Full wwPDB EM Validation Report ⓘ

Apr 14, 2024 – 12:36 AM JST

PDB ID	:	8XON
EMDB ID	:	EMD-38535
Title	:	Cryo-EM structure of the ClpC1:ClpP1P2 degradation complex in Streptomyces hawaiiensis
Authors	:	Xu, X.; Long, F.
Deposited on	:	2024-01-01
Resolution	:	1.96 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:

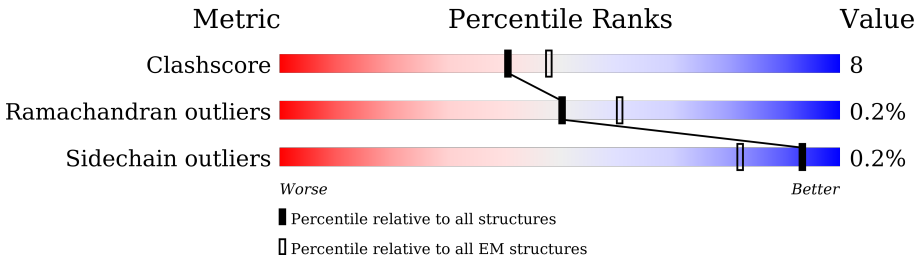
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.96 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	O	696	23% 61% 24% 15%
1	P	696	6% 68% 18% 15%
1	Q	696	70% 15% 15%
1	R	696	72% 14% 15%
1	S	696	69% 16% 15%
1	T	696	42% 61% 24% 15%
2	X	24	29% 92% 8%
3	A	226	62% 17% 21%

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Mol	Chain	Length	Quality of chain
3	B	226	60% 19% 21%
3	C	226	66% 12% 21%
3	D	226	68% 11% 21%
3	E	226	66% 13% 21%
3	F	226	66% 13% 21%
3	G	226	65% 13% 21%
4	H	207	76% 10% 14%
4	I	207	80% 8% 12%
4	J	207	71% 14% 15%
4	K	207	71% 14% 15%
4	L	207	72% 14% 14%
4	M	207	77% 9% 14%
4	N	207	74% 11% 14%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 47409 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NDP-hexose 4-ketoreductase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	S	592	Total	C	N	O	S	0	0
			4636	2915	826	886	9		
1	R	592	Total	C	N	O	S	0	0
			4636	2915	826	886	9		
1	Q	592	Total	C	N	O	S	0	0
			4636	2915	826	886	9		
1	P	592	Total	C	N	O	S	0	0
			4636	2915	826	886	9		
1	O	593	Total	C	N	O	S	0	0
			4640	2917	827	887	9		
1	T	592	Total	C	N	O	S	0	0
			4632	2912	825	886	9		

There are 234 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	121	MET	-	initiating methionine	UNP A0A6G5RIJ6
S	122	GLY	-	expression tag	UNP A0A6G5RIJ6
S	123	SER	-	expression tag	UNP A0A6G5RIJ6
S	124	SER	-	expression tag	UNP A0A6G5RIJ6
S	125	HIS	-	expression tag	UNP A0A6G5RIJ6
S	126	HIS	-	expression tag	UNP A0A6G5RIJ6
S	127	HIS	-	expression tag	UNP A0A6G5RIJ6
S	128	HIS	-	expression tag	UNP A0A6G5RIJ6
S	129	HIS	-	expression tag	UNP A0A6G5RIJ6
S	130	HIS	-	expression tag	UNP A0A6G5RIJ6
S	131	SER	-	expression tag	UNP A0A6G5RIJ6
S	132	SER	-	expression tag	UNP A0A6G5RIJ6
S	133	GLY	-	expression tag	UNP A0A6G5RIJ6
S	134	LEU	-	expression tag	UNP A0A6G5RIJ6
S	135	VAL	-	expression tag	UNP A0A6G5RIJ6
S	136	PRO	-	expression tag	UNP A0A6G5RIJ6
S	137	ARG	-	expression tag	UNP A0A6G5RIJ6
S	138	GLY	-	expression tag	UNP A0A6G5RIJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
S	139	SER	-	expression tag	UNP A0A6G5RIJ6
S	140	HIS	-	expression tag	UNP A0A6G5RIJ6
S	141	MET	-	expression tag	UNP A0A6G5RIJ6
S	142	ALA	-	expression tag	UNP A0A6G5RIJ6
S	143	SER	-	expression tag	UNP A0A6G5RIJ6
S	144	MET	-	expression tag	UNP A0A6G5RIJ6
S	145	THR	-	expression tag	UNP A0A6G5RIJ6
