-400	HIS	-	expression tag	UNP P0AEX9
V	-399	HIS	-	expression tag	UNP P0AEX9
V	-398	HIS	-	expression tag	UNP P0AEX9
V	-397	HIS	-	expression tag	UNP P0AEX9
V	-396	GLY	-	expression tag	UNP P0AEX9
V	-395	SER	-	expression tag	UNP P0AEX9
V	-394	SER	-	expression tag	UNP P0AEX9
V	-393	MET	-	expression tag	UNP P0AEX9
V	-26	ASN	-	linker	UNP P0AEX9
V	-25	SER	-	linker	UNP P0AEX9
V	-24	SER	-	linker	UNP P0AEX9
V	-23	SER	-	linker	UNP P0AEX9
V	-22	ASN	-	linker	UNP P0AEX9
V	-21	ASN	-	linker	UNP P0AEX9
V	-20	ASN	-	linker	UNP P0AEX9
V	-19	ASN	-	linker	UNP P0AEX9
V	-18	ASN	-	linker	UNP P0AEX9
V	-17	ASN	-	linker	UNP P0AEX9
V	-16	ASN	-	linker	UNP P0AEX9
V	-15	ASN	-	linker	UNP P0AEX9
V	-14	ASN	-	linker	UNP P0AEX9
V	-13	ASN	-	linker	UNP P0AEX9
V	-12	LEU	-	linker	UNP P0AEX9
V	-11	GLY	-	linker	UNP P0AEX9
V	-10	ILE	-	linker	UNP P0AEX9
V	-9	GLU	-	linker	UNP P0AEX9
V	-8	GLU	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
V	-7	ASN	-	linker	UNP P0AEX9
V	-6	LEU	-	linker	UNP P0AEX9
V	-5	TYR	-	linker	UNP P0AEX9
V	-4	PHE	-	linker	UNP P0AEX9
V	-3	GLN	-	linker	UNP P0AEX9
V	-2	SER	-	linker	UNP P0AEX9
V	-1	ASN	-	linker	UNP P0AEX9
V	0	ALA	-	linker	UNP P0AEX9
W	-406	MET	-	initiating methionine	UNP P0AEX9
W	-405	GLY	-	expression tag	UNP P0AEX9
W	-404	SER	-	expression tag	UNP P0AEX9
W	-403	SER	-	expression tag	UNP P0AEX9
W	-402	HIS	-	expression tag	UNP P0AEX9
W	-401	HIS	-	expression tag	UNP P0AEX9
W	-400	HIS	-	expression tag	UNP P0AEX9
W	-399	HIS	-	expression tag	UNP P0AEX9
W	-398	HIS	-	expression tag	UNP P0AEX9
W	-397	HIS	-	expression tag	UNP P0AEX9
W	-396	GLY	-	expression tag	UNP P0AEX9
W	-395	SER	-	expression tag	UNP P0AEX9
W	-394	SER	-	expression tag	UNP P0AEX9
W	-393	MET	-	expression tag	UNP P0AEX9
W	-26	ASN	-	linker	UNP P0AEX9
W	-25	SER	-	linker	UNP P0AEX9
W	-24	SER	-	linker	UNP P0AEX9
W	-23	SER	-	linker	UNP P0AEX9
W	-22	ASN	-	linker	UNP P0AEX9
W	-21	ASN	-	linker	UNP P0AEX9
W	-20	ASN	-	linker	UNP P0AEX9
W	-19	ASN	-	linker	UNP P0AEX9
W	-18	ASN	-	linker	UNP P0AEX9
W	-17	ASN	-	linker	UNP P0AEX9
W	-16	ASN	-	linker	UNP P0AEX9
W	-15	ASN	-	linker	UNP P0AEX9
W	-14	ASN	-	linker	UNP P0AEX9
W	-13	ASN	-	linker	UNP P0AEX9
W	-12	LEU	-	linker	UNP P0AEX9
W	-11	GLY	-	linker	UNP P0AEX9
W	-10	ILE	-	linker	UNP P0AEX9
W	-9	GLU	-	linker	UNP P0AEX9
W	-8	GLU	-	linker	UNP P0AEX9
W	-7	ASN	-	linker	UNP P0AEX9

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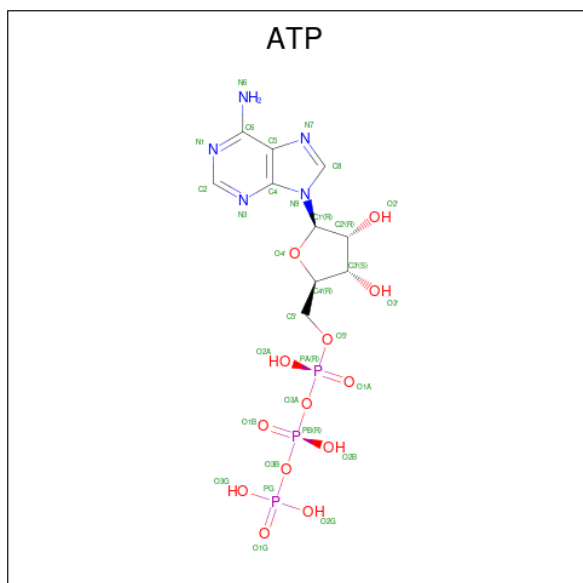
Chain	Residue	Modelled	Actual	Comment	Reference
W	-6	LEU	-	linker	UNP P0AEX9
W	-5	TYR	-	linker	UNP P0AEX9
W	-4	PHE	-	linker	UNP P0AEX9
W	-3	GLN	-	linker	UNP P0AEX9
W	-2	SER	-	linker	UNP P0AEX9
W	-1	ASN	-	linker	UNP P0AEX9
W	0	ALA	-	linker	UNP P0AEX9
X	-406	MET	-	initiating methionine	UNP P0AEX9
X	-405	GLY	-	expression tag	UNP P0AEX9
X	-404	SER	-	expression tag	UNP P0AEX9
X	-403	SER	-	expression tag	UNP P0AEX9
X	-402	HIS	-	expression tag	UNP P0AEX9
X	-401	HIS	-	expression tag	UNP P0AEX9
X	-400	HIS	-	expression tag	UNP P0AEX9
X	-399	HIS	-	expression tag	UNP P0AEX9
X	-398	HIS	-	expression tag	UNP P0AEX9
X	-397	HIS	-	expression tag	UNP P0AEX9
X	-396	GLY	-	expression tag	UNP P0AEX9
X	-395	SER	-	expression tag	UNP P0AEX9
X	-394	SER	-	expression tag	UNP P0AEX9
X	-393	MET	-	expression tag	UNP P0AEX9
X	-26	ASN	-	linker	UNP P0AEX9
X	-25	SER	-	linker	UNP P0AEX9
X	-24	SER	-	linker	UNP P0AEX9
X	-23	SER	-	linker	UNP P0AEX9
X	-22	ASN	-	linker	UNP P0AEX9
X	-21	ASN	-	linker	UNP P0AEX9
X	-20	ASN	-	linker	UNP P0AEX9
X	-19	ASN	-	linker	UNP P0AEX9
X	-18	ASN	-	linker	UNP P0AEX9
X	-17	ASN	-	linker	UNP P0AEX9
X	-16	ASN	-	linker	UNP P0AEX9
X	-15	ASN	-	linker	UNP P0AEX9
X	-14	ASN	-	linker	UNP P0AEX9
X	-13	ASN	-	linker	UNP P0AEX9
X	-12	LEU	-	linker	UNP P0AEX9
X	-11	GLY	-	linker	UNP P0AEX9
X	-10	ILE	-	linker	UNP P0AEX9
X	-9	GLU	-	linker	UNP P0AEX9
X	-8	GLU	-	linker	UNP P0AEX9
X	-7	ASN	-	linker	UNP P0AEX9
X	-6	LEU	-	linker	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-5	TYR	-	linker	UNP P0AEX9
X	-4	PHE	-	linker	UNP P0AEX9
X	-3	GLN	-	linker	UNP P0AEX9
X	-2	SER	-	linker	UNP P0AEX9
X	-1	ASN	-	linker	UNP P0AEX9
X	0	ALA	-	linker	UNP P0AEX9

- Molecule 10 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).

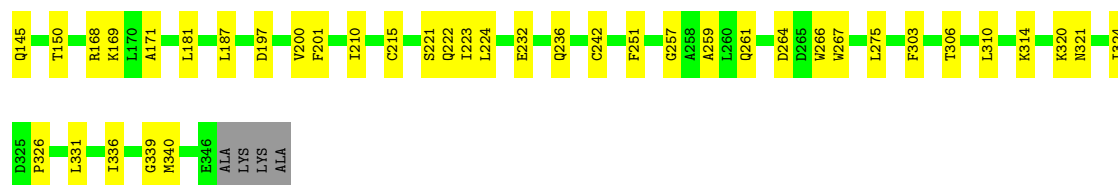


Mol	Chain	Residues	Atoms					AltConf
10	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	M	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	N	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	O	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	P	1	Total	C	N	O	P	0
			31	10	5	13	3	
10	Q	1	Total	C	N	O	P	0
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

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of

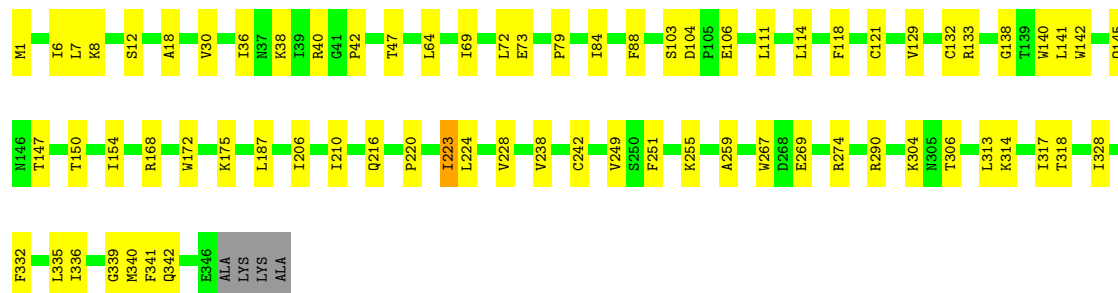
Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	K	1	Total 1	Mg 1	0
11	L	1	Total 1	Mg 1	0
11	M	1	Total 1	Mg 1	0
11	N	1	Total 1	Mg 1	0
11	O	1	Total 1	Mg 1	0
11	P	1	Total 1	Mg 1	0
11	Q	1	Total 1	Mg 1	0



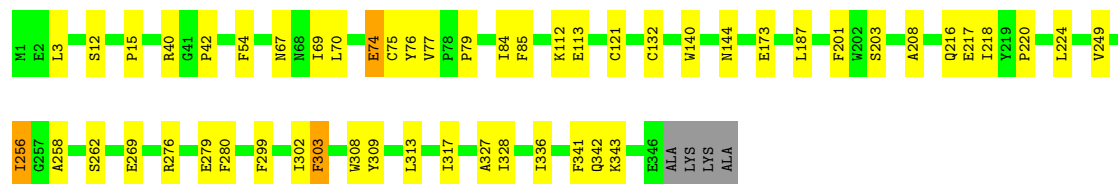
• Molecule 4: Cas7.1

Chain B: 78% 20%



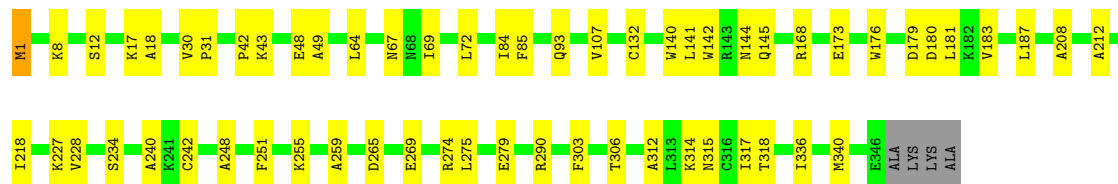
• Molecule 4: Cas7.1

Chain C: 84% 14%



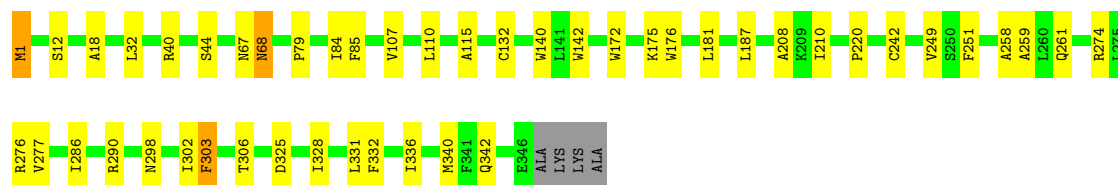
• Molecule 4: Cas7.1

Chain D: 82% 17%




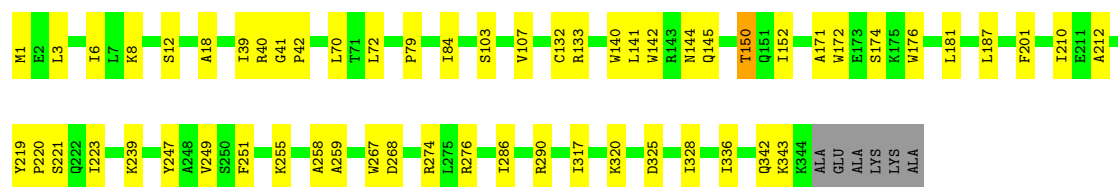
• Molecule 4: Cas7.1

Chain E: 85% 13%




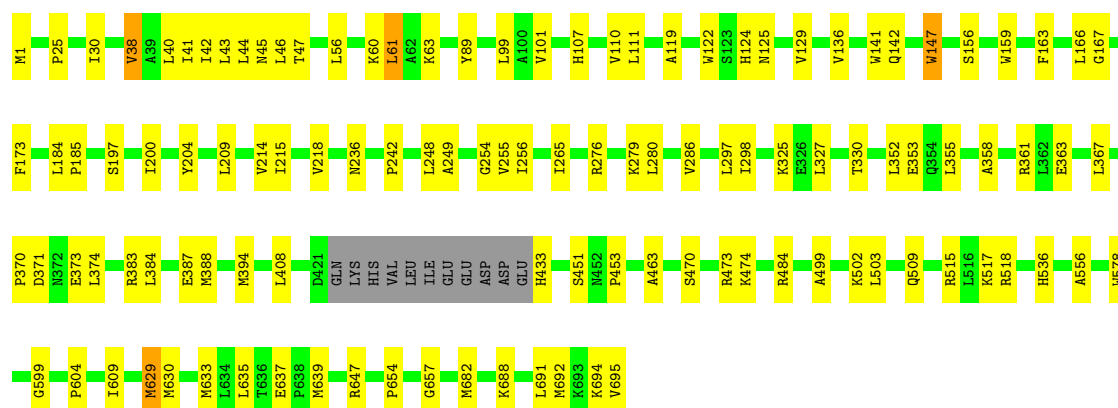
• Molecule 4: Cas7.1

Chain F:  82% 16%



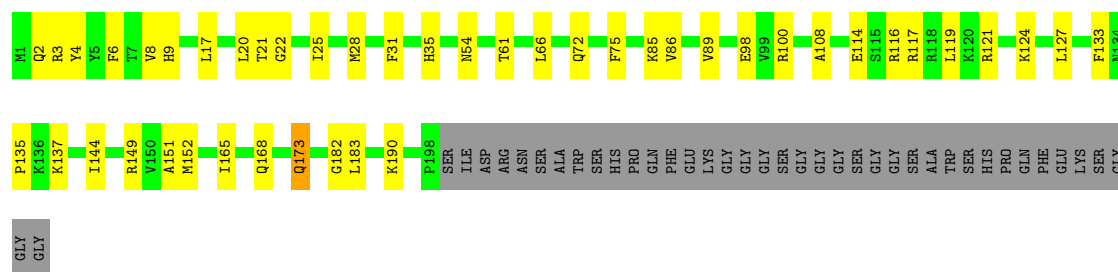
• Molecule 5: Cas8

Chain G:  82% 16%



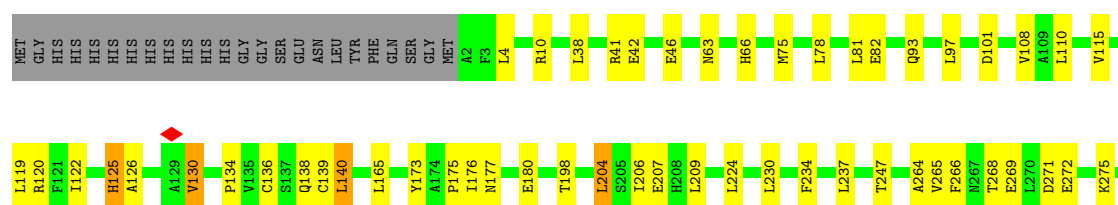
• Molecule 6: Cas6

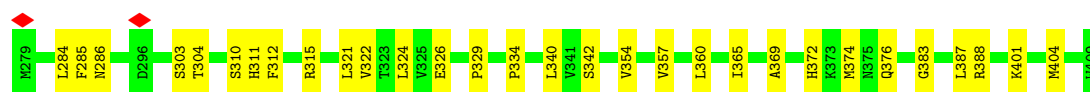
Chain H:  65% 19% 16%



• Molecule 7: TniQ.1

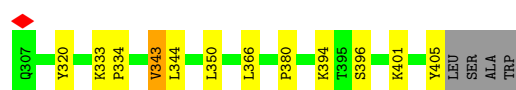
Chain I:  75% 18% 6%





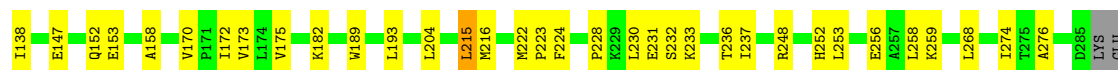
• Molecule 7: ThiQ.1

Chain J: 79% 13% 6%



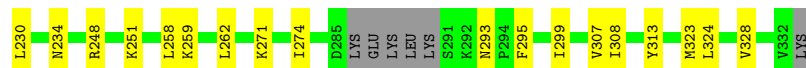
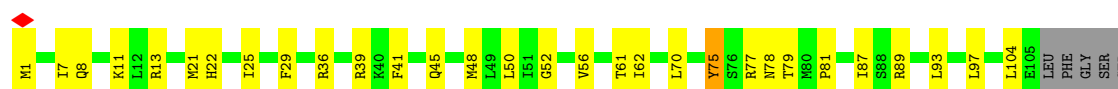
• Molecule 8: AAA+ ATPase domain-containing protein

Chain K: 77% 21% ..



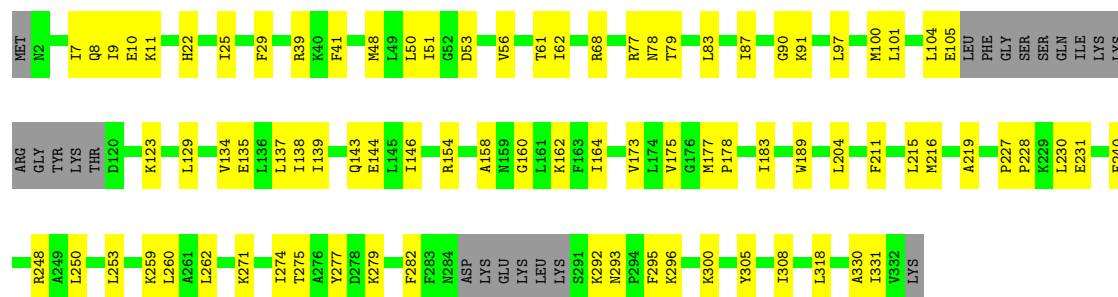
• Molecule 8: AAA+ ATPase domain-containing protein

Chain L: 71% 22% 6%



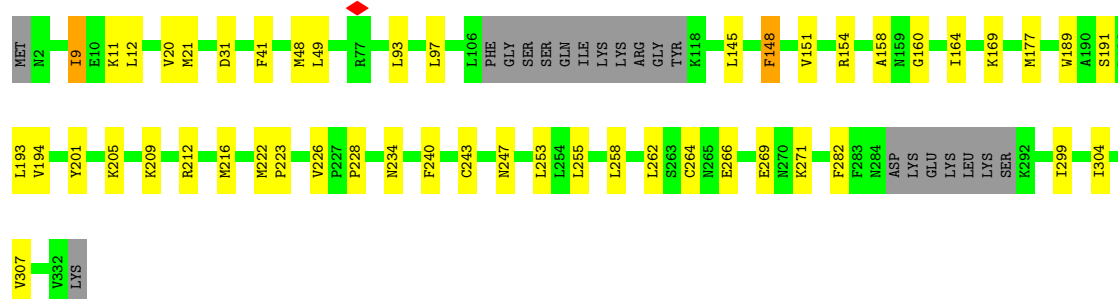
• Molecule 8: AAA+ ATPase domain-containing protein

Chain M: 68% 25% 7%



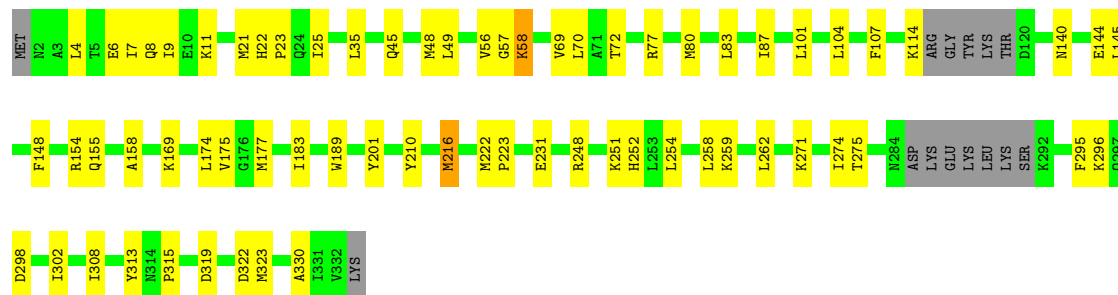
• Molecule 8: AAA+ ATPase domain-containing protein

Chain N: 79% 14% 6%



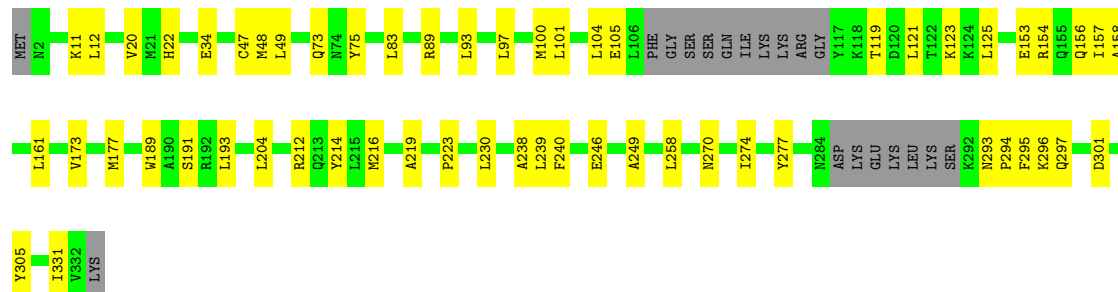
• Molecule 8: AAA+ ATPase domain-containing protein

Chain O: 75% 20% 5%




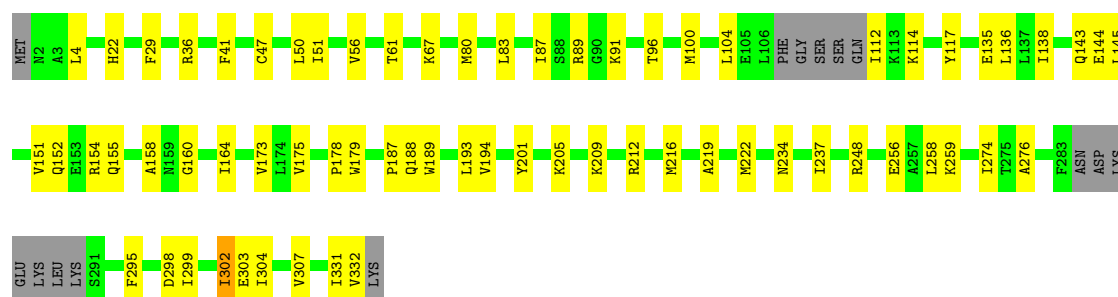
• Molecule 8: AAA+ ATPase domain-containing protein

Chain P: 77% 17% 6%



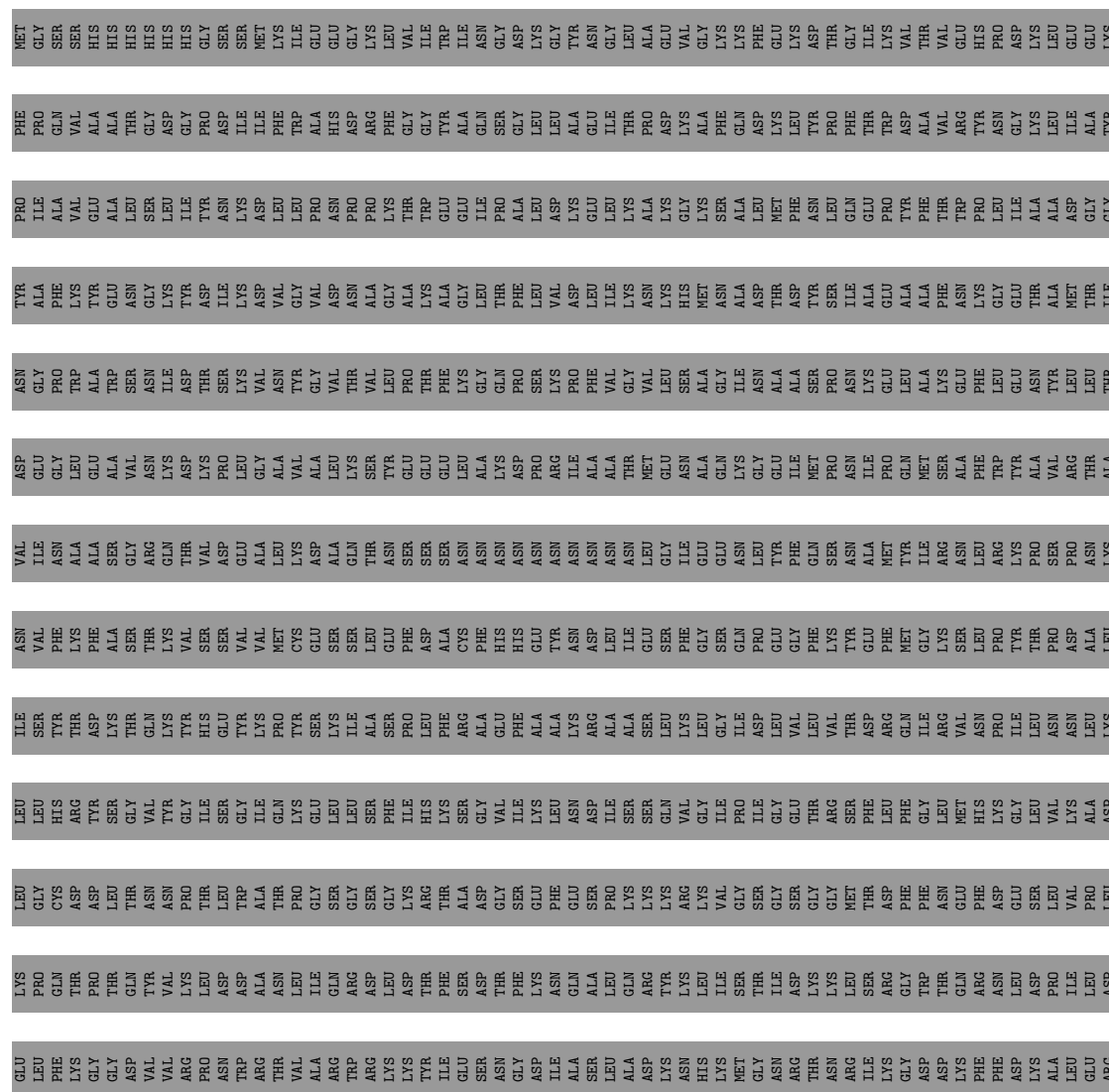
• Molecule 8: AAA+ ATPase domain-containing protein

Chain Q:  75% 20%



• Molecule 9: Maltose/maltodextrin-binding periplasmic protein,TnsA endonuclease N-terminal domain-containing protein,TnsB transposase

Chain R:  99%





- Molecule 9: Maltose/maltodextrin-binding periplasmic protein,TnsA endonuclease N-terminal domain-containing protein,TnsB transposase

99%

NET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	GLY	SER	SER	NET	LYS	LEU	GLU	GLU	GLY	LYS	LEU	VAL	TRP	ILE	ILE	ASN	GLY	GLY	ASP	LYS	GLY	TYR	ASN	GLY	LEU	ALA	GLU	VAL	GLY	LYS	LYS	PHE	GLY	LYS	ASP	THR	GLY	ILE	LYS	VAL	THR	VAL	GLU	HIS	PRO	ASP	LYS	LEU	GLU	GLY	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----



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WORLDWIDE
PDB
PROTEIN DATA BANK

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	138834	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60.95	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	38.365	Depositor
Minimum map value	-12.636	Depositor
Average map value	0.004	Depositor
Map value standard deviation	1.080	Depositor
Recommended contour level	4.3	Depositor
Map size (Å)	390.0, 390.0, 390.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.65, 0.65, 0.65	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.17	0/1447	0.40	0/2258
2	2	0.19	0/1587	0.48	0/2448
3	3	0.19	0/983	0.55	0/1509
4	A	0.14	0/2637	0.31	0/3565
4	B	0.17	0/2842	0.32	0/3846
4	C	0.14	0/2842	0.29	0/3846
4	D	0.15	0/2842	0.30	0/3846
4	E	0.13	0/2842	0.27	0/3846
4	F	0.21	0/2828	0.31	0/3827
5	G	0.13	0/5617	0.28	0/7609
6	H	0.15	0/1634	0.32	0/2201
7	I	0.14	0/3392	0.36	0/4595
7	J	0.13	0/3349	0.30	0/4534
8	K	0.13	0/2704	0.30	0/3635
8	L	0.13	0/2588	0.33	0/3481
8	M	0.14	0/2572	0.34	0/3460
8	N	0.13	0/2590	0.30	0/3484
8	O	0.20	0/2636	0.34	0/3543
8	P	0.14	0/2603	0.32	0/3502
8	Q	0.13	0/2642	0.28	0/3551
9	R	0.11	0/82	0.37	0/111
9	S	0.10	0/82	0.27	0/111
9	T	0.22	0/82	0.61	0/111
9	U	0.13	0/82	0.27	0/111
9	V	0.09	0/82	0.31	0/111
9	W	0.11	0/82	0.37	0/111
9	X	0.19	0/82	0.52	0/111
All	All	0.15	0/53751	0.33	0/73363