S	146	GLY	-	expression tag	UNP A0A6G5RIJ6
S	147	GLY	-	expression tag	UNP A0A6G5RIJ6
S	148	GLN	-	expression tag	UNP A0A6G5RIJ6
S	149	GLN	-	expression tag	UNP A0A6G5RIJ6
S	150	MET	-	expression tag	UNP A0A6G5RIJ6
S	151	GLY	-	expression tag	UNP A0A6G5RIJ6
S	152	ARG	-	expression tag	UNP A0A6G5RIJ6
S	153	GLY	-	expression tag	UNP A0A6G5RIJ6
S	154	SER	-	expression tag	UNP A0A6G5RIJ6
S	155	GLU	-	expression tag	UNP A0A6G5RIJ6
S	156	PHE	-	expression tag	UNP A0A6G5RIJ6
S	284	ALA	GLU	engineered mutation	UNP A0A6G5RIJ6
S	440	ALA	PHE	engineered mutation	UNP A0A6G5RIJ6
S	622	ALA	GLU	engineered mutation	UNP A0A6G5RIJ6
R	121	MET	-	initiating methionine	UNP A0A6G5RIJ6
R	122	GLY	-	expression tag	UNP A0A6G5RIJ6
R	123	SER	-	expression tag	UNP A0A6G5RIJ6
R	124	SER	-	expression tag	UNP A0A6G5RIJ6
R	125	HIS	-	expression tag	UNP A0A6G5RIJ6
R	126	HIS	-	expression tag	UNP A0A6G5RIJ6
R	127	HIS	-	expression tag	UNP A0A6G5RIJ6
R	128	HIS	-	expression tag	UNP A0A6G5RIJ6
R	129	HIS	-	expression tag	UNP A0A6G5RIJ6
R	130	HIS	-	expression tag	UNP A0A6G5RIJ6
R	131	SER	-	expression tag	UNP A0A6G5RIJ6
R	132	SER	-	expression tag	UNP A0A6G5RIJ6
R	133	GLY	-	expression tag	UNP A0A6G5RIJ6
R	134	LEU	-	expression tag	UNP A0A6G5RIJ6
R	135	VAL	-	expression tag	UNP A0A6G5RIJ6
R	136	PRO	-	expression tag	UNP A0A6G5RIJ6
R	137	ARG	-	expression tag	UNP A0A6G5RIJ6
R	138	GLY	-	expression tag	UNP A0A6G5RIJ6
R	139	SER	-	expression tag	UNP A0A6G5RIJ6
R	140	HIS	-	expression tag	UNP A0A6G5RIJ6
R	141	MET	-	expression tag	UNP A0A6G5RIJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
R	142	ALA	-	expression tag	UNP A0A6G5RIJ6
R	143	SER	-	expression tag	UNP A0A6G5RIJ6
R	144	MET	-	expression tag	UNP A0A6G5RIJ6
R	145	THR	-	expression tag	UNP A0A6G5RIJ6
R	146	GLY	-	expression tag	UNP A0A6G5RIJ6
R	147	GLY	-	expression tag	UNP A0A6G5RIJ6
R	148	GLN	-	expression tag	UNP A0A6G5RIJ6
R	149	GLN	-	expression tag	UNP A0A6G5RIJ6
R	150	MET	-	expression tag	UNP A0A6G5RIJ6
R	151	GLY	-	expression tag	UNP A0A6G5RIJ6
R	152	ARG	-	expression tag	UNP A0A6G5RIJ6
R	153	GLY	-	expression tag	UNP A0A6G5RIJ6
R	154	SER	-	expression tag	UNP A0A6G5RIJ6
R	155	GLU	-	expression tag	UNP A0A6G5RIJ6
R	156	PHE	-	expression tag	UNP A0A6G5RIJ6
R	284	ALA	GLU	engineered mutation	UNP A0A6G5RIJ6
R	440	ALA	PHE	engineered mutation	UNP A0A6G5RIJ6
R	622	ALA	GLU	engineered mutation	UNP A0A6G5RIJ6
Q	121	MET	-	initiating methionine	UNP A0A6G5RIJ6
Q	122	GLY	-	expression tag	UNP A0A6G5RIJ6
Q	123	SER	-	expression tag	UNP A0A6G5RIJ6
Q	124	SER	-	expression tag	UNP A0A6G5RIJ6
Q	125	HIS	-	expression tag	UNP A0A6G5RIJ6
Q	126	HIS	-	expression tag	UNP A0A6G5RIJ6
Q	127	HIS	-	expression tag	UNP A0A6G5RIJ6