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1291	0	648	32	0
2	2	1416	0	777	51	0
3	3	881	0	494	16	0
4	A	2580	0	2544	43	0
4	B	2777	0	2730	52	0
4	C	2777	0	2730	36	0
4	D	2777	0	2730	44	0
4	E	2777	0	2730	33	0
4	F	2763	0	2719	38	0
5	G	5489	0	5543	75	0
6	H	1599	0	1588	33	0
7	I	3311	0	3241	42	0
7	J	3271	0	3212	33	0
8	K	2658	0	2734	43	0
8	L	2545	0	2610	53	0
8	M	2529	0	2594	55	0
8	N	2547	0	2619	38	0
8	O	2592	0	2663	48	0
8	P	2559	0	2628	40	0
8	Q	2598	0	2681	49	0
9	R	80	0	58	0	0
9	S	80	0	58	0	0
9	T	80	0	58	1	0
9	U	80	0	58	4	0
9	V	80	0	58	0	0
9	W	80	0	58	2	0
9	X	80	0	58	3	0
10	K	31	0	12	1	0
10	L	31	0	12	2	0
10	M	31	0	12	1	0
10	N	31	0	12	1	0
10	O	31	0	12	2	0
10	P	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	Q	31	0	12	1	0
11	K	1	0	0	0	0
11	L	1	0	0	0	0
11	M	1	0	0	0	0
11	N	1	0	0	0	0
11	O	1	0	0	0	0
11	P	1	0	0	0	0
11	Q	1	0	0	0	0
All	All	52521	0	50705	759	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (759) 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)
8:L:77:ARG:HD2	8:L:78:ASN:H	1.29	0.94
4:D:43:LYS:HB3	4:D:48:GLU:HG2	1.57	0.84
4:C:40:ARG:HG3	4:C:67:ASN:HD22	1.42	0.82
8:O:216:MET:HE1	8:O:231:GLU:HB3	1.63	0.80
5:G:695:VAL:HG11	8:O:77:ARG:HE	1.49	0.78
4:C:309:TYR:HB3	4:C:328:ILE:HD11	1.68	0.75
4:D:31:PRO:HB3	4:D:248:ALA:HB2	1.70	0.74
7:J:162:GLN:HG2	7:J:206:ILE:HG13	1.71	0.72
8:M:41:PHE:HE1	8:N:9:ILE:HD13	1.54	0.71
8:O:274:ILE:HD12	8:O:296:LYS:HG3	1.72	0.71
4:E:258:ALA:HA	4:E:276:ARG:HE	1.58	0.69
4:D:84:ILE:HD13	4:D:218:ILE:HD11	1.75	0.69
4:D:242:CYS:HA	4:E:79:PRO:HD2	1.75	0.69
8:L:158:ALA:HB1	8:L:189:TRP:HE1	1.57	0.69
4:D:1:MET:HE3	4:D:306:THR:HG21	1.74	0.68
8:N:31:ASP:HB3	8:N:48:MET:HE1	1.75	0.68
1:1:3:A:H1'	4:F:8:LYS:HD2	1.75	0.68
4:F:286:ILE:HG13	4:F:290:ARG:HH21	1.59	0.68
8:O:21:MET:HA	8:O:21:MET:HE3	1.75	0.67
7:I:134:PRO:HB2	7:I:165:LEU:HB3	1.75	0.67
4:E:286:ILE:HG13	4:E:290:ARG:HH21	1.58	0.66
3:3:49:DT:H2'	3:3:50:DA:C8	2.31	0.66
4:E:12:SER:HB2	4:E:336:ILE:HG23	1.78	0.66
5:G:384:LEU:HG	5:G:388:MET:HE3	1.76	0.66
8:L:213:GLN:HA	8:L:216:MET:HG3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:11:LYS:HB3	8:K:223:PRO:HB3	1.77	0.65
2:2:-46:DG:H1	3:3:46:DC:H5	1.45	0.65
7:I:404:MET:HE1	7:J:100:SER:HA	1.79	0.65
2:2:2:DC:H4'	5:G:125:ASN:HB2	1.78	0.65
8:L:248:ARG:HB2	10:L:402:ATP:H5'2	1.78	0.64
3:3:38:DA:H2'	3:3:39:DG:C8	2.32	0.64
4:F:18:ALA:HB3	4:F:251:PHE:HB2	1.80	0.64
4:D:18:ALA:HB3	4:D:251:PHE:HB2	1.78	0.64
5:G:204:TYR:HB2	5:G:209:LEU:HD22	1.79	0.64
5:G:630:MET:HG2	5:G:657:GLY:HA3	1.80	0.64
1:1:-5:G:H4'	1:1:-4:A:H5'	1.79	0.64
5:G:107:HIS:HB3	5:G:110:VAL:HG22	1.79	0.64
8:Q:212:ARG:O	8:Q:216:MET:HG3	1.98	0.63
8:M:158:ALA:HB1	8:M:189:TRP:HE1	1.63	0.63
7:I:108:VAL:HB	7:I:119:LEU:HD12	1.79	0.63
8:L:234:ASN:HA	8:L:299:ILE:HD11	1.80	0.63
8:M:160:GLY:O	8:M:164:ILE:HG12	1.99	0.63
8:Q:248:ARG:HB2	10:Q:401:ATP:H5'2	1.81	0.63
4:B:36:ILE:HG12	4:B:73:GLU:HG3	1.81	0.63
8:N:12:LEU:HD21	8:N:258:LEU:HB3	1.81	0.62
8:P:48:MET:HB3	8:P:173:VAL:HG22	1.80	0.62
1:1:23:G:H1'	4:C:42:PRO:HD2	1.82	0.62
1:1:17:G:H1'	4:D:42:PRO:HD2	1.81	0.62
1:1:7:G:H5''	4:F:40:ARG:HG3	1.80	0.62
4:E:1:MET:HE3	4:E:107:VAL:HG13	1.81	0.62
4:C:121:CYS:HB3	4:C:317:ILE:HG22	1.81	0.61
5:G:25:PRO:HB2	5:G:248:LEU:HD13	1.82	0.61
5:G:101:VAL:HG21	5:G:635:LEU:HB3	1.82	0.61
8:Q:158:ALA:HB1	8:Q:189:TRP:HE1	1.65	0.61
4:E:40:ARG:HD3	4:E:67:ASN:HD21	1.64	0.61
5:G:41:ILE:HG22	5:G:166:LEU:HD21	1.81	0.61
8:O:148:PHE:HE1	8:O:323:MET:HE2	1.64	0.61
8:N:240:PHE:HD2	8:N:304:ILE:HD11	1.66	0.61
7:J:223:PRO:HG3	7:J:262:TRP:HB3	1.83	0.61
8:Q:80:MET:HE3	8:Q:104:LEU:HD12	1.83	0.61
8:L:77:ARG:HH11	8:L:78:ASN:HA	1.66	0.61
8:K:129:LEU:HD22	8:K:134:VAL:HG11	1.82	0.60
1:1:42:C:H5	6:H:121:ARG:HH12	1.49	0.60
8:O:158:ALA:HB1	8:O:189:TRP:HE1	1.66	0.60
4:A:320:LYS:HA	4:A:320:LYS:HE3	1.83	0.60
8:N:212:ARG:O	8:N:216:MET:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:12:A:HB3'	4:E:40:ARG:HB2	1.84	0.59
2:2:-11:DG:H22	4:E:44:SER:H	1.49	0.59
8:M:248:ARG:HB2	10:M:401:ATP:H5'2	1.84	0.59
8:O:223:PRO:HD2	8:O:258:LEU:HD21	1.84	0.59
4:A:266:TRP:HB3	4:A:326:PRO:HB3	1.85	0.59
7:I:312:PHE:HA	7:I:315:ARG:HD2	1.85	0.59
6:H:9:HIS:HB3	6:H:85:LYS:HB3	1.85	0.59
6:H:151:ALA:O	6:H:152:MET:HE2	2.03	0.59
4:B:142:TRP:CZ2	4:B:259:ALA:HB2	2.37	0.58
8:Q:222:MET:SD	8:Q:258:LEU:HD11	2.43	0.58
8:L:62:ILE:HD12	8:L:138:ILE:HG21	1.85	0.58
4:F:325:ASP:HB3	4:F:328:ILE:HD12	1.84	0.58
8:P:270:ASN:O	8:P:274:ILE:HD12	2.03	0.58
1:1:30:G:H3'	4:B:40:ARG:HB2	1.84	0.58
4:B:147:THR:HG21	4:B:216:GLN:HE22	1.69	0.58
7:J:105:ASN:HD21	7:J:300:ALA:HA	1.68	0.58
8:Q:4:LEU:HD11	8:Q:259:LYS:HG3	1.86	0.58
2:2:-3:DT:H5''	4:E:342:GLN:HE21	1.66	0.58
4:A:18:ALA:HB3	4:A:251:PHE:HB2	1.86	0.58
8:L:77:ARG:HD2	8:L:78:ASN:N	2.11	0.58
8:Q:219:ALA:HA	8:Q:222:MET:HG3	1.85	0.58
8:N:151:VAL:HA	8:N:154:ARG:HG3	1.85	0.58
4:F:12:SER:HB2	4:F:336:ILE:HG23	1.85	0.58
4:B:114:LEU:HG	4:B:332:PHE:HZ	1.69	0.58
1:1:29:U:H1'	4:B:42:PRO:HD2	1.85	0.57
8:L:153:GLU:O	8:L:157:ILE:HG12	2.04	0.57
8:M:7:ILE:HG13	8:M:11:LYS:HZ2	1.67	0.57
5:G:42:ILE:HG23	5:G:56:LEU:HD12	1.86	0.57
5:G:184:LEU:HD12	5:G:185:PRO:HD2	1.86	0.57
1:1:5:U:H1'	4:F:42:PRO:HD2	1.87	0.57
5:G:124:HIS:CG	5:G:125:ASN:H	2.23	0.57
8:Q:83:LEU:HD22	8:Q:104:LEU:HD13	1.87	0.57
4:B:150:THR:HG22	4:B:210:ILE:HG23	1.87	0.57
8:Q:274:ILE:HG12	8:Q:295:PHE:HB2	1.87	0.57
4:B:114:LEU:HD22	4:B:306:THR:HG23	1.86	0.56
5:G:1:MET:HE3	5:G:1:MET:N	2.20	0.56
8:P:158:ALA:HB1	8:P:189:TRP:HE1	1.69	0.56
5:G:119:ALA:HB3	5:G:218:VAL:HG22	1.87	0.56
8:M:177:MET:HE3	8:M:178:PRO:HD2	1.87	0.56
2:2:-15:DT:H5'	4:C:342:GLN:HE21	1.69	0.56
4:E:40:ARG:HD3	4:E:67:ASN:ND2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:87:ILE:HD11	8:O:144:GLU:HB2	1.86	0.56
8:M:48:MET:HG2	8:M:173:VAL:HG13	1.86	0.56
8:O:22:HIS:CE1	8:O:25:ILE:HG12	2.41	0.56
4:C:15:PRO:HB2	4:C:256:ILE:HD11	1.87	0.56
8:K:68:ARG:O	8:K:72:THR:HG23	2.06	0.56
8:Q:234:ASN:HB3	8:Q:299:ILE:HD11	1.88	0.56
8:P:34:GLU:HG2	8:Q:259:LYS:HZ1	1.71	0.56
8:O:8:GLN:HG2	8:O:262:LEU:HD13	1.88	0.56
7:J:104:PHE:HE1	7:J:235:ALA:HB2	1.71	0.56
4:E:175:LYS:HE3	4:E:175:LYS:HA	1.87	0.55
6:H:28:MET:HE1	6:H:182:GLY:HA3	1.88	0.55
7:J:285:PHE:HB2	7:J:334:PRO:HB2	1.87	0.55
8:M:41:PHE:CE1	8:N:9:ILE:HD13	2.39	0.55
6:H:173:GLN:HE21	6:H:173:GLN:C	2.13	0.55
8:M:177:MET:HB3	8:M:178:PRO:HD2	1.89	0.55
2:2:3:DG:H2''	2:2:4:DT:H5''	1.89	0.55
7:J:56:PRO:HG2	7:J:61:ARG:HB2	1.88	0.55
8:O:45:GLN:HE22	8:O:169:LYS:HG2	1.70	0.55
4:E:1:MET:HG3	4:E:110:LEU:HD23	1.89	0.55
8:L:79:THR:HG23	8:L:133:GLN:HB2	1.88	0.55
2:2:-59:DG:H2''	2:2:-58:DA:C8	2.42	0.55
4:A:150:THR:HG22	4:A:210:ILE:HG23	1.88	0.55
8:N:240:PHE:CD2	8:N:304:ILE:HD11	2.42	0.55
1:1:21:A:H1'	4:B:8:LYS:HD2	1.89	0.55
8:N:234:ASN:HA	8:N:299:ILE:HD11	1.88	0.55
7:I:120:ARG:HH21	7:I:247:THR:HG23	1.70	0.55
8:K:259:LYS:HD3	8:Q:41:PHE:HZ	1.72	0.55
2:2:-62:DA:H2''	2:2:-61:DA:C8	2.41	0.55
7:I:97:LEU:HD13	7:I:110:LEU:HD23	1.88	0.55
8:P:101:LEU:HD22	8:P:125:LEU:HD13	1.90	0.55
6:H:100:ARG:HD2	6:H:168:GLN:HE21	1.72	0.54
4:A:121:CYS:HB3	4:A:324:ILE:HD11	1.88	0.54
8:L:251:LYS:HG3	10:L:402:ATP:H1'	1.89	0.54
8:P:12:LEU:HD23	8:P:258:LEU:HD23	1.89	0.54
4:B:18:ALA:HB3	4:B:251:PHE:HB2	1.89	0.54
4:B:114:LEU:HG	4:B:332:PHE:CZ	2.43	0.54
8:Q:138:ILE:HG12	8:Q:173:VAL:HB	1.90	0.54
2:2:-57:DG:H2''	2:2:-56:DG:C8	2.43	0.54
4:D:84:ILE:HG13	4:D:212:ALA:HB2	1.90	0.54
4:E:325:ASP:HB3	4:E:328:ILE:HD12	1.90	0.54
5:G:298:ILE:HG13	5:G:394:MET:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:372:HIS:HB3	7:I:374:MET:HE3	1.89	0.54
7:J:45:HIS:HA	8:Q:117:TYR:HD2	1.71	0.54
8:K:41:PHE:HZ	8:L:259:LYS:HD3	1.72	0.54
4:A:78:PRO:HG2	4:A:81:VAL:HG21	1.89	0.54
5:G:30:ILE:HD12	5:G:30:ILE:O	2.07	0.54
8:M:260:LEU:HD13	8:M:275:THR:HG23	1.90	0.54
8:M:274:ILE:HD13	8:M:296:LYS:HG2	1.90	0.54
8:O:216:MET:HE1	8:O:231:GLU:CB	2.37	0.54
6:H:8:VAL:HG13	6:H:86:VAL:HG22	1.89	0.53
8:N:209:LYS:HG3	9:U:847:LEU:HD22	1.90	0.53
4:F:220:PRO:HG3	4:F:249:VAL:HB	1.90	0.53
7:I:130:VAL:HG23	7:I:175:PRO:HG3	1.90	0.53
8:L:215:LEU:HB3	8:L:230:LEU:HD13	1.91	0.53
5:G:63:LYS:HZ3	5:G:167:GLY:HA3	1.74	0.53
1:1:31:A:O2'	4:A:222:GLN:HB2	2.09	0.53
4:D:265:ASP:HB3	4:D:274:ARG:HG2	1.91	0.53
8:M:87:ILE:HD11	8:M:144:GLU:HB2	1.90	0.53
8:N:11:LYS:HB3	8:N:223:PRO:HG3	1.91	0.53
8:P:73:GLN:HB3	8:P:75:TYR:CE1	2.44	0.53
8:N:41:PHE:CZ	8:O:259:LYS:HD3	2.45	0.52
8:P:83:LEU:HD22	8:P:104:LEU:HD23	1.91	0.52
2:2:-36:DT:H73	3:3:36:DA:H2	1.74	0.52
4:F:258:ALA:HA	4:F:276:ARG:HH11	1.75	0.52
6:H:31:PHE:O	6:H:35:HIS:HD2	1.92	0.52
4:B:314:LYS:O	4:B:318:THR:HG23	2.09	0.52
2:2:-58:DA:H2''	2:2:-57:DG:C8	2.44	0.52
3:3:36:DA:H5''	7:J:344:LEU:HD21	1.92	0.52
5:G:451:SER:HB2	5:G:629:MET:HB3	1.91	0.52
7:J:12:PHE:HB2	7:J:15:GLU:HB2	1.92	0.52
8:K:293:ASN:HB3	8:K:296:LYS:HG2	1.91	0.52
8:M:274:ILE:HG12	8:M:295:PHE:HB2	1.91	0.52
1:1:4:G:C2	4:E:340:MET:HG3	2.45	0.52
2:2:-4:DC:C6	2:2:-3:DT:H73	2.44	0.52
4:A:310:LEU:O	4:A:314:LYS:HG2	2.08	0.52
7:I:75:MET:HE2	7:J:396:SER:HA	1.91	0.52
8:O:319:ASP:HB3	8:O:322:ASP:HB2	1.91	0.52
8:P:11:LYS:HD2	8:P:223:PRO:HB2	1.92	0.52
4:E:18:ALA:HB3	4:E:251:PHE:HB2	1.90	0.52
7:I:310:SER:H	7:I:315:ARG:HH21	1.57	0.52
8:K:47:CYS:HB3	8:K:193:LEU:HD23	1.91	0.52
5:G:371:ASP:HA	5:G:374:LEU:HG	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:J:124:HIS:CE1	7:J:131:ASP:HB3	2.45	0.52
7:J:350:LEU:HA	7:J:394:LYS:HD3	1.91	0.52
8:M:253:LEU:HD21	8:M:295:PHE:HZ	1.74	0.52
8:N:21:MET:HE3	8:N:21:MET:HA	1.92	0.52
8:N:158:ALA:HB1	8:N:189:TRP:HE1	1.75	0.52
7:J:138:GLN:HE21	7:J:198:THR:HG21	1.74	0.52
8:Q:216:MET:HE2	9:X:849:ALA:HB2	1.92	0.52
4:D:176:TRP:HB2	4:D:181:LEU:HD22	1.91	0.51
4:F:239:LYS:HB3	4:F:247:TYR:HB3	1.92	0.51
8:P:219:ALA:HB2	8:P:230:LEU:HD12	1.92	0.51
2:2:-56:DG:H2''	2:2:-55:DA:C8	2.46	0.51
4:B:313:LEU:HD11	4:B:328:ILE:HG21	1.92	0.51
4:C:74:GLU:HG3	4:C:76:TYR:HE1	1.75	0.51
2:2:-61:DA:H2''	2:2:-60:DG:C8	2.46	0.51
4:A:224:LEU:HB3	4:B:38:LYS:HB2	1.92	0.51
4:A:232:GLU:HG3	6:H:149:ARG:HH12	1.74	0.51
8:M:29:PHE:HD2	8:M:68:ARG:HH21	1.58	0.51
8:P:191:SER:OG	8:Q:248:ARG:HD2	2.11	0.51
8:Q:87:ILE:HD11	8:Q:144:GLU:HB2	1.93	0.51
6:H:17:LEU:HD11	6:H:54:ASN:HA	1.91	0.51
8:K:48:MET:HB3	8:K:173:VAL:HG22	1.91	0.51
4:C:3:LEU:HB2	4:C:343:LYS:HE3	1.91	0.51
8:N:41:PHE:HZ	8:O:259:LYS:HD3	1.73	0.51
8:Q:50:LEU:HD23	8:Q:175:VAL:HG22	1.93	0.51
2:2:-55:DA:H2''	2:2:-54:DG:C8	2.46	0.51
4:A:171:ALA:HB2	7:I:41:ARG:HH21	1.75	0.51
4:F:142:TRP:CZ2	4:F:259:ALA:HB2	2.46	0.51
5:G:327:LEU:HD21	5:G:408:LEU:HD23	1.91	0.51
1:1:31:A:H5''	4:A:224:LEU:HD12	1.93	0.51
2:2:-11:DG:N2	4:E:44:SER:H	2.09	0.51
4:C:132:CYS:SG	4:C:187:LEU:HB3	2.51	0.51
4:C:279:GLU:HB3	4:C:299:PHE:HB3	1.93	0.51
4:D:8:LYS:HA	4:D:340:MET:HA	1.93	0.51
7:J:95:LEU:HD23	7:J:95:LEU:O	2.11	0.51
4:A:224:LEU:HD21	4:B:69:ILE:HD12	1.93	0.50
7:I:78:LEU:O	7:I:82:GLU:HG3	2.10	0.50
8:K:224:PHE:HE2	8:K:268:LEU:HD13	1.77	0.50
8:L:159:ASN:HA	8:L:162:LYS:HE2	1.93	0.50
8:P:104:LEU:O	8:P:105:GLU:HG3	2.11	0.50
2:2:-5:DA:H5'	2:2:-5:DA:C8	2.47	0.50
4:D:142:TRP:CZ2	4:D:259:ALA:HB2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:274:ILE:HG12	8:L:295:PHE:HB2	1.94	0.50
8:Q:47:CYS:HB3	8:Q:193:LEU:HD23	1.92	0.50
5:G:280:LEU:HD23	5:G:355:LEU:HD22	1.94	0.50
3:3:-3:DC:H2''	3:3:-2:DG:C8	2.47	0.50
4:B:175:LYS:HE3	4:B:175:LYS:HA	1.94	0.50
4:F:142:TRP:CE2	4:F:259:ALA:HB2	2.47	0.50
1:1:-5:G:H22	5:G:654:PRO:HB3	1.77	0.50
8:O:222:MET:HE1	8:O:254:LEU:HD22	1.93	0.50
2:2:-38:DT:H3	3:3:38:DA:H62	1.59	0.49
7:I:286:ASN:HB3	7:I:334:PRO:HB3	1.93	0.49
8:K:216:MET:HG2	8:K:231:GLU:HG2	1.94	0.49
2:2:-28:DC:H4'	4:B:47:THR:HG21	1.95	0.49
8:K:158:ALA:HB1	8:K:189:TRP:HE1	1.77	0.49
8:M:216:MET:HB3	8:M:231:GLU:OE1	2.11	0.49
8:P:274:ILE:HG13	8:P:295:PHE:HB2	1.94	0.49
2:2:-63:DG:H2''	2:2:-62:DA:C8	2.48	0.49
2:2:-19:DT:C4	4:D:69:ILE:HD11	2.47	0.49
4:C:313:LEU:O	4:C:317:ILE:HG23	2.13	0.49
4:E:132:CYS:SG	4:E:187:LEU:HB3	2.52	0.49
7:I:372:HIS:CD2	7:I:374:MET:H	2.30	0.49
8:M:129:LEU:HD22	8:M:134:VAL:HG21	1.93	0.49
4:A:12:SER:HB2	4:A:336:ILE:HG23	1.93	0.49
8:L:7:ILE:O	8:L:11:LYS:HG3	2.12	0.49
4:D:132:CYS:SG	4:D:187:LEU:HB3	2.52	0.49
8:P:223:PRO:HD2	8:P:258:LEU:HD21	1.95	0.49
3:3:1:DT:H2'	3:3:2:DG:C5	2.48	0.49
4:B:142:TRP:CE2	4:B:259:ALA:HB2	2.47	0.49
5:G:503:LEU:HD11	5:G:518:ARG:HH11	1.78	0.49
8:K:21:MET:HE1	8:K:29:PHE:CE2	2.47	0.49
8:L:75:TYR:HE1	8:L:81:PRO:HD3	1.77	0.49
8:M:216:MET:HE3	9:T:849:ALA:HB2	1.94	0.49
8:M:308:ILE:HD13	8:M:330:ALA:HB2	1.94	0.49
8:O:140:ASN:HA	8:O:175:VAL:HB	1.94	0.49
4:D:275:LEU:H	4:D:275:LEU:HD23	1.77	0.49
8:L:36:ARG:O	8:L:39:ARG:HG2	2.13	0.49
8:M:51:ILE:HD13	8:M:178:PRO:HA	1.95	0.49
8:P:119:THR:HG22	8:P:121:LEU:H	1.78	0.49
8:P:216:MET:HE3	9:W:849:ALA:HB2	1.95	0.49
8:P:277:TYR:HD1	8:P:277:TYR:O	1.95	0.49
8:Q:36:ARG:HG2	8:Q:135:GLU:HB3	1.95	0.48
1:1:38:C:H2'	1:1:39:U:C6	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:271:LYS:O	8:O:275:THR:HG22	2.12	0.48
4:A:79:PRO:HG3	6:H:119:LEU:HD13	1.95	0.48
7:I:177:ASN:HB3	7:I:180:GLU:HG2	1.96	0.48
7:I:342:SER:HA	7:I:383:GLY:HA2	1.95	0.48
4:C:76:TYR:CE2	4:C:217:GLU:HB2	2.48	0.48
5:G:484:ARG:HE	8:O:107:PHE:HE2	1.60	0.48
7:I:284:LEU:HD12	7:I:285:PHE:H	1.79	0.48
8:N:212:ARG:HD2	9:U:843:TRP:CZ3	2.48	0.48
8:O:251:LYS:HE3	10:O:402:ATP:N3	2.29	0.48
2:2:-54:DG:H2''	2:2:-53:DG:C8	2.49	0.48
2:2:-42:DC:H2''	2:2:-41:DG:C8	2.48	0.48
4:C:140:TRP:CD1	4:C:140:TRP:H	2.29	0.48
4:D:314:LYS:O	4:D:317:ILE:HG22	2.14	0.48
8:L:22:HIS:CE1	8:L:25:ILE:HG12	2.49	0.48
8:Q:303:GLU:HG2	8:Q:331:ILE:HD13	1.95	0.48
1:1:27:G:H1'	4:A:8:LYS:HD2	1.96	0.48
4:D:142:TRP:CE2	4:D:259:ALA:HB2	2.48	0.48
4:E:242:CYS:HA	4:F:79:PRO:HD2	1.95	0.48
8:O:7:ILE:HG22	8:O:11:LYS:HE3	1.94	0.48
8:P:49:LEU:HB2	8:P:193:LEU:HD22	1.96	0.48
8:M:39:ARG:HD2	8:M:135:GLU:HA	1.95	0.48
4:D:1:MET:HG3	4:D:107:VAL:HG22	1.94	0.48
8:P:230:LEU:HD22	8:P:239:LEU:HD11	1.95	0.48
8:Q:160:GLY:O	8:Q:164:ILE:HG12	2.14	0.48
4:C:77:VAL:HG23	4:C:216:GLN:O	2.14	0.48
4:F:1:MET:HE2	4:F:107:VAL:HG22	1.95	0.48
5:G:578:TRP:H	5:G:578:TRP:CD1	2.31	0.48
7:J:134:PRO:HB2	7:J:165:LEU:HD23	1.96	0.48
8:K:22:HIS:CE1	8:K:25:ILE:HG12	2.49	0.48
8:L:21:MET:HE3	8:L:21:MET:HB3	1.81	0.48
1:1:-6:U:H1'	5:G:463:ALA:HA	1.96	0.47
5:G:141:TRP:O	5:G:142:GLN:HG3	2.14	0.47
6:H:165:ILE:HG13	6:H:183:LEU:HD21	1.95	0.47
7:J:21:LEU:HD11	7:J:81:LEU:HD13	1.95	0.47
8:L:77:ARG:NH1	8:L:78:ASN:HA	2.27	0.47
8:L:77:ARG:CD	8:L:78:ASN:H	2.13	0.47
8:L:143:GLN:HB3	8:L:177:MET:H	1.79	0.47
2:2:-60:DG:H2''	2:2:-59:DG:C8	2.50	0.47
4:F:286:ILE:HG13	4:F:290:ARG:NH2	2.26	0.47
5:G:265:ILE:HD12	5:G:599:GLY:HA2	1.96	0.47
8:M:219:ALA:HB2	8:M:230:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:142:TRP:CE2	4:A:259:ALA:HB2	2.50	0.47
4:A:201:PHE:CD2	4:B:168:ARG:HD3	2.50	0.47
4:B:104:ASP:OD1	4:B:106:GLU:HG2	2.14	0.47
4:E:1:MET:SD	4:E:306:THR:HG21	2.53	0.47
5:G:604:PRO:HB2	5:G:694:LYS:HB2	1.95	0.47
8:O:11:LYS:HD3	8:O:223:PRO:HB2	1.96	0.47
8:P:47:CYS:HB3	8:P:193:LEU:HD23	1.94	0.47
8:P:93:LEU:HG	8:P:97:LEU:HD23	1.95	0.47
8:P:177:MET:HE3	8:P:177:MET:HB3	1.80	0.47
8:P:297:GLN:HB3	8:P:301:ASP:HB3	1.96	0.47
4:A:264:ASP:HB3	4:A:275:LEU:HB2	1.97	0.47
4:D:141:LEU:HB2	4:D:145:GLN:HA	1.96	0.47
7:J:343:VAL:HG22	7:J:380:PRO:HA	1.94	0.47
8:M:62:ILE:HD12	8:M:138:ILE:HD13	1.97	0.47
8:M:271:LYS:O	8:M:275:THR:HG22	2.15	0.47
8:K:62:ILE:HD12	8:K:138:ILE:HD13	1.95	0.47
8:P:293:ASN:HB3	8:P:296:LYS:HG3	1.96	0.47
1:1:10:C:H41	4:D:340:MET:CE	2.28	0.47
1:1:10:C:H4'	1:1:11:C:OP1	2.14	0.47
4:B:223:ILE:HG22	4:B:238:VAL:HG22	1.96	0.47
4:E:84:ILE:HG12	4:E:210:ILE:HB	1.96	0.47
5:G:470:SER:O	5:G:474:LYS:HG3	2.14	0.47
8:N:145:LEU:O	8:N:148:PHE:HB2	2.14	0.47
8:O:4:LEU:HD11	8:O:259:LYS:HG3	1.97	0.47
8:O:83:LEU:HD22	8:O:104:LEU:HD13	1.96	0.47
4:A:221:SER:HB2	4:A:251:PHE:HA	1.96	0.47
4:A:223:ILE:HB	4:A:236:GLN:HB2	1.97	0.47
4:D:140:TRP:H	4:D:140:TRP:CD1	2.33	0.47
7:I:63:ASN:HB2	7:I:66:HIS:HD2	1.79	0.47
8:L:323:MET:HB2	8:L:324:LEU:HD22	1.97	0.47
8:M:228:PRO:HB2	8:M:230:LEU:HD12	1.95	0.47
8:M:277:TYR:CD2	8:M:293:ASN:HA	2.50	0.47
5:G:44:LEU:O	5:G:47:THR:HG22	2.15	0.47
5:G:637:GLU:O	5:G:639:MET:HE3	2.15	0.47
8:K:300:LYS:HD3	8:K:300:LYS:N	2.29	0.47
8:M:8:GLN:HB3	8:M:262:LEU:HD23	1.97	0.47
6:H:114:GLU:CD	6:H:117:ARG:HH22	2.22	0.47
8:L:48:MET:HB3	8:L:173:VAL:HG13	1.97	0.47
8:L:136:LEU:HD11	8:L:173:VAL:HG23	1.97	0.47
8:Q:22:HIS:CD2	8:Q:22:HIS:H	2.33	0.47
8:Q:91:LYS:HA	8:Q:91:LYS:HD3	1.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:205:LYS:HB2	8:Q:332:VAL:HG11	1.97	0.47
4:B:7:LEU:H	4:B:342:GLN:HB3	1.79	0.46
4:C:75:CYS:SG	4:C:218:ILE:HD11	2.55	0.46
5:G:122:TRP:CZ3	5:G:129:VAL:HG12	2.50	0.46
5:G:688:LYS:HD3	5:G:688:LYS:HA	1.74	0.46
8:K:318:LEU:H	8:K:318:LEU:HD23	1.79	0.46
4:A:142:TRP:NE1	4:A:259:ALA:HB2	2.31	0.46
7:I:303:SER:O	7:I:304:THR:HG22	2.15	0.46
4:D:142:TRP:O	4:D:145:GLN:HB2	2.15	0.46
4:F:150:THR:HG22	4:F:210:ILE:HG23	1.97	0.46
8:M:29:PHE:HE1	8:M:61:THR:HG23	1.81	0.46
8:M:300:LYS:N	8:M:300:LYS:HE2	2.29	0.46
2:2:-47:DG:H2''	2:2:-46:DG:C8	2.50	0.46
4:D:312:ALA:HA	4:D:315:ASN:ND2	2.30	0.46
7:I:329:PRO:HA	7:I:388:ARG:HH12	1.80	0.46
8:K:222:MET:SD	8:K:258:LEU:HD11	2.56	0.46
8:O:35:LEU:HD11	8:O:48:MET:HB2	1.97	0.46
6:H:3:ARG:HG2	6:H:61:THR:HG22	1.97	0.46
7:J:47:LEU:HD21	7:J:76:ARG:HG3	1.98	0.46
5:G:297:LEU:HD22	5:G:330:THR:HG21	1.98	0.46
8:P:100:MET:HE1	8:P:161:LEU:HD21	1.98	0.46
4:A:257:GLY:O	4:A:261:GLN:HG3	2.16	0.46
4:C:201:PHE:CD2	4:D:168:ARG:HG2	2.51	0.46
4:E:303:PHE:HD1	4:E:331:LEU:HD11	1.80	0.46
8:M:177:MET:HE3	8:M:177:MET:HB3	1.77	0.46
8:M:215:LEU:HD21	8:M:250:LEU:HD11	1.98	0.46
2:2:-48:DA:H2''	2:2:-47:DG:H8	1.81	0.46
4:A:215:CYS:HB2	6:H:116:ARG:HG3	1.97	0.46
4:B:314:LYS:O	4:B:317:ILE:HG22	2.15	0.46
5:G:60:LYS:HD3	5:G:61:LEU:HD22	1.98	0.46
6:H:98:GLU:HG3	6:H:173:GLN:HB2	1.98	0.46
7:I:125:HIS:CE1	7:I:126:ALA:HB2	2.51	0.46
8:M:22:HIS:CE1	8:M:25:ILE:HG12	2.51	0.46
8:M:83:LEU:HD23	8:M:137:LEU:HD12	1.98	0.46
8:Q:29:PHE:HE1	8:Q:61:THR:HG23	1.80	0.46
8:Q:256:GLU:HB3	8:Q:276:ALA:HB1	1.97	0.46
4:F:144:ASN:HD21	4:F:219:TYR:H	1.64	0.46
6:H:85:LYS:HE2	6:H:85:LYS:HB2	1.79	0.46
8:L:223:PRO:HD2	8:L:258:LEU:HD21	1.97	0.46
8:M:77:ARG:HA	8:M:77:ARG:NE	2.30	0.46
8:M:318:LEU:HD22	8:M:318:LEU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:2:DC:H2''	2:2:3:DG:C8	2.51	0.46
4:A:169:LYS:HA	7:I:38:LEU:HD13	1.99	0.46
4:A:197:ASP:HB3	4:A:200:VAL:HG12	1.98	0.46
4:C:280:PHE:CG	4:D:64:LEU:HD13	2.51	0.46
5:G:370:PRO:HG2	5:G:373:GLU:HG2	1.98	0.46
7:I:401:LYS:HA	7:I:401:LYS:HD2	1.75	0.46
7:J:71:SER:O	7:J:75:MET:HG2	2.16	0.46
8:Q:298:ASP:O	8:Q:302:ILE:HG13	2.16	0.46
4:C:220:PRO:HG3	4:C:249:VAL:HB	1.97	0.45
4:C:224:LEU:HD21	4:D:69:ILE:HG12	1.98	0.45
4:C:262:SER:HA	4:C:276:ARG:HA	1.97	0.45
4:F:41:GLY:HA3	4:F:70:LEU:HD11	1.98	0.45
4:F:140:TRP:H	4:F:140:TRP:CD1	2.32	0.45
8:K:228:PRO:HB2	8:K:230:LEU:HD13	1.97	0.45
2:2:-36:DT:H72	3:3:37:DA:C2	2.52	0.45
4:F:176:TRP:HB2	4:F:181:LEU:HG	1.98	0.45
7:I:230:LEU:HD12	7:I:230:LEU:H	1.81	0.45
7:I:322:VAL:O	7:I:326:GLU:HG2	2.17	0.45
8:K:50:LEU:O	8:K:175:VAL:HA	2.16	0.45
8:M:90:GLY:C	8:M:91:LYS:HD3	2.41	0.45
4:F:172:TRP:CE2	4:F:274:ARG:HD3	2.51	0.45
4:F:343:LYS:HB2	4:F:343:LYS:HE2	1.72	0.45
7:I:10:ARG:HA	7:I:10:ARG:HD3	1.63	0.45
8:K:256:GLU:HB3	8:K:276:ALA:HB1	1.96	0.45
8:N:253:LEU:HD13	8:N:282:PHE:HE2	1.81	0.45
4:C:269:GLU:H	4:C:269:GLU:CD	2.24	0.45
4:E:140:TRP:CD1	4:E:140:TRP:H	2.32	0.45
4:F:221:SER:OG	4:F:255:LYS:HD3	2.16	0.45
8:L:308:ILE:HG13	8:L:328:VAL:HG23	1.97	0.45
8:O:6:GLU:O	8:O:9:ILE:HG22	2.15	0.45
1:1:22:G:N1	4:B:340:MET:HE2	2.31	0.45
1:1:28:G:O4'	4:A:339:GLY:HA2	2.17	0.45
2:2:-9:DC:H5'	2:2:-9:DC:C6	2.52	0.45
4:A:314:LYS:HE2	4:A:314:LYS:HB3	1.81	0.45
4:B:118:PHE:HD1	4:B:313:LEU:HD21	1.82	0.45
4:E:172:TRP:CE2	4:E:274:ARG:HD3	2.51	0.45
8:K:253:LEU:HD21	8:K:295:PHE:HZ	1.82	0.45
8:Q:212:ARG:HD2	9:X:843:TRP:CZ3	2.52	0.45
4:A:168:ARG:HH11	7:I:42:GLU:HG2	1.80	0.45
4:B:84:ILE:HG12	4:B:210:ILE:HB	1.98	0.45
6:H:6:PHE:HB3	6:H:89:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:140:LEU:HA	7:I:140:LEU:HD12	1.77	0.45
8:L:45:GLN:HE22	8:L:169:LYS:HB3	1.81	0.45
8:L:177:MET:HE3	8:L:177:MET:HB3	1.75	0.45
8:N:49:LEU:HB2	8:N:193:LEU:HD13	1.97	0.45
2:2:-27:DC:H2''	2:2:-26:DA:C8	2.52	0.45
2:2:-12:DT:H4'	4:E:68:ASN:HB3	1.98	0.45
2:2:4:DT:H2''	2:2:5:DG:H5'	1.99	0.45
4:A:38:LYS:HE3	4:A:69:ILE:HG21	1.98	0.45
4:B:242:CYS:HA	4:C:79:PRO:HD2	1.99	0.45
8:K:248:ARG:HB2	10:K:401:ATP:H5'2	1.99	0.45
5:G:242:PRO:HB3	5:G:254:GLY:HA2	1.98	0.45
7:J:10:ARG:HA	7:J:10:ARG:HD3	1.75	0.45
8:P:34:GLU:HG2	8:Q:259:LYS:NZ	2.32	0.45
8:Q:87:ILE:HA	8:Q:96:THR:HG23	1.99	0.45
4:F:317:ILE:HD13	4:F:320:LYS:HZ1	1.81	0.45
6:H:100:ARG:CZ	6:H:190:LYS:HG3	2.47	0.45
8:L:123:LYS:HB3	8:L:123:LYS:HE3	1.78	0.45
8:L:219:ALA:HB1	8:L:228:PRO:HD2	1.98	0.45
4:C:12:SER:HB2	4:C:336:ILE:HG23	1.99	0.45
4:D:85:PHE:HA	4:D:208:ALA:O	2.17	0.45
4:A:39:ILE:HG22	6:H:144:ILE:HB	1.99	0.44
4:F:39:ILE:HD11	4:F:72:LEU:HD12	1.99	0.44
7:I:110:LEU:HD22	7:I:122:ILE:HG13	1.99	0.44
7:I:340:LEU:HD11	7:I:369:ALA:HB3	1.99	0.44
8:K:147:GLU:HG2	8:K:313:TYR:CE1	2.52	0.44
8:L:219:ALA:HB2	8:L:230:LEU:HD11	1.99	0.44
8:N:269:GLU:HG3	8:N:271:LYS:HG3	1.99	0.44
4:B:141:LEU:HB2	4:B:145:GLN:HA	1.99	0.44
8:L:11:LYS:HB3	8:L:223:PRO:HB3	1.99	0.44
8:Q:67:LYS:HB3	8:Q:67:LYS:HE3	1.84	0.44
3:3:1:DT:H5''	3:3:1:DT:H6	1.82	0.44
4:F:132:CYS:SG	4:F:187:LEU:HB3	2.57	0.44
5:G:647:ARG:HB3	5:G:647:ARG:CZ	2.47	0.44
8:N:194:VAL:HG11	8:O:252:HIS:HD2	1.81	0.44
1:I:19:A:C4	4:C:224:LEU:HG	2.52	0.44
2:2:-53:DG:H21	8:K:115:ARG:NH2	2.16	0.44
2:2:-48:DA:H2''	2:2:-47:DG:C8	2.53	0.44
5:G:215:ILE:HD13	5:G:453:PRO:HB2	2.00	0.44
5:G:682:MET:HG2	5:G:695:VAL:HG22	1.98	0.44
7:I:63:ASN:HB2	7:I:66:HIS:CD2	2.53	0.44
7:I:271:ASP:O	7:I:275:LYS:HG2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:O:298:ASP:O	8:O:302:ILE:HG13	2.18	0.44
8:P:123:LYS:HD3	8:Q:112:ILE:N	2.33	0.44
8:P:212:ARG:HD2	9:W:843:TRP:CZ3	2.52	0.44
8:Q:237:ILE:HG23	8:Q:304:ILE:HD11	2.00	0.44
2:2:-44:DT:H2''	2:2:-43:DG:C8	2.52	0.44
2:2:-32:DG:H2''	2:2:-31:DT:O4'	2.17	0.44
5:G:63:LYS:NZ	5:G:167:GLY:HA3	2.31	0.44
5:G:99:LEU:HD23	5:G:214:VAL:HG11	1.99	0.44
5:G:156:SER:HB3	5:G:159:TRP:HD1	1.82	0.44
8:K:91:LYS:HB3	8:K:95:ALA:HB3	2.00	0.44
8:N:160:GLY:O	8:N:164:ILE:HG12	2.17	0.44
6:H:108:ALA:HB1	6:H:114:GLU:HG3	1.99	0.44
8:P:246:GLU:HG2	8:P:249:ALA:H	1.82	0.44
8:P:305:TYR:CE1	8:P:331:ILE:HG13	2.52	0.44
4:B:304:LYS:HD3	4:C:54:PHE:CE2	2.53	0.44
4:C:302:ILE:HD12	4:C:327:ALA:HB1	2.00	0.44
6:H:4:TYR:HB2	6:H:66:LEU:HD12	1.99	0.44
8:K:112:ILE:HD11	8:K:124:LYS:HG3	1.99	0.44
8:K:204:LEU:HD23	8:K:204:LEU:HA	1.83	0.44
8:M:143:GLN:HB3	8:M:177:MET:H	1.83	0.44
8:M:296:LYS:HB2	8:M:296:LYS:HZ3	1.83	0.44
8:O:145:LEU:O	8:O:154:ARG:HG2	2.18	0.44
5:G:236:ASN:HB2	5:G:255:VAL:HG13	2.00	0.44
6:H:124:LYS:HB2	6:H:124:LYS:HE3	1.72	0.44
7:I:204:LEU:HA	7:I:207:GLU:HG2	2.00	0.44
7:J:366:LEU:HD23	7:J:366:LEU:HA	1.84	0.44
7:J:401:LYS:HE3	7:J:401:LYS:HB2	1.75	0.44
8:L:93:LEU:HD23	8:L:157:ILE:HA	2.00	0.44
8:O:57:GLY:HA2	10:O:402:ATP:O1A	2.17	0.44
8:O:145:LEU:HD12	8:O:145:LEU:HA	1.86	0.44
1:1:46:U:C5	6:H:137:LYS:HB3	2.53	0.44
4:D:176:TRP:HB3	4:D:180:ASP:HB2	1.99	0.44
4:D:17:LYS:HD3	4:D:240:ALA:HB2	1.99	0.43
4:E:85:PHE:HA	4:E:208:ALA:O	2.18	0.43
5:G:43:LEU:HD12	5:G:43:LEU:HA	1.82	0.43
8:L:271:LYS:H	8:L:271:LYS:HG2	1.66	0.43
3:3:41:DC:H2''	3:3:42:DG:C8	2.53	0.43
3:3:55:DT:H2''	3:3:56:DC:C6	2.53	0.43
4:B:1:MET:HE1	4:B:111:LEU:HD21	1.99	0.43
4:B:140:TRP:H	4:B:140:TRP:CD1	2.35	0.43
4:D:314:LYS:O	4:D:318:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:232:SER:O	8:K:236:THR:HG23	2.18	0.43
8:N:169:LYS:HE2	8:N:169:LYS:HB2	1.78	0.43
8:N:222:MET:SD	8:N:258:LEU:HD11	2.58	0.43
4:E:298:ASN:O	4:E:302:ILE:HG12	2.18	0.43
4:F:258:ALA:HA	4:F:276:ARG:HD3	2.00	0.43
6:H:72:GLN:HB2	6:H:75:PHE:HD2	1.83	0.43
8:L:93:LEU:HD13	8:L:97:LEU:HG	1.99	0.43
8:N:191:SER:OG	8:O:248:ARG:HD2	2.17	0.43
2:2:-27:DC:H6	2:2:-27:DC:H2'	1.67	0.43
4:A:267:TRP:H	4:A:267:TRP:CD1	2.35	0.43
4:D:290:ARG:HD2	4:D:290:ARG:N	2.34	0.43
4:E:32:LEU:HD12	4:E:32:LEU:HA	1.79	0.43
4:E:115:ALA:HA	4:E:332:PHE:CZ	2.54	0.43
8:O:313:TYR:CE2	8:O:315:PRO:HB3	2.54	0.43
5:G:358:ALA:HB1	5:G:361:ARG:HG3	2.00	0.43
8:K:215:LEU:HD13	8:K:215:LEU:HA	1.87	0.43
8:L:274:ILE:HG23	8:L:293:ASN:ND2	2.33	0.43
8:N:264:CYS:SG	8:N:266:GLU:HB3	2.58	0.43
8:O:114:LYS:HA	8:O:114:LYS:HD3	1.84	0.43
4:A:132:CYS:SG	4:A:187:LEU:HB3	2.59	0.43
4:A:340:MET:HE3	4:A:340:MET:HB3	1.80	0.43
4:B:154:ILE:HG23	4:B:206:ILE:HG12	2.01	0.43
5:G:502:LYS:HZ2	5:G:502:LYS:HG2	1.71	0.43
7:I:82:GLU:OE2	7:I:93:GLN:HG3	2.19	0.43
8:M:50:LEU:O	8:M:175:VAL:HA	2.19	0.43
8:M:183:ILE:HD12	8:M:183:ILE:HA	1.87	0.43
3:3:53:DC:H2''	3:3:54:DC:C6	2.54	0.43
4:F:267:TRP:CE3	4:F:268:ASP:HB2	2.54	0.43
5:G:45:ASN:HB2	5:G:56:LEU:HD13	2.01	0.43
8:L:8:GLN:HG2	8:L:262:LEU:HD12	2.00	0.43
1:1:18:G:OP2	4:C:258:ALA:HB2	2.19	0.43
4:B:138:GLY:O	4:B:145:GLN:HG3	2.18	0.43
4:C:308:TRP:CD1	4:C:308:TRP:C	2.97	0.43
4:D:227:LYS:HD2	4:D:227:LYS:HA	1.76	0.43
8:K:137:LEU:HD23	8:K:172:ILE:HG12	2.00	0.43
8:L:29:PHE:HE1	8:L:61:THR:HG23	1.84	0.43
8:L:39:ARG:HH12	8:L:170:VAL:HG12	1.84	0.43
8:N:20:VAL:H	10:N:402:ATP:HN62	1.65	0.43
4:A:1:MET:HE1	4:A:111:LEU:HD21	2.01	0.43
7:I:266:PHE:O	7:I:269:GLU:HG2	2.19	0.43
8:K:274:ILE:HG13	8:K:295:PHE:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Q:212:ARG:HG2	8:Q:212:ARG:HH11	1.84	0.43
2:2:-10:DG:C2	4:D:340:MET:HE2	2.54	0.42
2:2:4:DT:H2''	2:2:5:DG:H8	1.84	0.42
4:F:133:ARG:HB3	4:F:172:TRP:CZ3	2.54	0.42
5:G:89:TYR:HE1	5:G:453:PRO:HB3	1.83	0.42
5:G:325:LYS:HB2	5:G:325:LYS:HE3	1.87	0.42
7:J:270:LEU:HB3	7:J:320:TYR:CE2	2.53	0.42
8:L:1:MET:HE3	8:L:1:MET:N	2.33	0.42
2:2:-3:DT:H6	2:2:-3:DT:H2'	1.60	0.42
4:A:69:ILE:C	4:A:70:LEU:HD23	2.44	0.42
5:G:276:ARG:HD2	5:G:286:VAL:HG13	2.01	0.42
8:K:53:ASP:O	8:K:56:VAL:HG22	2.19	0.42
8:K:215:LEU:HD12	8:K:230:LEU:HD23	2.00	0.42
8:L:70:LEU:HD23	8:L:70:LEU:HA	1.88	0.42
8:N:48:MET:HE2	8:N:48:MET:HB2	1.92	0.42
8:N:177:MET:HB3	8:N:177:MET:HE3	1.80	0.42
3:3:43:DC:H2''	3:3:44:DA:C8	2.54	0.42
4:F:6:ILE:HG22	4:F:103:SER:HB3	2.01	0.42
4:F:84:ILE:HD13	4:F:212:ALA:HB2	2.02	0.42
5:G:249:ALA:HA	5:G:256:ILE:HD11	2.01	0.42
5:G:515:ARG:HD3	5:G:517:LYS:HE2	2.01	0.42
8:O:308:ILE:HD13	8:O:330:ALA:HB2	2.02	0.42
8:P:212:ARG:O	8:P:216:MET:HG2	2.19	0.42
2:2:-46:DG:H2''	2:2:-45:DA:C8	2.53	0.42
4:B:290:ARG:HA	4:B:290:ARG:HD3	1.75	0.42
4:E:176:TRP:HB2	4:E:181:LEU:HG	2.00	0.42
5:G:633:MET:SD	5:G:691:LEU:HD21	2.59	0.42
7:J:306:LYS:HA	7:J:306:LYS:HD3	1.84	0.42
8:L:87:ILE:HD11	8:L:144:GLU:HB2	2.00	0.42
8:M:292:LYS:HE2	8:M:292:LYS:HB2	1.69	0.42
1:1:37:C:H5	6:H:149:ARG:HE	1.67	0.42
4:D:12:SER:HB2	4:D:336:ILE:HG23	2.01	0.42
4:D:173:GLU:CD	4:D:173:GLU:H	2.27	0.42
5:G:124:HIS:CG	5:G:125:ASN:N	2.87	0.42
5:G:473:ARG:HE	5:G:473:ARG:HB3	1.60	0.42
6:H:133:PHE:CZ	6:H:135:PRO:HG3	2.54	0.42
7:J:41:ARG:NE	7:J:49:PHE:HZ	2.18	0.42
8:K:83:LEU:HD23	8:K:137:LEU:HD13	2.01	0.42
8:Q:56:VAL:HG22	8:Q:201:TYR:CE1	2.54	0.42
2:2:-54:DG:H2''	2:2:-53:DG:H8	1.84	0.42
4:B:220:PRO:HG3	4:B:249:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:383:ARG:O	5:G:387:GLU:HG2	2.20	0.42
7:I:354:VAL:O	7:I:357:VAL:HG22	2.19	0.42
8:K:75:TYR:CD2	8:K:81:PRO:HG3	2.54	0.42
8:Q:89:ARG:HD3	8:Q:89:ARG:HA	1.88	0.42
2:2:-29:DA:H2''	2:2:-28:DC:C6	2.55	0.42
4:A:181:LEU:HD23	4:A:181:LEU:HA	1.82	0.42
4:B:172:TRP:CZ2	4:B:274:ARG:HD3	2.54	0.42
4:B:332:PHE:CD1	4:B:335:LEU:HD12	2.55	0.42
4:D:179:ASP:O	4:D:183:VAL:HG12	2.20	0.42
4:D:279:GLU:HB2	4:E:44:SER:HB2	2.01	0.42
4:E:261:GLN:O	4:E:277:VAL:HG23	2.20	0.42
4:F:3:LEU:HD23	4:F:3:LEU:HA	1.77	0.42
4:F:320:LYS:HD3	4:F:320:LYS:HA	1.88	0.42
5:G:692:MET:HE3	5:G:692:MET:HB3	1.77	0.42
8:K:134:VAL:HG13	8:K:170:VAL:HG11	2.01	0.42
8:O:56:VAL:HG22	8:O:201:TYR:CE1	2.54	0.42
8:O:70:LEU:HD23	8:O:70:LEU:HA	1.83	0.42
8:P:156:GLN:HG3	8:Q:89:ARG:HG3	2.01	0.42
8:P:204:LEU:HG	8:P:240:PHE:CD2	2.54	0.42
1:1:9:G:H1'	4:D:8:LYS:HD3	2.01	0.42
4:B:142:TRP:NE1	4:B:255:LYS:HG2	2.35	0.42
5:G:43:LEU:HD12	5:G:46:LEU:HD12	2.02	0.42
5:G:111:LEU:HD12	5:G:111:LEU:HA	1.88	0.42
8:L:179:TRP:CG	8:L:313:TYR:HB3	2.53	0.42
4:B:88:PHE:CZ	4:B:206:ILE:HD12	2.55	0.42
8:Q:145:LEU:HD13	8:Q:154:ARG:HG3	2.02	0.42
1:1:22:G:O4'	4:B:339:GLY:HA2	2.20	0.42
4:A:303:PHE:CD1	4:A:331:LEU:HD21	2.55	0.42
5:G:147:TRP:N	5:G:147:TRP:CD1	2.88	0.42
7:J:187:CYS:HB2	7:J:193:LEU:HD21	2.02	0.42
8:L:89:ARG:HD3	8:L:144:GLU:HB3	2.01	0.42
8:M:279:LYS:HB2	8:M:279:LYS:HE2	1.75	0.42
8:Q:51:ILE:HD13	8:Q:178:PRO:HA	2.01	0.42
8:Q:114:LYS:HD2	8:Q:114:LYS:HA	1.59	0.42
8:Q:136:LEU:O	8:Q:138:ILE:HG13	2.20	0.42
2:2:4:DT:H2''	2:2:5:DG:C8	2.55	0.41
3:3:62:DT:H2''	3:3:63:DC:C6	2.55	0.41
4:B:133:ARG:HG2	4:B:172:TRP:CE3	2.54	0.41
4:B:267:TRP:CD1	4:B:267:TRP:H	2.38	0.41
5:G:38:VAL:HA	5:G:41:ILE:HG12	2.01	0.41
5:G:163:PHE:HD2	5:G:173:PHE:CD1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:9:ILE:HG13	8:M:10:GLU:N	2.35	0.41
8:M:228:PRO:HB2	8:M:230:LEU:CD1	2.50	0.41
8:N:205:LYS:HB2	8:N:205:LYS:HE2	1.71	0.41
8:Q:209:LYS:HZ3	9:X:847:LEU:HD22	1.85	0.41
1:1:10:C:OP2	1:1:10:C:H2'	2.19	0.41
4:B:332:PHE:CE1	4:B:335:LEU:HD12	2.56	0.41
8:M:53:ASP:O	8:M:56:VAL:HG22	2.19	0.41
8:M:139:ILE:HD13	8:M:139:ILE:HA	1.89	0.41
1:1:-6:U:H5''	5:G:200:ILE:HB	2.02	0.41
4:B:317:ILE:HD12	4:B:317:ILE:HA	1.81	0.41
4:D:269:GLU:CD	4:D:269:GLU:H	2.28	0.41
4:E:220:PRO:HG3	4:E:249:VAL:HB	2.02	0.41
8:M:97:LEU:O	8:M:101:LEU:HG	2.21	0.41
8:M:146:ILE:HD13	8:M:154:ARG:HD2	2.01	0.41
8:N:212:ARG:HD2	9:U:843:TRP:HZ3	1.85	0.41
8:N:216:MET:HE2	9:U:849:ALA:HB2	2.01	0.41
8:P:22:HIS:CD2	8:P:22:HIS:H	2.38	0.41
8:Q:201:TYR:HD2	8:Q:307:VAL:HG11	1.84	0.41
4:F:201:PHE:HB2	5:G:556:ALA:HA	2.01	0.41
5:G:536:HIS:CG	8:O:77:ARG:HH12	2.39	0.41
6:H:127:LEU:HD12	6:H:127:LEU:HA	1.90	0.41
7:I:264:ALA:O	7:I:268:THR:HG23	2.21	0.41
7:J:55:PHE:HB2	7:J:73:PHE:CD1	2.55	0.41
7:J:281:LEU:HD23	7:J:281:LEU:HA	1.90	0.41
7:J:299:LEU:HD23	7:J:299:LEU:HA	1.86	0.41
8:K:233:LYS:O	8:K:237:ILE:HG12	2.20	0.41
8:L:104:LEU:HD23	8:L:128:SER:HB3	2.02	0.41
8:O:183:ILE:HD12	8:O:183:ILE:HA	1.84	0.41
8:P:238:ALA:HA	8:P:294:PRO:HB2	2.02	0.41
1:1:29:U:O4	4:B:72:LEU:HD11	2.21	0.41
4:D:49:ALA:HB2	4:D:64:LEU:HD21	2.02	0.41
4:F:171:ALA:HB3	4:F:174:SER:HB3	2.03	0.41
5:G:1:MET:HE3	5:G:1:MET:H1	1.84	0.41
5:G:695:VAL:HG11	8:O:77:ARG:NE	2.25	0.41
7:I:321:LEU:HD13	7:I:387:LEU:HD11	2.03	0.41
8:O:274:ILE:HD13	8:O:295:PHE:HB2	2.02	0.41
4:B:12:SER:OG	4:B:336:ILE:HG23	2.21	0.41
6:H:20:LEU:HD21	7:J:282:ILE:HA	2.01	0.41
8:K:54:THR:HG21	8:Q:187:PRO:C	2.46	0.41
8:K:252:HIS:HD2	8:Q:194:VAL:HG11	1.86	0.41
8:L:52:GLY:HA3	8:L:56:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:M:104:LEU:O	8:M:105:GLU:HG3	2.21	0.41
8:N:93:LEU:HG	8:N:97:LEU:HG	2.02	0.41
8:N:262:LEU:HD23	8:N:262:LEU:HA	1.94	0.41
8:Q:143:GLN:HB2	8:Q:179:TRP:NE1	2.36	0.41
8:Q:151:VAL:O	8:Q:155:GLN:HG2	2.21	0.41
2:2:-51:DC:H2''	2:2:-50:DT:O5'	2.20	0.41
4:A:23:LYS:HG2	4:A:28:ASP:O	2.21	0.41
4:A:114:LEU:HD22	4:A:306:THR:HG23	2.03	0.41
4:C:224:LEU:HD22	4:D:69:ILE:HG23	2.03	0.41
5:G:279:LYS:HE2	5:G:279:LYS:HB3	1.84	0.41
7:J:209:LEU:HD23	7:J:209:LEU:HA	1.76	0.41
8:L:39:ARG:HB2	8:L:39:ARG:NH1	2.36	0.41
8:O:271:LYS:HA	8:O:274:ILE:HB	2.02	0.41
4:A:232:GLU:HG3	6:H:149:ARG:NH1	2.36	0.41
4:E:142:TRP:NE1	4:E:259:ALA:HB2	2.35	0.41
5:G:1:MET:HE3	5:G:1:MET:H3	1.86	0.41
5:G:363:GLU:O	5:G:367:LEU:HG	2.21	0.41
6:H:21:THR:O	6:H:25:ILE:HG12	2.20	0.41
7:I:374:MET:O	7:I:376:GLN:HG2	2.21	0.41
8:M:282:PHE:HD1	8:M:282:PHE:HA	1.80	0.41
8:N:222:MET:SD	8:N:228:PRO:HG2	2.61	0.41
8:Q:50:LEU:O	8:Q:175:VAL:HA	2.21	0.41
4:B:121:CYS:HA	4:B:317:ILE:HD13	2.02	0.41
4:B:132:CYS:SG	4:B:187:LEU:HB3	2.61	0.41
4:B:269:GLU:H	4:B:269:GLU:CD	2.26	0.41
4:D:228:VAL:HG21	4:D:234:SER:HA	2.02	0.41
7:I:269:GLU:HA	7:I:272:GLU:CD	2.45	0.41
7:J:228:MET:HE3	7:J:232:GLU:CB	2.51	0.41
8:K:106:LEU:HD23	8:K:106:LEU:HA	1.95	0.41
8:M:162:LYS:HG3	8:M:189:TRP:CZ2	2.56	0.41
8:O:49:LEU:HD12	8:O:174:LEU:HB2	2.03	0.41
8:O:80:MET:HE3	8:O:80:MET:HB2	1.71	0.41
8:P:20:VAL:HB	8:P:214:TYR:HE1	1.85	0.41
2:2:-19:DT:H2''	4:D:67:ASN:O	2.20	0.41
4:F:141:LEU:HB2	4:F:145:GLN:HA	2.02	0.41
6:H:22:GLY:HA3	6:H:151:ALA:O	2.21	0.41
8:M:211:PHE:HE2	8:M:240:PHE:HB2	1.86	0.41
8:N:201:TYR:CD2	8:N:307:VAL:HG21	2.55	0.41
8:O:58:LYS:NZ	8:O:177:MET:SD	2.94	0.41
8:P:153:GLU:O	8:P:157:ILE:HG12	2.20	0.41
1:1:39:U:OP2	6:H:117:ARG:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:-47:DG:H2''	2:2:-46:DG:H8	1.86	0.40
2:2:-39:DC:H2'	2:2:-38:DT:H71	2.03	0.40
4:A:321:ASN:OD1	4:A:321:ASN:C	2.63	0.40
4:B:6:ILE:HG13	4:B:103:SER:HB3	2.04	0.40
4:B:224:LEU:HD22	4:C:69:ILE:HG23	2.02	0.40
5:G:639:MET:HE2	5:G:639:MET:HB3	1.88	0.40
8:K:182:LYS:HA	8:K:182:LYS:HD2	1.89	0.40
8:O:23:PRO:HG2	8:O:210:TYR:HE2	1.86	0.40
8:P:240:PHE:HD1	8:P:240:PHE:O	2.04	0.40
2:2:-53:DG:H2''	2:2:-52:DC:C5	2.56	0.40
2:2:-25:DA:C5	4:C:69:ILE:HD11	2.57	0.40
4:A:242:CYS:HA	4:B:79:PRO:HD2	2.03	0.40
4:C:112:LYS:HE3	4:C:112:LYS:HB2	1.84	0.40
4:F:223:ILE:HD11	5:G:499:ALA:C	2.47	0.40
5:G:353:GLU:OE1	5:G:353:GLU:HA	2.22	0.40
7:I:234:PHE:HA	7:I:237:LEU:HD12	2.02	0.40
8:L:41:PHE:HZ	8:M:259:LYS:HD3	1.87	0.40
8:M:227:PRO:HA	8:M:228:PRO:HD3	1.96	0.40
8:O:155:GLN:HG3	8:P:89:ARG:HH21	1.86	0.40
8:P:154:ARG:HE	8:P:154:ARG:HB3	1.60	0.40
4:D:142:TRP:CE2	4:D:255:LYS:HE3	2.57	0.40
4:F:150:THR:HA	4:F:210:ILE:HA	2.03	0.40
8:L:50:LEU:O	8:L:175:VAL:HA	2.20	0.40
8:L:201:TYR:CD2	8:L:307:VAL:HG11	2.55	0.40
8:O:101:LEU:HD23	8:O:101:LEU:HA	1.88	0.40
2:2:-23:DC:N4	4:C:70:LEU:HD22	2.36	0.40
3:3:55:DT:H2''	3:3:56:DC:C5	2.56	0.40
4:C:85:PHE:HA	4:C:208:ALA:O	2.22	0.40
4:C:303:PHE:HD1	4:C:303:PHE:HA	1.70	0.40
7:I:360:LEU:HD22	7:I:365:ILE:HG21	2.03	0.40
8:M:305:TYR:CE1	8:M:331:ILE:HG13	2.57	0.40
8:N:158:ALA:HB1	8:N:189:TRP:NE1	2.35	0.40
4:C:77:VAL:CG2	4:C:84:ILE:HD11	2.51	0.40
8:K:5:THR:HG23	8:K:8:GLN:H	1.86	0.40
8:K:36:ARG:O	8:K:39:ARG:HG2	2.22	0.40
8:L:251:LYS:HB3	8:L:251:LYS:HE2	1.82	0.40
8:N:240:PHE:HA	8:N:243:CYS:SG	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	317/350 (91%)	307 (97%)	10 (3%)	0	100	100
4	B	344/350 (98%)	340 (99%)	4 (1%)	0	100	100
4	C	344/350 (98%)	335 (97%)	9 (3%)	0	100	100
4	D	344/350 (98%)	337 (98%)	7 (2%)	0	100	100
4	E	344/350 (98%)	337 (98%)	7 (2%)	0	100	100
4	F	342/350 (98%)	336 (98%)	6 (2%)	0	100	100
5	G	680/695 (98%)	668 (98%)	12 (2%)	0	100	100
6	H	196/237 (83%)	190 (97%)	6 (3%)	0	100	100
7	I	406/432 (94%)	386 (95%)	20 (5%)	0	100	100
7	J	400/432 (93%)	391 (98%)	9 (2%)	0	100	100
8	K	323/333 (97%)	319 (99%)	4 (1%)	0	100	100
8	L	307/333 (92%)	295 (96%)	12 (4%)	0	100	100
8	M	305/333 (92%)	298 (98%)	7 (2%)	0	100	100
8	N	307/333 (92%)	298 (97%)	9 (3%)	0	100	100
8	O	313/333 (94%)	305 (97%)	8 (3%)	0	100	100
8	P	308/333 (92%)	299 (97%)	9 (3%)	0	100	100
8	Q	313/333 (94%)	306 (98%)	7 (2%)	0	100	100
9	R	7/1258 (1%)	7 (100%)	0	0	100	100
9	S	7/1258 (1%)	7 (100%)	0	0	100	100
9	T	7/1258 (1%)	7 (100%)	0	0	100	100
9	U	7/1258 (1%)	7 (100%)	0	0	100	100
9	V	7/1258 (1%)	7 (100%)	0	0	100	100
9	W	7/1258 (1%)	7 (100%)	0	0	100	100
9	X	7/1258 (1%)	6 (86%)	1 (14%)	0	100	100
All	All	5942/15033 (40%)	5795 (98%)	147 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	
4	A	282/307 (92%)	281 (100%)	1 (0%)	84	94
4	B	305/307 (99%)	299 (98%)	6 (2%)	48	78
4	C	305/307 (99%)	297 (97%)	8 (3%)	40	73
4	D	305/307 (99%)	299 (98%)	6 (2%)	48	78
4	E	305/307 (99%)	302 (99%)	3 (1%)	68	89
4	F	304/307 (99%)	301 (99%)	3 (1%)	68	89
5	G	603/614 (98%)	592 (98%)	11 (2%)	51	80
6	H	174/200 (87%)	172 (99%)	2 (1%)	65	88
7	I	363/383 (95%)	342 (94%)	21 (6%)	18	49
7	J	359/383 (94%)	348 (97%)	11 (3%)	35	69
8	K	295/301 (98%)	290 (98%)	5 (2%)	53	82
8	L	283/301 (94%)	280 (99%)	3 (1%)	65	88
8	M	281/301 (93%)	276 (98%)	5 (2%)	51	80
8	N	283/301 (94%)	278 (98%)	5 (2%)	51	80
8	O	288/301 (96%)	284 (99%)	4 (1%)	59	85
8	P	284/301 (94%)	284 (100%)	0	100	100
8	Q	288/301 (96%)	284 (99%)	4 (1%)	59	85
9	R	8/1085 (1%)	8 (100%)	0	100	100
9	S	8/1085 (1%)	8 (100%)	0	100	100
9	T	8/1085 (1%)	8 (100%)	0	100	100
9	U	8/1085 (1%)	8 (100%)	0	100	100
9	V	8/1085 (1%)	8 (100%)	0	100	100
9	W	8/1085 (1%)	8 (100%)	0	100	100
9	X	8/1085 (1%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5363/13124 (41%)	5265 (98%)	98 (2%)	51 80