Q	128	HIS	-	expression tag	UNP A0A6G5RIJ6
Q	129	HIS	-	expression tag	UNP A0A6G5RIJ6
Q	130	HIS	-	expression tag	UNP A0A6G5RIJ6
Q	131	SER	-	expression tag	UNP A0A6G5RIJ6
Q	132	SER	-	expression tag	UNP A0A6G5RIJ6
Q	133	GLY	-	expression tag	UNP A0A6G5RIJ6
Q	134	LEU	-	expression tag	UNP A0A6G5RIJ6
Q	135	VAL	-	expression tag	UNP A0A6G5RIJ6
Q	136	PRO	-	expression tag	UNP A0A6G5RIJ6
Q	137	ARG	-	expression tag	UNP A0A6G5RIJ6
Q	138	GLY	-	expression tag	UNP A0A6G5RIJ6
Q	139	SER	-	expression tag	UNP A0A6G5RIJ6
Q	140	HIS	-	expression tag	UNP A0A6G5RIJ6
Q	141	MET	-	expression tag	UNP A0A6G5RIJ6
Q	142	ALA	-	expression tag	UNP A0A6G5RIJ6
Q	143	SER	-	expression tag	UNP A0A6G5RIJ6
Q	144	MET	-	expression tag	UNP A0A6G5RIJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
Q	145	THR	-	expression tag	UNP A0A6G5RIJ6
Q	146	GLY	-	expression tag	UNP A0A6G5RIJ6
Q	147	GLY	-	expression tag	UNP A0A6G5RIJ6
Q	148	GLN	-	expression tag	UNP A0A6G5RIJ6
Q	149	GLN	-	expression tag	UNP A0A6G5RIJ6
Q	150	MET	-	expression tag	UNP A0A6G5RIJ6
Q	151	GLY	-	expression tag	UNP A0A6G5RIJ6
Q	152	ARG	-	expression tag	UNP A0A6G5RIJ6
Q	153	GLY	-	expression tag	UNP A0A6G5RIJ6
Q	154	SER	-	expression tag	UNP A0A6G5RIJ6
Q	155	GLU	-	expression tag	UNP A0A6G5RIJ6
Q	156	PHE	-	expression tag	UNP A0A6G5RIJ6
Q	284	ALA	GLU	engineered mutation	UNP A0A6G5RIJ6
Q	440	ALA	PHE	engineered mutation	UNP A0A6G5RIJ6
Q	622	ALA	GLU	engineered mutation	UNP A0A6G5RIJ6
P	121	MET	-	initiating methionine	UNP A0A6G5RIJ6
P	122	GLY	-	expression tag	UNP A0A6G5RIJ6
P	123	SER	-	expression tag	UNP A0A6G5RIJ6
P	124	SER	-	expression tag	UNP A0A6G5RIJ6
P	125	HIS	-	expression tag	UNP A0A6G5RIJ6
P	126	HIS	-	expression tag	UNP A0A6G5RIJ6
P	127	HIS	-	expression tag	UNP A0A6G5RIJ6
P	128	HIS	-	expression tag	UNP A0A6G5RIJ6
P	129	HIS	-	expression tag	UNP A0A6G5RIJ6
P	130	HIS	-	expression tag	UNP A0A6G5RIJ6
P	131	SER	-	expression tag	UNP A0A6G5RIJ6
P	132	SER	-	expression tag	UNP A0A6G5RIJ6
P	133	GLY	-	expression tag	UNP A0A6G5RIJ6
P	134	LEU	-	expression tag	UNP A0A6G5RIJ6
P	135	VAL	-	expression tag	UNP A0A6G5RIJ6
P	136	PRO	-	expression tag	UNP A0A6G5RIJ6
P	137	ARG	-	expression tag	UNP A0A6G5RIJ6
P	138	GLY	-	expression tag	UNP A0A6G5RIJ6
P	139	SER	-	expression tag	UNP A0A6G5RIJ6
P	140	HIS	-	expression tag	UNP A0A6G5RIJ6
P	141	MET	-	expression tag	UNP A0A6G5RIJ6
P	142	ALA	-	expression tag	UNP A0A6G5RIJ6
P	143	SER	-	expression tag	UNP A0A6G5RIJ6
P	144	MET	-	expression tag	UNP A0A6G5RIJ6
P	145	THR	-	expression tag	UNP A0A6G5RIJ6
P	146	GLY	-	expression tag	UNP A0A6G5RIJ6
P	147	GLY	-	expression tag	UNP A0A6G5RIJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
P	148	GLN	-	expression tag	UNP A0A6G5RIJ6
P	149	GLN	-	expression tag	UNP A0A6G5RIJ6
P	150	MET	-	expression tag	UNP A0A6G5RIJ6
P	151	GLY	-	expression tag	UNP A0A6G5RIJ6
P	152	ARG	-	expression tag	UNP A0A6G5RIJ6
P	153	GLY	-	expression tag	UNP A0A6G5RIJ6
P	154	SER	-	expression tag	UNP A0A6G5RIJ6
P	155	GLU	-	expression tag	UNP A0A6G5RIJ6
P	156	PHE	-	expression tag	UNP A0A6G5RIJ6
P	284	ALA	GLU	engineered mutation	UNP A0A6G5RIJ6
P	440	ALA	PHE	engineered mutation	UNP A0A6G5RIJ6
P	622	ALA	GLU	engineered mutation	UNP A0A6G5RIJ6
O	121	MET	-	initiating methionine	UNP A0A6G5RIJ6
O	122	GLY	-	expression tag	UNP A0A6G5RIJ6
O	123	SER	-	expression tag	UNP A0A6G5RIJ6
O	124	SER	-	expression tag	UNP A0A6G5RIJ6
O	125	HIS	-	expression tag	UNP A0A6G5RIJ6
O	126	HIS	-	expression tag	UNP A0A6G5RIJ6
O	127	HIS	-	expression tag	UNP A0A6G5RIJ6
O	128	HIS	-	expression tag	UNP A0A6G5RIJ6
O	129	HIS	-	expression tag	UNP A0A6G5RIJ6
O	130	HIS	-	expression tag	UNP A0A6G5RIJ6
O	131	SER	-	expression tag	UNP A0A6G5RIJ6
O	132	SER	-	expression tag	UNP A0A6G5RIJ6
O	133	GLY	-	expression tag	UNP A0A6G5RIJ6
O	134	LEU	-	expression tag	UNP A0A6G5RIJ6
O	135	VAL	-	expression tag	UNP A0A6G5RIJ6
O	136	PRO	-	expression tag	UNP A0A6G5RIJ6
O	137	ARG	-	expression tag	UNP A0A6G5RIJ6
O	138	GLY	-	expression tag	UNP A0A6G5RIJ6
O	139	SER	-	expression tag	UNP A0A6G5RIJ6
O	140	HIS	-	expression tag	UNP A0A6G5RIJ6
O	141	MET	-	expression tag	UNP A0A6G5RIJ6
O	142	ALA	-	expression tag	UNP A0A6G5RIJ6
O	143	SER	-	expression tag	UNP A0A6G5RIJ6
O	144	MET	-	expression tag	UNP A0A6G5RIJ6
O	145	THR	-	expression tag	UNP A0A6G5RIJ6
O	146	GLY	-	expression tag	UNP A0A6G5RIJ6
O	147	GLY	-	expression tag	UNP A0A6G5RIJ6
O	148	GLN	-	expression tag	UNP A0A6G5RIJ6
O	149	GLN	-	expression tag	UNP A0A6G5RIJ6
O	150	MET	-	expression tag	UNP A0A6G5RIJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
O	151	GLY	-	expression tag	UNP A0A6G5RIJ6
O	152	ARG	-	expression tag	UNP A0A6G5RIJ6
O	153	GLY	-	expression tag	UNP A0A6G5RIJ6
O	154	SER	-	expression tag	UNP A0A6G5RIJ6
O	155	GLU	-	expression tag	UNP A0A6G5RIJ6
O	156	PHE	-	expression tag	UNP A0A6G5RIJ6
O	284	ALA	GLU	engineered mutation	UNP A0A6G5RIJ6
O	440	ALA	PHE	engineered mutation	UNP A0A6G5RIJ6
O	622	ALA	GLU	engineered mutation	UNP A0A6G5RIJ6
T	121	MET	-	initiating methionine	UNP A0A6G5RIJ6
T	122	GLY	-	expression tag	UNP A0A6G5RIJ6
T	123	SER	-	expression tag	UNP A0A6G5RIJ6
T	124	SER	-	expression tag	UNP A0A6G5RIJ6
T	125	HIS	-	expression tag	UNP A0A6G5RIJ6
T	126	HIS	-	expression tag	UNP A0A6G5RIJ6
T	127	HIS	-	expression tag	UNP A0A6G5RIJ6
T	128	HIS	-	expression tag	UNP A0A6G5RIJ6
T	129	HIS	-	expression tag	UNP A0A6G5RIJ6
T	130	HIS	-	expression tag	UNP A0A6G5RIJ6
T	131	SER	-	expression tag	UNP A0A6G5RIJ6