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	145	GLN
4	B	30	VAL
4	B	64	LEU
4	B	129	VAL
4	B	223	ILE
4	B	228	VAL
4	B	341	PHE
4	C	74	GLU
4	C	113	GLU
4	C	144	ASN
4	C	173	GLU
4	C	203	SER
4	C	256	ILE
4	C	303	PHE
4	C	341	PHE
4	D	1	MET
4	D	30	VAL
4	D	72	LEU
4	D	93	GLN
4	D	144	ASN
4	D	303	PHE
4	E	1	MET
4	E	68	ASN
4	E	303	PHE
4	F	150	THR
4	F	152	ILE
4	F	342	GLN
5	G	38	VAL
5	G	40	LEU
5	G	61	LEU
5	G	136	VAL
5	G	147	TRP
5	G	197	SER
5	G	352	LEU
5	G	433	HIS
5	G	509	GLN
5	G	609	ILE

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Mol	Chain	Res	Type
5	G	629	MET
6	H	2	GLN
6	H	173	GLN
7	I	4	LEU
7	I	46	GLU
7	I	81	LEU
7	I	101	ASP
7	I	115	VAL
7	I	125	HIS
7	I	130	VAL
7	I	136	CYS
7	I	138	GLN
7	I	139	CYS
7	I	140	LEU
7	I	173	TYR
7	I	176	ILE
7	I	198	THR
7	I	204	LEU
7	I	206	ILE
7	I	209	LEU
7	I	224	LEU
7	I	265	VAL
7	I	311	HIS
7	I	324	LEU
7	J	21	LEU
7	J	62	LEU
7	J	122	ILE
7	J	162	GLN
7	J	185	THR
7	J	213	LEU
7	J	265	VAL
7	J	288	THR
7	J	333	LYS
7	J	343	VAL
7	J	405	TYR
8	K	112	ILE
8	K	152	GLN
8	K	153	GLU
8	K	215	LEU
8	K	325	THR
8	L	13	ARG
8	L	75	TYR