T	132	SER	-	expression tag	UNP A0A6G5RIJ6
T	133	GLY	-	expression tag	UNP A0A6G5RIJ6
T	134	LEU	-	expression tag	UNP A0A6G5RIJ6
T	135	VAL	-	expression tag	UNP A0A6G5RIJ6
T	136	PRO	-	expression tag	UNP A0A6G5RIJ6
T	137	ARG	-	expression tag	UNP A0A6G5RIJ6
T	138	GLY	-	expression tag	UNP A0A6G5RIJ6
T	139	SER	-	expression tag	UNP A0A6G5RIJ6
T	140	HIS	-	expression tag	UNP A0A6G5RIJ6
T	141	MET	-	expression tag	UNP A0A6G5RIJ6
T	142	ALA	-	expression tag	UNP A0A6G5RIJ6
T	143	SER	-	expression tag	UNP A0A6G5RIJ6
T	144	MET	-	expression tag	UNP A0A6G5RIJ6
T	145	THR	-	expression tag	UNP A0A6G5RIJ6
T	146	GLY	-	expression tag	UNP A0A6G5RIJ6
T	147	GLY	-	expression tag	UNP A0A6G5RIJ6
T	148	GLN	-	expression tag	UNP A0A6G5RIJ6
T	149	GLN	-	expression tag	UNP A0A6G5RIJ6
T	150	MET	-	expression tag	UNP A0A6G5RIJ6
T	151	GLY	-	expression tag	UNP A0A6G5RIJ6
T	152	ARG	-	expression tag	UNP A0A6G5RIJ6
T	153	GLY	-	expression tag	UNP A0A6G5RIJ6

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Chain	Residue	Modelled	Actual	Comment	Reference
T	154	SER	-	expression tag	UNP A0A6G5RIJ6
T	155	GLU	-	expression tag	UNP A0A6G5RIJ6
T	156	PHE	-	expression tag	UNP A0A6G5RIJ6
T	284	ALA	GLU	engineered mutation	UNP A0A6G5RIJ6
T	440	ALA	PHE	engineered mutation	UNP A0A6G5RIJ6
T	622	ALA	GLU	engineered mutation	UNP A0A6G5RIJ6

- Molecule 2 is a protein called casein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	X	24	Total	C	N	O	0	0
			120	72	24	24		

- Molecule 3 is a protein called ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	178	Total	C	N	O	S	0	0
			1369	863	234	266	6		
3	B	178	Total	C	N	O	S	0	0
			1369	863	234	266	6		
3	C	178	Total	C	N	O	S	0	0
			1369	863	234	266	6		
3	D	178	Total	C	N	O	S	0	0
			1369	863	234	266	6		
3	E	178	Total	C	N	O	S	0	0
			1369	863	234	266	6		
3	F	178	Total	C	N	O	S	0	0
			1369	863	234	266	6		
3	G	178	Total	C	N	O	S	0	0
			1369	863	234	266	6		

There are 259 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP A0A5B9BGY8
A	-5	GLY	-	expression tag	UNP A0A5B9BGY8
A	-4	SER	-	expression tag	UNP A0A5B9BGY8
A	-3	SER	-	expression tag	UNP A0A5B9BGY8
A	-2	HIS	-	expression tag	UNP A0A5B9BGY8
A	-1	HIS	-	expression tag	UNP A0A5B9BGY8
A	0	HIS	-	expression tag	UNP A0A5B9BGY8
A	1	HIS	-	expression tag	UNP A0A5B9BGY8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2	HIS	-	expression tag	UNP A0A5B9BGY8
A	3	HIS	-	expression tag	UNP A0A5B9BGY8
A	4	SER	-	expression tag	UNP A0A5B9BGY8
A	5	SER	-	expression tag	UNP A0A5B9BGY8
A	6	GLY	-	expression tag	UNP A0A5B9BGY8
A	7	LEU	-	expression tag	UNP A0A5B9BGY8
A	8	VAL	-	expression tag	UNP A0A5B9BGY8
A	9	PRO	-	expression tag	UNP A0A5B9BGY8
A	10	ARG	-	expression tag	UNP A0A5B9BGY8
A	11	GLY	-	expression tag	UNP A0A5B9BGY8
A	12	SER	-	expression tag	UNP A0A5B9BGY8
A	13	HIS	-	expression tag	UNP A0A5B9BGY8
A	14	MET	-	expression tag	UNP A0A5B9BGY8
A	15	ALA	-	expression tag	UNP A0A5B9BGY8
A	16	SER	-	expression tag	UNP A0A5B9BGY8
A	17	MET	-	expression tag	UNP A0A5B9BGY8
A	18	THR	-	expression tag	UNP A0A5B9BGY8
A	19	GLY	-	expression tag	UNP A0A5B9BGY8
A	20	GLY	-	expression tag	UNP A0A5B9BGY8
A	21	GLN	-	expression tag	UNP A0A5B9BGY8
A	22	GLN	-	expression tag	UNP A0A5B9BGY8
A	23	MET	-	expression tag	UNP A0A5B9BGY8
A	24	GLY	-	expression tag	UNP A0A5B9BGY8
A	25	ARG	-	expression tag	UNP A0A5B9BGY8
A	26	GLY	-	expression tag	UNP A0A5B9BGY8
A	27	SER	-	expression tag	UNP A0A5B9BGY8
A	28	GLU	-	expression tag	UNP A0A5B9BGY8
A	29	PHE	-	expression tag	UNP A0A5B9BGY8
A	113	ALA	SER	engineered mutation	UNP A0A5B9BGY8
B	-6	MET	-	initiating methionine	UNP A0A5B9BGY8
B	-5	GLY	-	expression tag	UNP A0A5B9BGY8
B	-4	SER	-	expression tag	UNP A0A5B9BGY8
B	-3	SER	-	expression tag	UNP A0A5B9BGY8
B	-2	HIS	-	expression tag	UNP A0A5B9BGY8
B	-1	HIS	-	expression tag	UNP A0A5B9BGY8
B	0	HIS	-	expression tag	UNP A0A5B9BGY8
B	1	HIS	-	expression tag	UNP A0A5B9BGY8
B	2	HIS	-	expression tag	UNP A0A5B9BGY8
B	3	HIS	-	expression tag	UNP A0A5B9BGY8
B	4	SER	-	expression tag	UNP A0A5B9BGY8
B	5	SER	-	expression tag	UNP A0A5B9BGY8
B	6	GLY	-	expression tag	UNP A0A5B9BGY8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	7	LEU	-	expression tag	UNP A0A5B9BGY8
B	8	VAL	-	expression tag	UNP A0A5B9BGY8
B	9	PRO	-	expression tag	UNP A0A5B9BGY8
B	10	ARG	-	expression tag	UNP A0A5B9BGY8
B	11	GLY	-	expression tag	UNP A0A5B9BGY8
B	12	SER	-	expression tag	UNP A0A5B9BGY8
B	13	HIS	-	expression tag	UNP A0A5B9BGY8
B	14	MET	-	expression tag	UNP A0A5B9BGY8
B	15	ALA	-	expression tag	UNP A0A5B9BGY8
B	16	SER	-	expression tag	UNP A0A5B9BGY8
B	17	MET	-	expression tag	UNP A0A5B9BGY8
B	18	THR	-	expression tag	UNP A0A5B9BGY8
B	19	GLY	-	expression tag	UNP A0A5B9BGY8
B	20	GLY	-	expression tag	UNP A0A5B9BGY8
B	21	GLN	-	expression tag	UNP A0A5B9BGY8
B	22	GLN	-	expression tag	UNP A0A5B9BGY8
B	23	MET	-	expression tag	UNP A0A5B9BGY8
B	24	GLY	-	expression tag	UNP A0A5B9BGY8
B	25	ARG	-	expression tag	UNP A0A5B9BGY8
B	26	GLY	-	expression tag	UNP A0A5B9BGY8
B	27	SER	-	expression tag	UNP A0A5B9BGY8
B	28	GLU	-	expression tag	UNP A0A5B9BGY8
B	29	PHE	-	expression tag	UNP A0A5B9BGY8
B	113	ALA	SER	engineered mutation	UNP A0A5B9BGY8
C	-6	MET	-	initiating methionine	UNP A0A5B9BGY8
C	-5	GLY	-	expression tag	UNP A0A5B9BGY8
C	-4	SER	-	expression tag	UNP A0A5B9BGY8
C	-3	SER	-	expression tag	UNP A0A5B9BGY8
C	-2	HIS	-	expression tag	UNP A0A5B9BGY8
C	-1	HIS	-	expression tag	UNP A0A5B9BGY8