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Mol	Chain	Res	Type
8	L	137	LEU
8	M	78	ASN
8	M	79	THR
8	M	100	MET
8	M	123	LYS
8	M	204	LEU
8	N	9	ILE
8	N	148	PHE
8	N	226	VAL
8	N	247	ASN
8	N	255	LEU
8	O	58	LYS
8	O	69	VAL
8	O	72	THR
8	O	216	MET
8	Q	100	MET
8	Q	152	GLN
8	Q	188	GLN
8	Q	302	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	5	ASN
4	C	67	ASN
4	C	83	HIS
4	C	321	ASN
4	C	342	GLN
4	D	62	GLN
4	D	67	ASN
4	E	37	ASN
4	E	145	GLN
4	E	230	GLN
4	F	37	ASN
4	F	144	ASN
4	F	199	ASN
5	G	64	GLN
5	G	130	ASN
5	G	282	ASN
5	G	568	HIS
5	G	607	HIS
6	H	2	GLN

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Mol	Chain	Res	Type
6	H	9	HIS
6	H	29	HIS
6	H	173	GLN
7	I	249	ASN
7	I	276	ASN
7	I	356	GLN
7	I	389	HIS
7	J	105	ASN
7	J	112	ASN
7	J	148	GLN
7	J	307	GLN
7	J	328	ASN
7	J	335	ASN
7	J	372	HIS
8	K	42	GLN
8	K	64	HIS
8	L	24	GLN
8	L	42	GLN
8	L	155	GLN
8	L	252	HIS
8	L	293	ASN
8	M	73	GLN
8	N	42	GLN
8	N	247	ASN
8	O	99	GLN
8	O	156	GLN
8	O	213	GLN
8	O	252	HIS
8	P	22	HIS
8	P	73	GLN
8	Q	42	GLN
8	Q	213	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	59/93 (63%)	26 (44%)	3 (5%)

All (26) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	-5	G
1	1	-4	A
1	1	1	A
1	1	2	C
1	1	6	G
1	1	7	G
1	1	8	G
1	1	10	C
1	1	11	C
1	1	13	C
1	1	14	U
1	1	18	G
1	1	19	A
1	1	20	C
1	1	24	A
1	1	25	U
1	1	26	U
1	1	28	G
1	1	31	A
1	1	32	C
1	1	33	G
1	1	35	G
1	1	36	A
1	1	37	C
1	1	47	A
1	1	52	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	-5	G
1	1	10	C
1	1	31	A

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	ATP	N	402	11	29,33,33	0.36	0	44,52,52	0.52	1 (2%)
10	ATP	K	401	11	29,33,33	0.36	0	44,52,52	0.53	1 (2%)
10	ATP	O	402	11	29,33,33	0.34	0	44,52,52	0.50	1 (2%)
10	ATP	M	401	11	29,33,33	0.34	0	44,52,52	0.52	1 (2%)
10	ATP	P	401	11	29,33,33	0.33	0	44,52,52	0.51	1 (2%)
10	ATP	Q	401	11	29,33,33	0.35	0	44,52,52	0.52	1 (2%)
10	ATP	L	402	11	29,33,33	0.34	0	44,52,52	0.52	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ATP	N	402	11	-	3/22/38/38	0/3/3/3
10	ATP	K	401	11	-	4/22/38/38	0/3/3/3
10	ATP	O	402	11	-	4/22/38/38	0/3/3/3
10	ATP	M	401	11	-	2/22/38/38	0/3/3/3
10	ATP	P	401	11	-	4/22/38/38	0/3/3/3
10	ATP	Q	401	11	-	3/22/38/38	0/3/3/3
10	ATP	L	402	11	-	7/22/38/38	0/3/3/3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	401	ATP	PB-O3B-PG	2.05	139.86	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	M	401	ATP	PB-O3B-PG	2.03	139.80	132.83
10	K	401	ATP	PB-O3B-PG	2.03	139.78	132.83
10	Q	401	ATP	PB-O3B-PG	2.01	139.74	132.83
10	O	402	ATP	PB-O3B-PG	2.01	139.72	132.83
10	L	402	ATP	PB-O3B-PG	2.01	139.71	132.83
10	N	402	ATP	PB-O3B-PG	2.00	139.69	132.83

There are no chirality outliers.

All (27) torsion outliers are listed below:

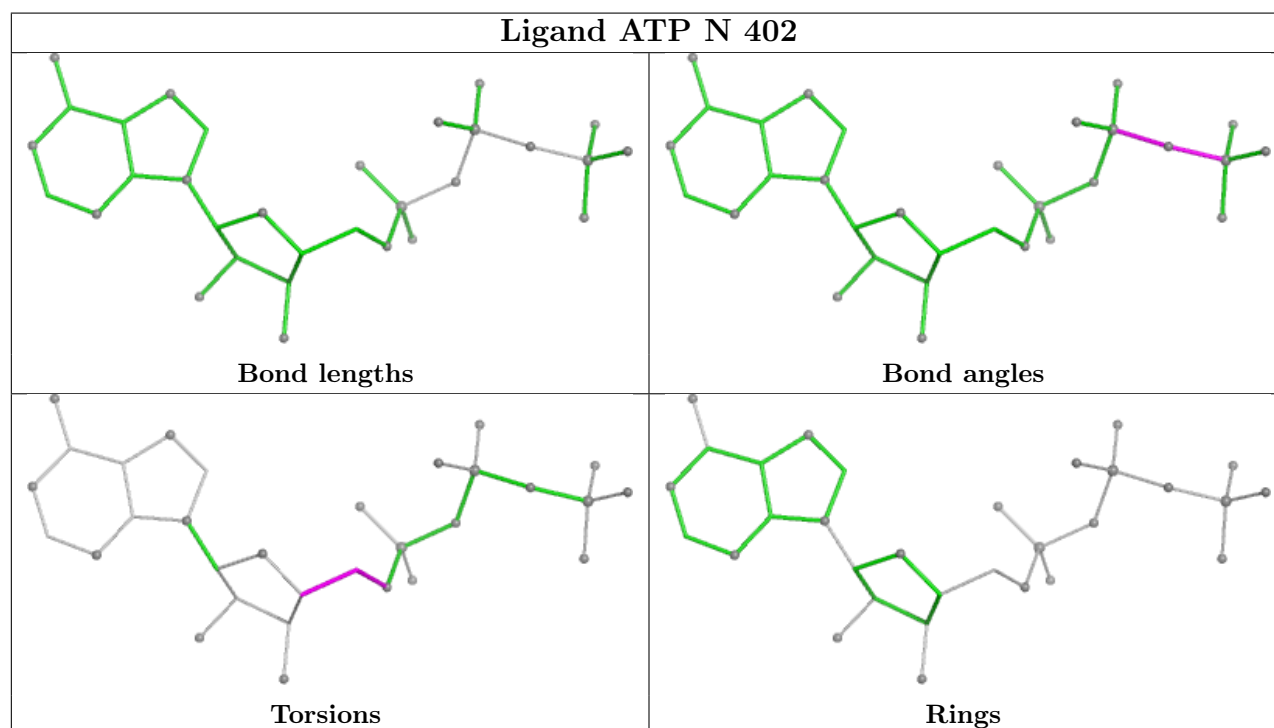
Mol	Chain	Res	Type	Atoms
10	K	401	ATP	O4'-C4'-C5'-O5'
10	L	402	ATP	PB-O3B-PG-O2G
10	L	402	ATP	O4'-C4'-C5'-O5'
10	M	401	ATP	O4'-C4'-C5'-O5'
10	P	401	ATP	PB-O3B-PG-O2G
10	Q	401	ATP	O4'-C4'-C5'-O5'
10	N	402	ATP	O4'-C4'-C5'-O5'
10	O	402	ATP	O4'-C4'-C5'-O5'
10	O	402	ATP	C3'-C4'-C5'-O5'
10	P	401	ATP	O4'-C4'-C5'-O5'
10	Q	401	ATP	C3'-C4'-C5'-O5'
10	K	401	ATP	C3'-C4'-C5'-O5'
10	L	402	ATP	C3'-C4'-C5'-O5'
10	M	401	ATP	C3'-C4'-C5'-O5'
10	N	402	ATP	C3'-C4'-C5'-O5'
10	P	401	ATP	C3'-C4'-C5'-O5'
10	K	401	ATP	PB-O3B-PG-O1G
10	L	402	ATP	PB-O3B-PG-O1G
10	O	402	ATP	PB-O3B-PG-O1G
10	K	401	ATP	PB-O3B-PG-O2G
10	O	402	ATP	PB-O3B-PG-O2G
10	P	401	ATP	PB-O3B-PG-O1G
10	N	402	ATP	C4'-C5'-O5'-PA
10	L	402	ATP	C4'-C5'-O5'-PA
10	Q	401	ATP	C4'-C5'-O5'-PA
10	L	402	ATP	PG-O3B-PB-O2B
10	L	402	ATP	PA-O3A-PB-O2B

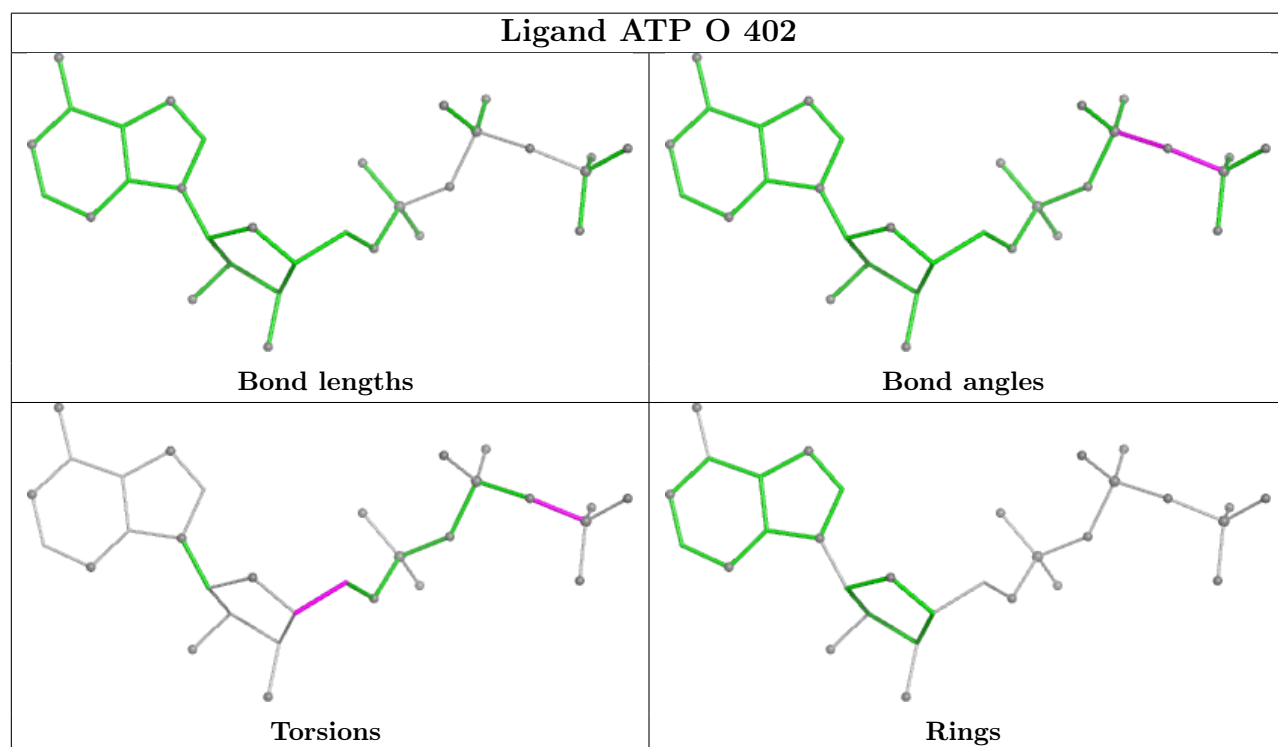
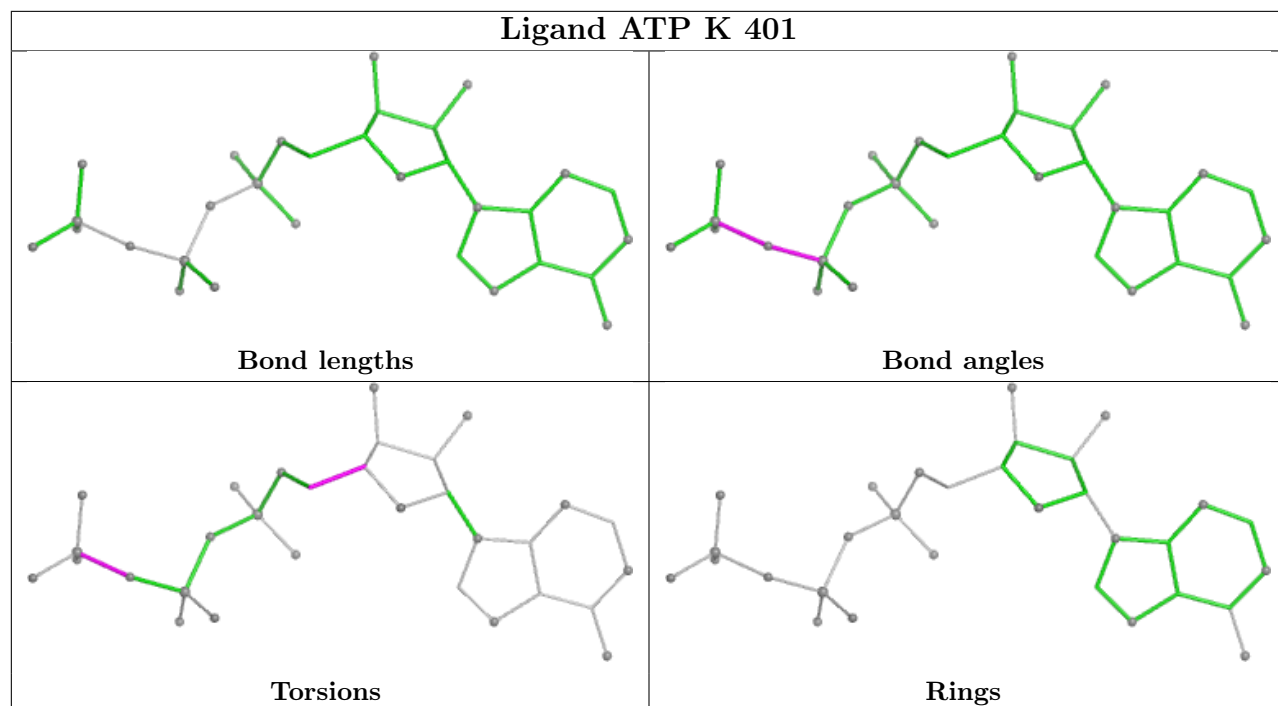
There are no ring outliers.