C	0	HIS	-	expression tag	UNP A0A5B9BGY8
C	1	HIS	-	expression tag	UNP A0A5B9BGY8
C	2	HIS	-	expression tag	UNP A0A5B9BGY8
C	3	HIS	-	expression tag	UNP A0A5B9BGY8
C	4	SER	-	expression tag	UNP A0A5B9BGY8
C	5	SER	-	expression tag	UNP A0A5B9BGY8
C	6	GLY	-	expression tag	UNP A0A5B9BGY8
C	7	LEU	-	expression tag	UNP A0A5B9BGY8
C	8	VAL	-	expression tag	UNP A0A5B9BGY8
C	9	PRO	-	expression tag	UNP A0A5B9BGY8
C	10	ARG	-	expression tag	UNP A0A5B9BGY8
C	11	GLY	-	expression tag	UNP A0A5B9BGY8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	12	SER	-	expression tag	UNP A0A5B9BGY8
C	13	HIS	-	expression tag	UNP A0A5B9BGY8
C	14	MET	-	expression tag	UNP A0A5B9BGY8
C	15	ALA	-	expression tag	UNP A0A5B9BGY8
C	16	SER	-	expression tag	UNP A0A5B9BGY8
C	17	MET	-	expression tag	UNP A0A5B9BGY8
C	18	THR	-	expression tag	UNP A0A5B9BGY8
C	19	GLY	-	expression tag	UNP A0A5B9BGY8
C	20	GLY	-	expression tag	UNP A0A5B9BGY8
C	21	GLN	-	expression tag	UNP A0A5B9BGY8
C	22	GLN	-	expression tag	UNP A0A5B9BGY8
C	23	MET	-	expression tag	UNP A0A5B9BGY8
C	24	GLY	-	expression tag	UNP A0A5B9BGY8
C	25	ARG	-	expression tag	UNP A0A5B9BGY8
C	26	GLY	-	expression tag	UNP A0A5B9BGY8
C	27	SER	-	expression tag	UNP A0A5B9BGY8
C	28	GLU	-	expression tag	UNP A0A5B9BGY8
C	29	PHE	-	expression tag	UNP A0A5B9BGY8
C	113	ALA	SER	engineered mutation	UNP A0A5B9BGY8
D	-6	MET	-	initiating methionine	UNP A0A5B9BGY8
D	-5	GLY	-	expression tag	UNP A0A5B9BGY8
D	-4	SER	-	expression tag	UNP A0A5B9BGY8
D	-3	SER	-	expression tag	UNP A0A5B9BGY8
D	-2	HIS	-	expression tag	UNP A0A5B9BGY8
D	-1	HIS	-	expression tag	UNP A0A5B9BGY8
D	0	HIS	-	expression tag	UNP A0A5B9BGY8
D	1	HIS	-	expression tag	UNP A0A5B9BGY8
D	2	HIS	-	expression tag	UNP A0A5B9BGY8
D	3	HIS	-	expression tag	UNP A0A5B9BGY8
D	4	SER	-	expression tag	UNP A0A5B9BGY8
D	5	SER	-	expression tag	UNP A0A5B9BGY8
D	6	GLY	-	expression tag	UNP A0A5B9BGY8
D	7	LEU	-	expression tag	UNP A0A5B9BGY8
D	8	VAL	-	expression tag	UNP A0A5B9BGY8
D	9	PRO	-	expression tag	UNP A0A5B9BGY8
D	10	ARG	-	expression tag	UNP A0A5B9BGY8
D	11	GLY	-	expression tag	UNP A0A5B9BGY8
D	12	SER	-	expression tag	UNP A0A5B9BGY8
D	13	HIS	-	expression tag	UNP A0A5B9BGY8
D	14	MET	-	expression tag	UNP A0A5B9BGY8
D	15	ALA	-	expression tag	UNP A0A5B9BGY8
D	16	SER	-	expression tag	UNP A0A5B9BGY8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	17	MET	-	expression tag	UNP A0A5B9BGY8
D	18	THR	-	expression tag	UNP A0A5B9BGY8
D	19	GLY	-	expression tag	UNP A0A5B9BGY8
D	20	GLY	-	expression tag	UNP A0A5B9BGY8
D	21	GLN	-	expression tag	UNP A0A5B9BGY8
D	22	GLN	-	expression tag	UNP A0A5B9BGY8
D	23	MET	-	expression tag	UNP A0A5B9BGY8
D	24	GLY	-	expression tag	UNP A0A5B9BGY8