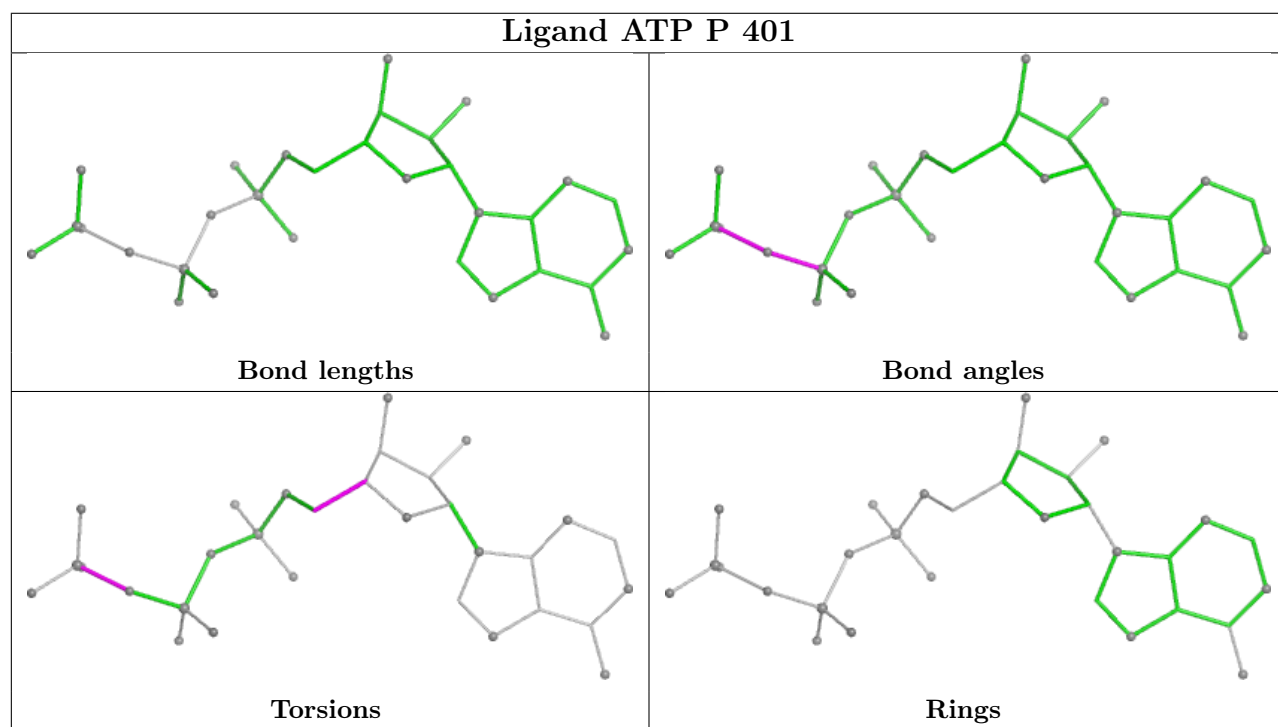
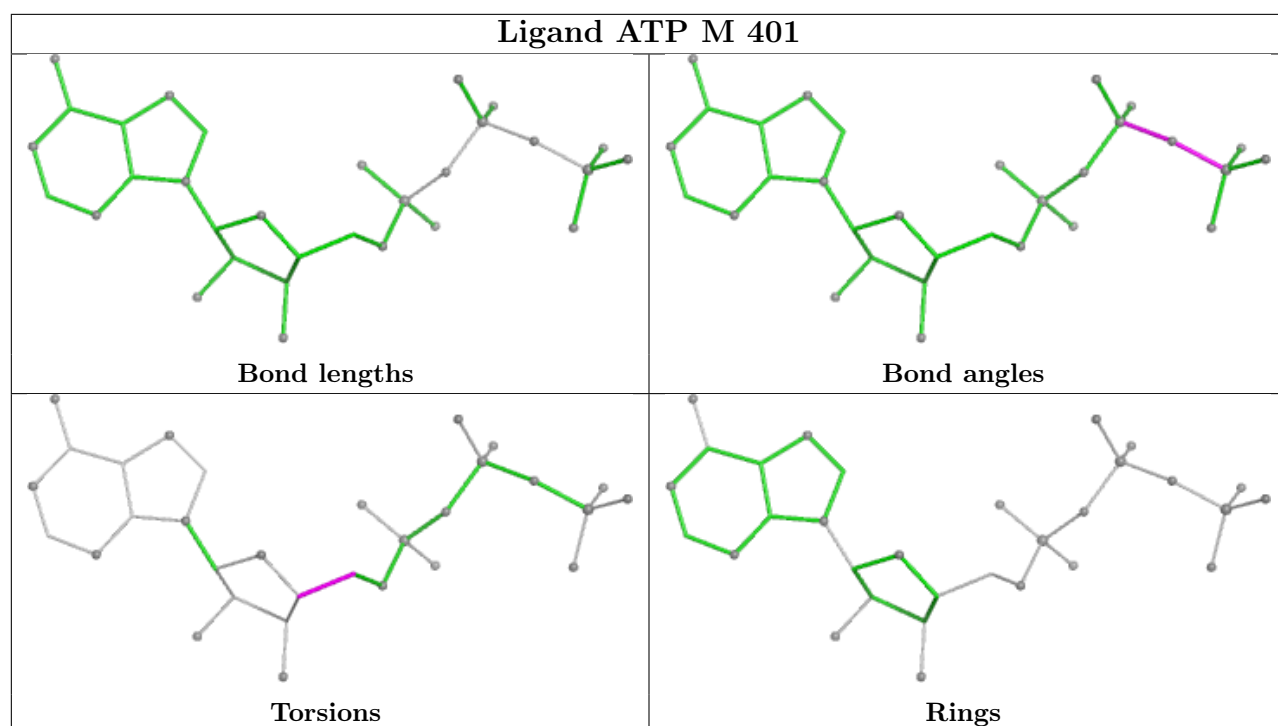
6 monomers are involved in 8 short contacts:

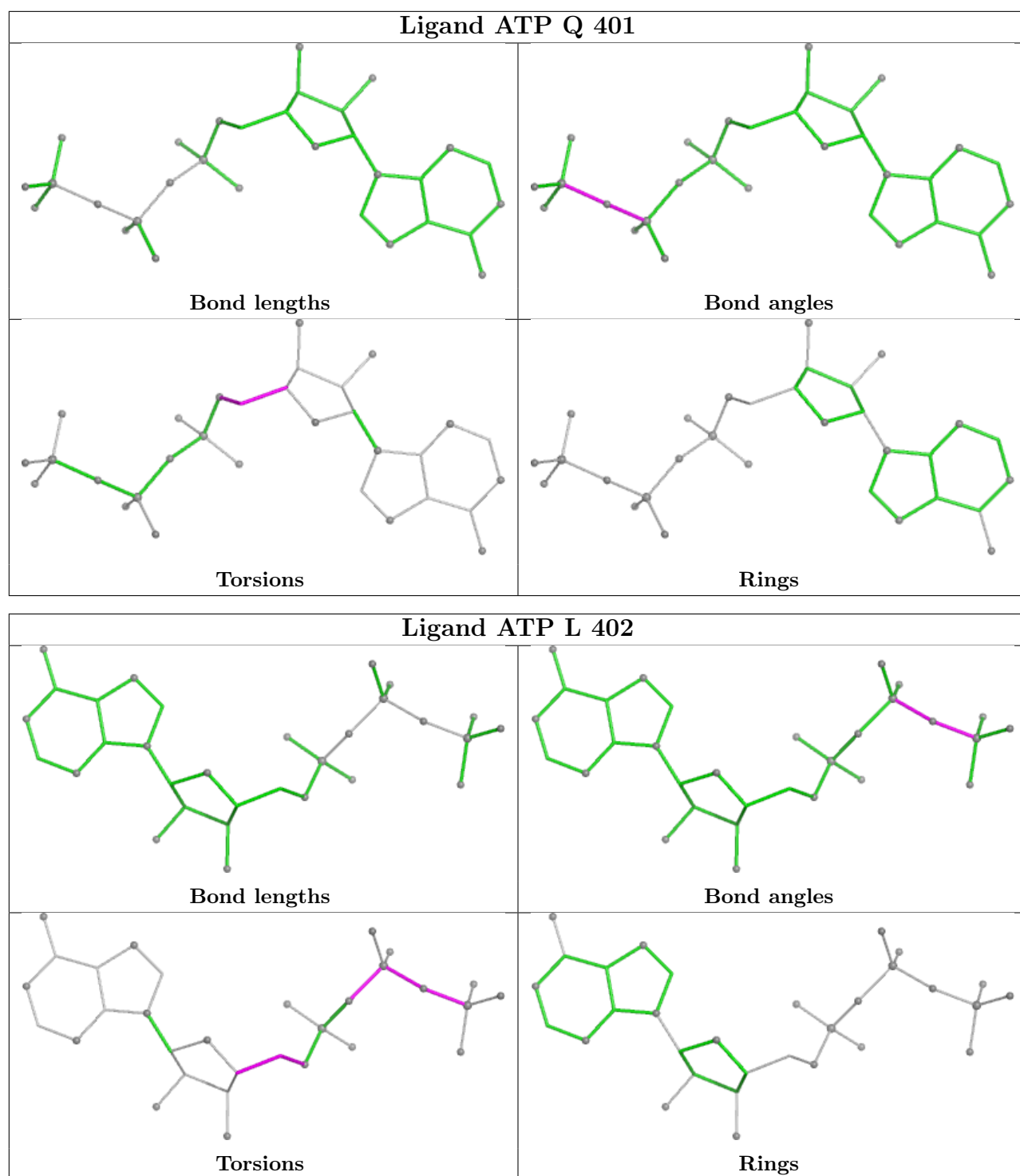
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	N	402	ATP	1	0
10	K	401	ATP	1	0
10	O	402	ATP	2	0
10	M	401	ATP	1	0
10	Q	401	ATP	1	0
10	L	402	ATP	2	0

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









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

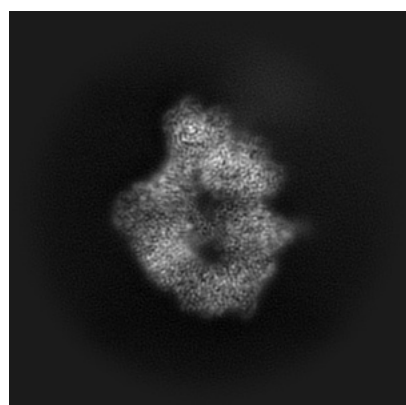
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57739. These allow visual inspection of the internal detail of the map and identification of artifacts.

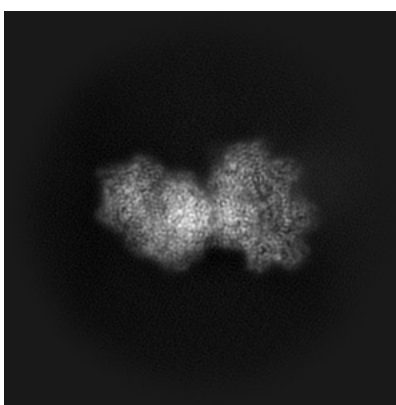
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

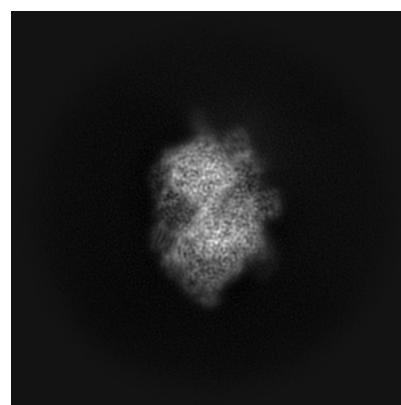
6.1.1 Primary map



X



Y

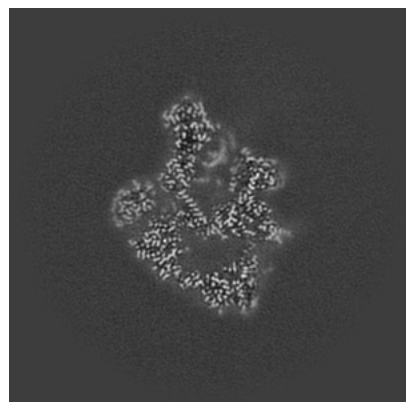


Z

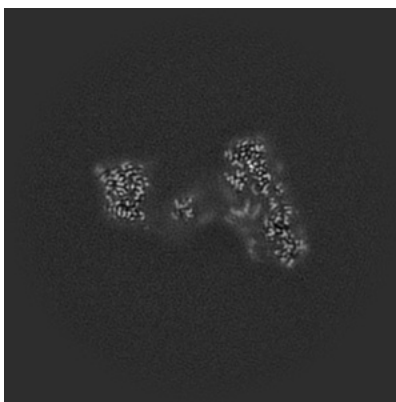
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

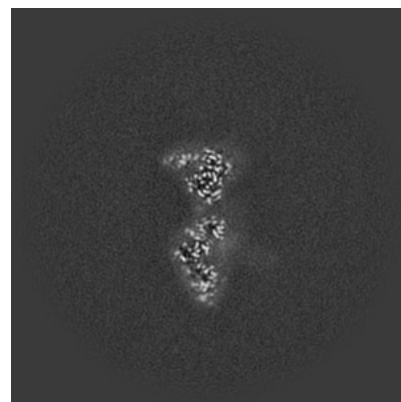
6.2.1 Primary map



X Index: 300



Y Index: 300

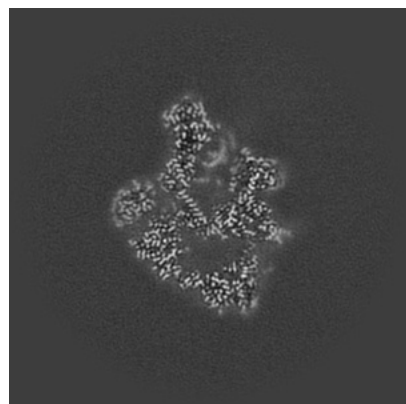


Z Index: 300

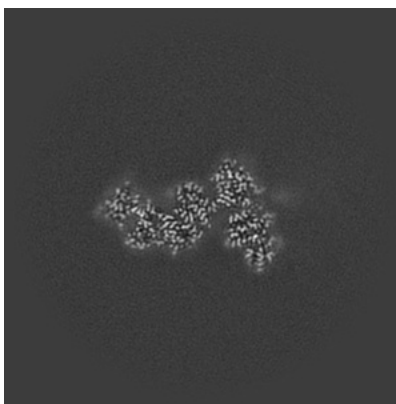
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

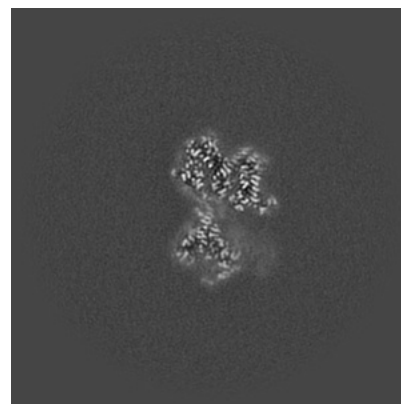
6.3.1 Primary map



X Index: 300



Y Index: 349

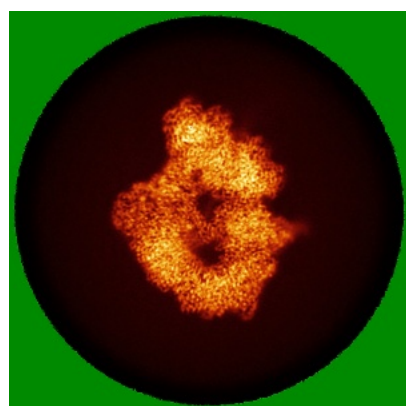


Z Index: 341

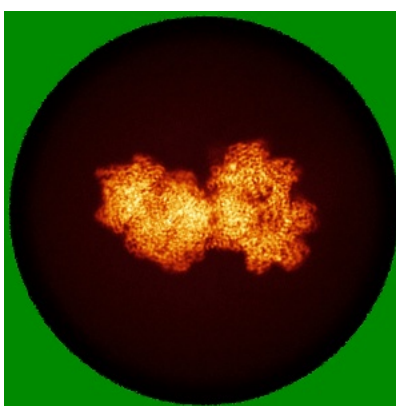
The images above show the largest variance slices of the map in three orthogonal directions.

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

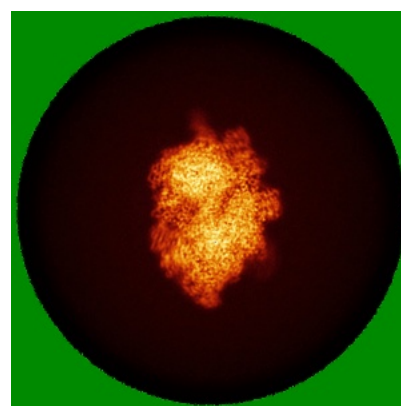
6.4.1 Primary map



X



Y

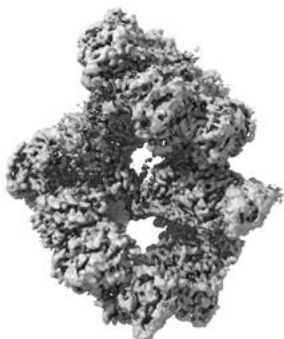


Z

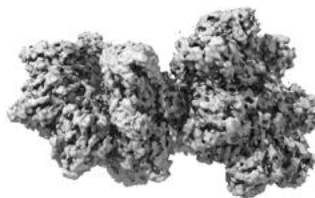
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

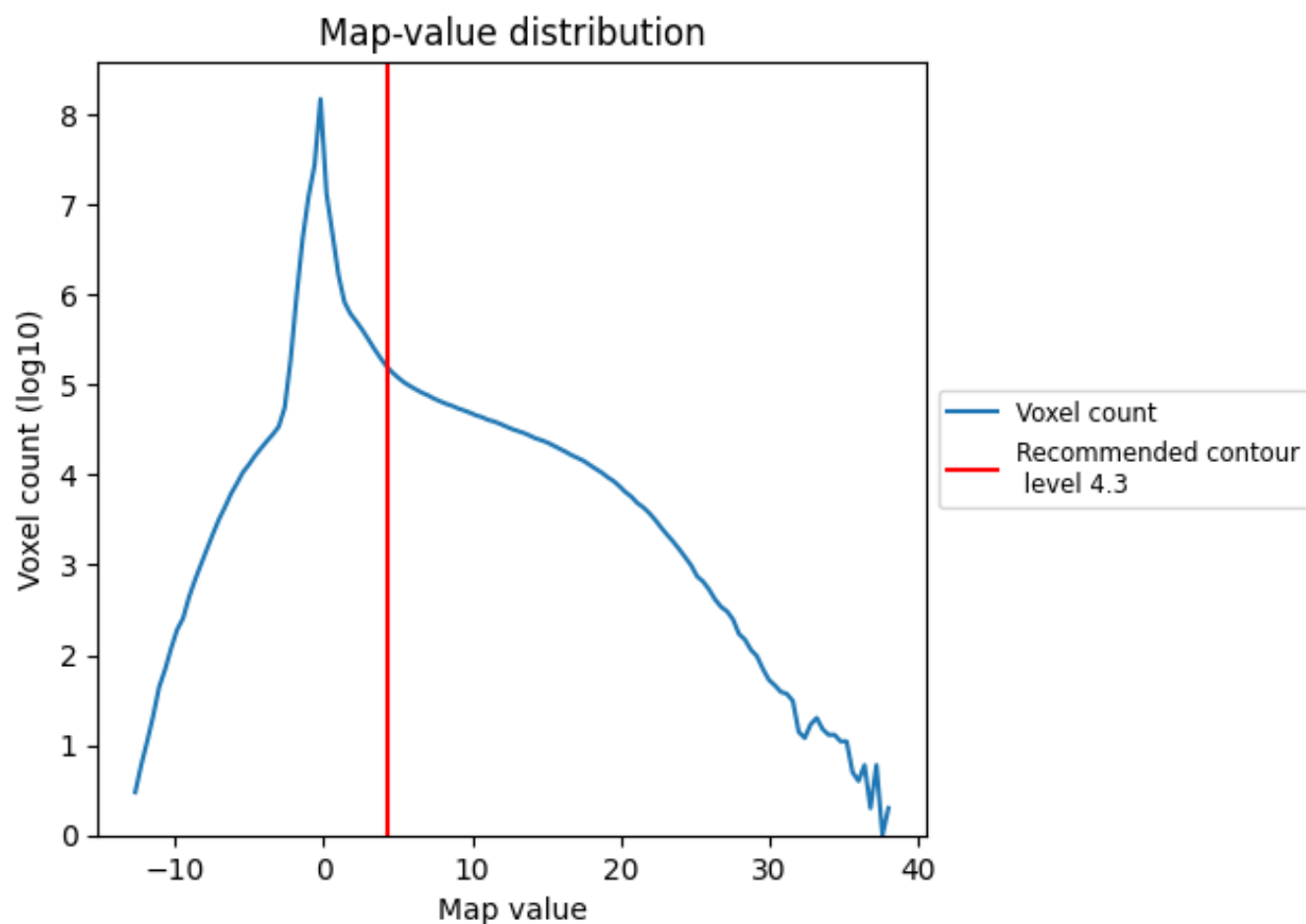
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

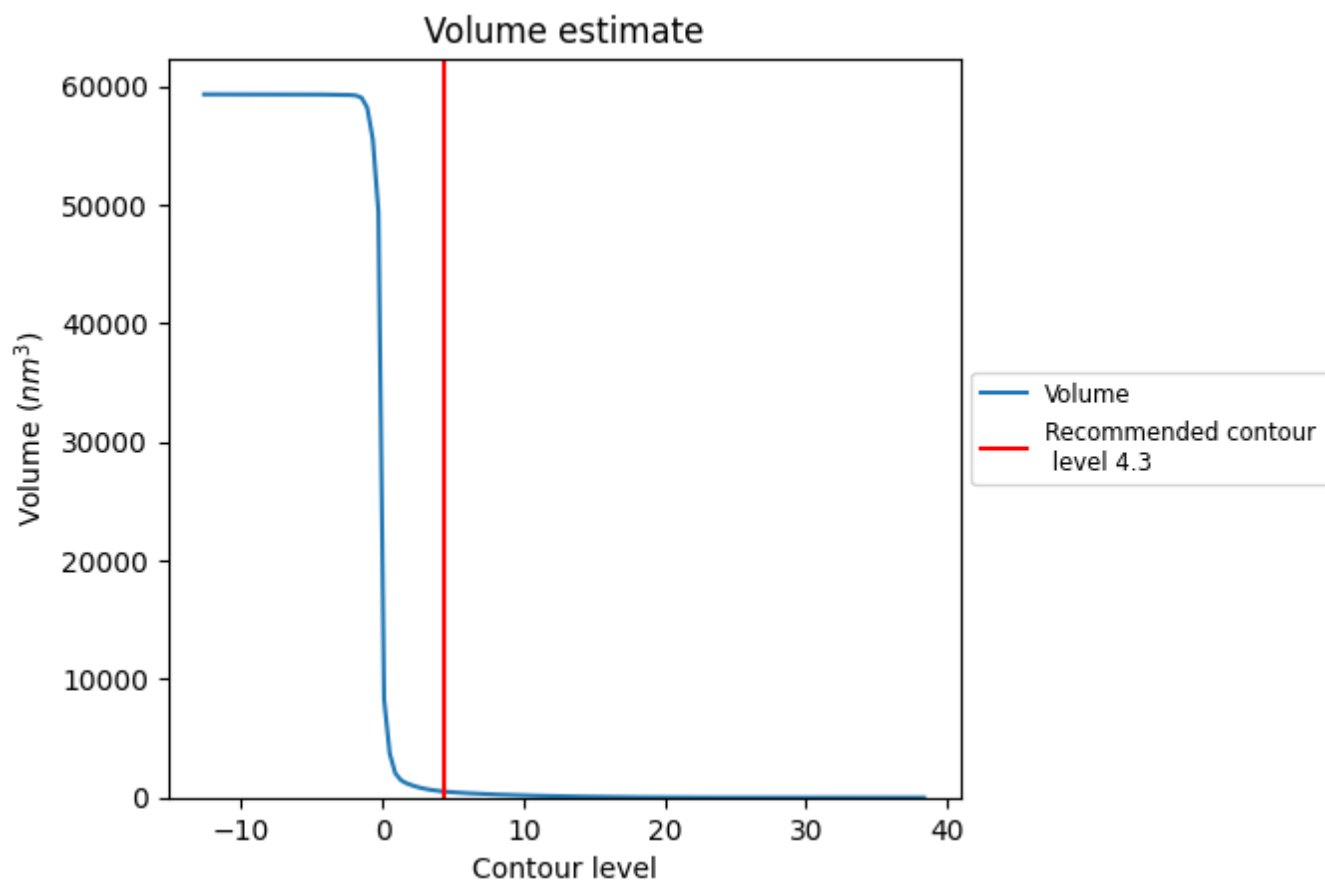
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

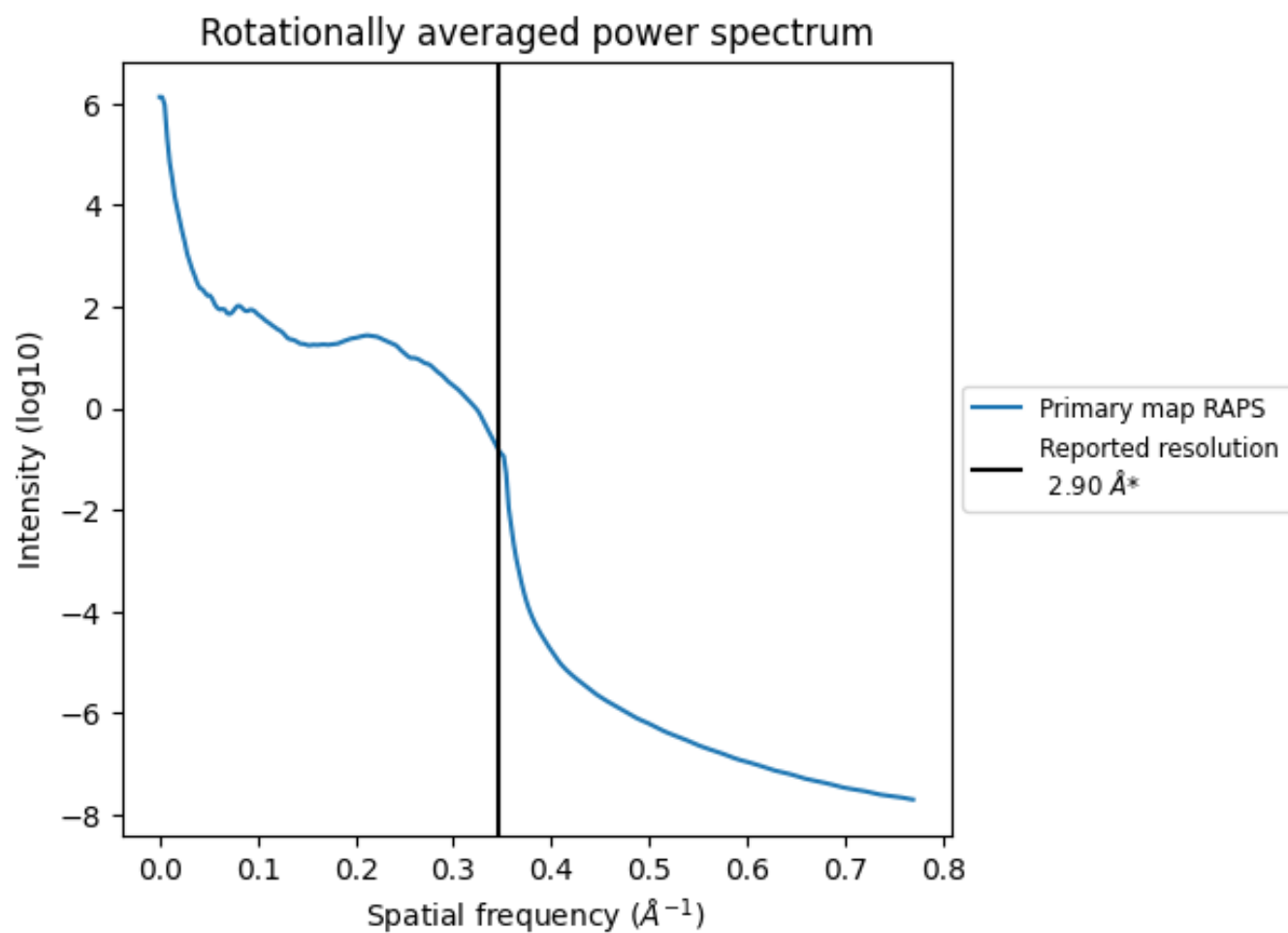
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 517 nm^3 ; this corresponds to an approximate mass of 467 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 0.345 Å⁻¹

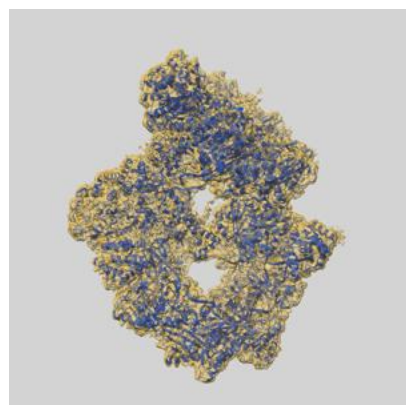
8 Fourier-Shell correlation ⓘ

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

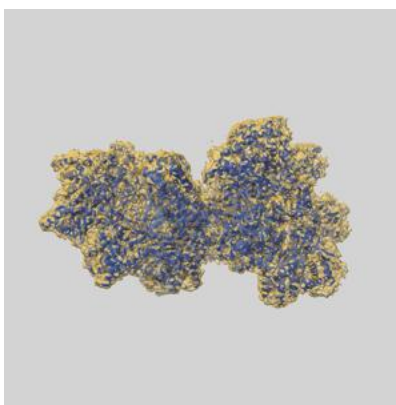
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-57739 and PDB model 30GB. Per-residue inclusion information can be found in [section 3](#) on [page 21](#).

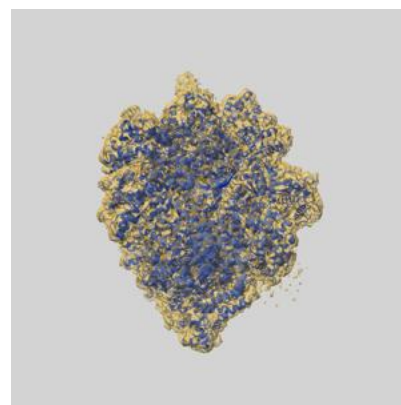
9.1 Map-model overlay [i](#)



X



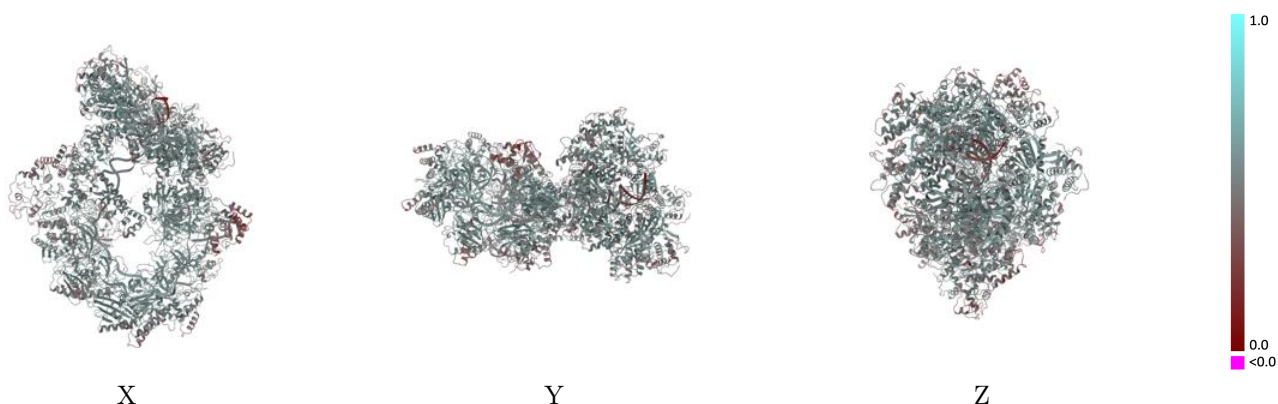
Y



Z

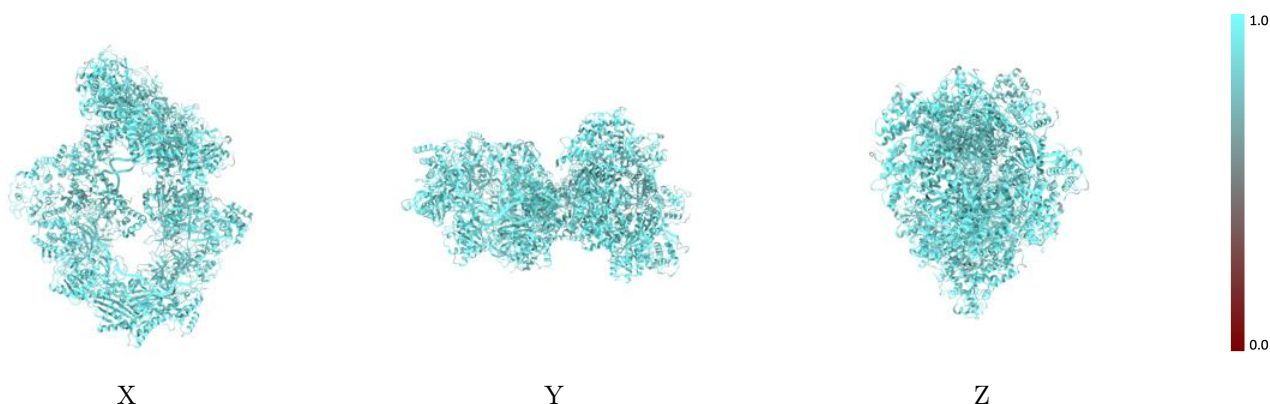
The images above show the 3D surface view of the map at the recommended contour level 4.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



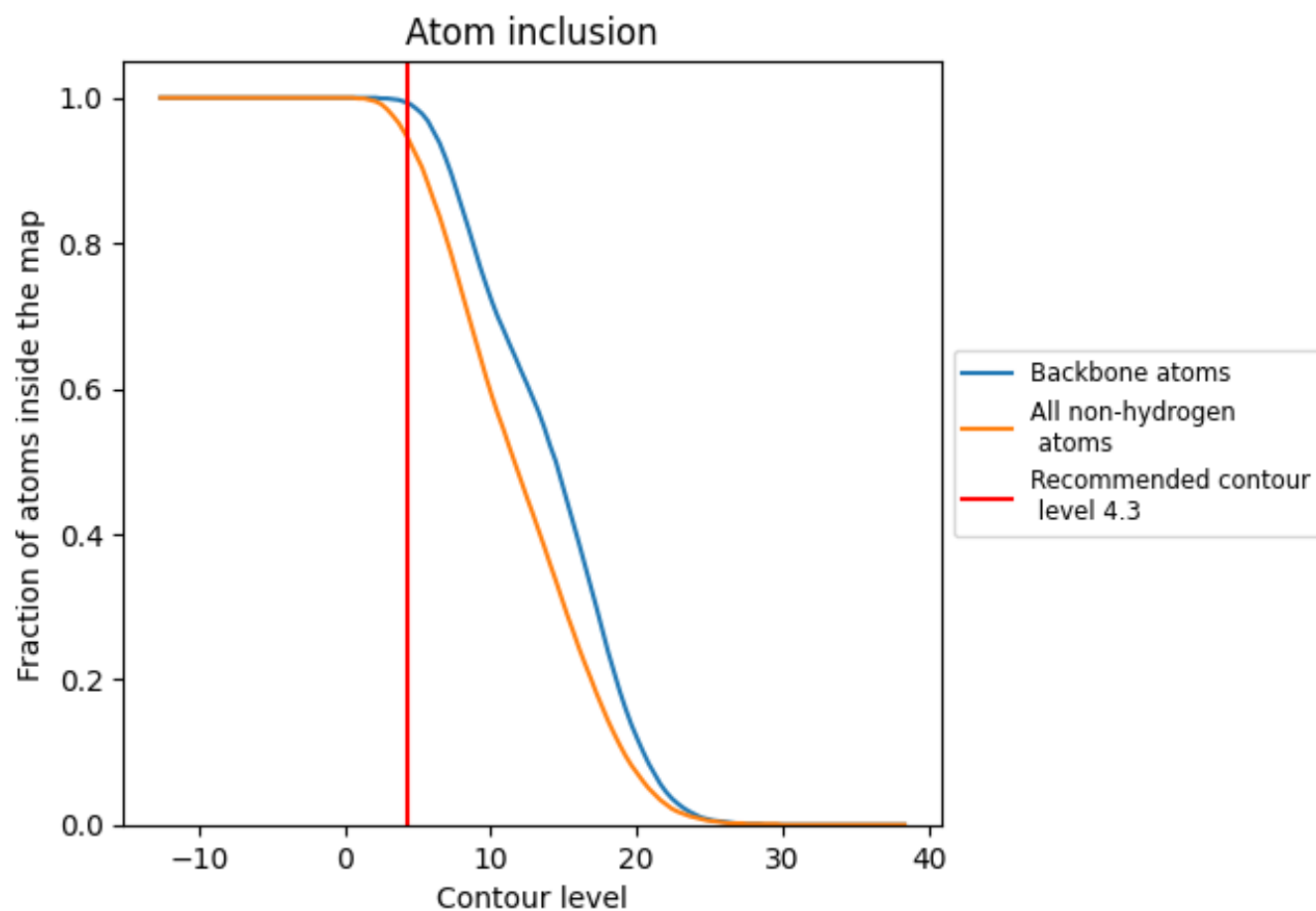
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.3).

























































9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 94% 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 (4.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9450	 0.5170
1	 0.9820	 0.5320
2	 0.9760	 0.4860
3	 0.9720	 0.4490
A	 0.9510	 0.5410
B	 0.9540	 0.5420
C	 0.9580	 0.5380
D	 0.9600	 0.5410
E	 0.9510	 0.5400
F	 0.9450	 0.5330
G	 0.9420	 0.5180
H	 0.9250	 0.4470
I	 0.9320	 0.4650
J	 0.9520	 0.5210
K	 0.9500	 0.5330
L	 0.9330	 0.5020
M	 0.9270	 0.5040
N	 0.9420	 0.5230
O	 0.9450	 0.5260
P	 0.9470	 0.5130
Q	 0.9520	 0.5320
R	 0.6960	 0.3400
S	 0.6960	 0.3590
T	 0.6960	 0.3710
U	 0.7220	 0.3610
V	 0.7220	 0.3660
W	 0.6960	 0.4190
X	 0.6960	 0.4120