D	25	ARG	-	expression tag	UNP A0A5B9BGY8
D	26	GLY	-	expression tag	UNP A0A5B9BGY8
D	27	SER	-	expression tag	UNP A0A5B9BGY8
D	28	GLU	-	expression tag	UNP A0A5B9BGY8
D	29	PHE	-	expression tag	UNP A0A5B9BGY8
D	113	ALA	SER	engineered mutation	UNP A0A5B9BGY8
E	-6	MET	-	initiating methionine	UNP A0A5B9BGY8
E	-5	GLY	-	expression tag	UNP A0A5B9BGY8
E	-4	SER	-	expression tag	UNP A0A5B9BGY8
E	-3	SER	-	expression tag	UNP A0A5B9BGY8
E	-2	HIS	-	expression tag	UNP A0A5B9BGY8
E	-1	HIS	-	expression tag	UNP A0A5B9BGY8
E	0	HIS	-	expression tag	UNP A0A5B9BGY8
E	1	HIS	-	expression tag	UNP A0A5B9BGY8
E	2	HIS	-	expression tag	UNP A0A5B9BGY8
E	3	HIS	-	expression tag	UNP A0A5B9BGY8
E	4	SER	-	expression tag	UNP A0A5B9BGY8
E	5	SER	-	expression tag	UNP A0A5B9BGY8
E	6	GLY	-	expression tag	UNP A0A5B9BGY8
E	7	LEU	-	expression tag	UNP A0A5B9BGY8
E	8	VAL	-	expression tag	UNP A0A5B9BGY8
E	9	PRO	-	expression tag	UNP A0A5B9BGY8
E	10	ARG	-	expression tag	UNP A0A5B9BGY8
E	11	GLY	-	expression tag	UNP A0A5B9BGY8
E	12	SER	-	expression tag	UNP A0A5B9BGY8
E	13	HIS	-	expression tag	UNP A0A5B9BGY8
E	14	MET	-	expression tag	UNP A0A5B9BGY8
E	15	ALA	-	expression tag	UNP A0A5B9BGY8
E	16	SER	-	expression tag	UNP A0A5B9BGY8
E	17	MET	-	expression tag	UNP A0A5B9BGY8
E	18	THR	-	expression tag	UNP A0A5B9BGY8
E	19	GLY	-	expression tag	UNP A0A5B9BGY8
E	20	GLY	-	expression tag	UNP A0A5B9BGY8
E	21	GLN	-	expression tag	UNP A0A5B9BGY8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	22	GLN	-	expression tag	UNP A0A5B9BGY8
E	23	MET	-	expression tag	UNP A0A5B9BGY8
E	24	GLY	-	expression tag	UNP A0A5B9BGY8
E	25	ARG	-	expression tag	UNP A0A5B9BGY8
E	26	GLY	-	expression tag	UNP A0A5B9BGY8
E	27	SER	-	expression tag	UNP A0A5B9BGY8
E	28	GLU	-	expression tag	UNP A0A5B9BGY8
E	29	PHE	-	expression tag	UNP A0A5B9BGY8
E	113	ALA	SER	engineered mutation	UNP A0A5B9BGY8
F	-6	MET	-	initiating methionine	UNP A0A5B9BGY8
F	-5	GLY	-	expression tag	UNP A0A5B9BGY8
F	-4	SER	-	expression tag	UNP A0A5B9BGY8
F	-3	SER	-	expression tag	UNP A0A5B9BGY8
F	-2	HIS	-	expression tag	UNP A0A5B9BGY8
F	-1	HIS	-	expression tag	UNP A0A5B9BGY8
F	0	HIS	-	expression tag	UNP A0A5B9BGY8
F	1	HIS	-	expression tag	UNP A0A5B9BGY8
F	2	HIS	-	expression tag	UNP A0A5B9BGY8
F	3	HIS	-	expression tag	UNP A0A5B9BGY8
F	4	SER	-	expression tag	UNP A0A5B9BGY8
F	5	SER	-	expression tag	UNP A0A5B9BGY8
F	6	GLY	-	expression tag	UNP A0A5B9BGY8
F	7	LEU	-	expression tag	UNP A0A5B9BGY8
F	8	VAL	-	expression tag	UNP A0A5B9BGY8
F	9	PRO	-	expression tag	UNP A0A5B9BGY8
F	10	ARG	-	expression tag	UNP A0A5B9BGY8
F	11	GLY	-	expression tag	UNP A0A5B9BGY8
F	12	SER	-	expression tag	UNP A0A5B9BGY8
F	13	HIS	-	expression tag	UNP A0A5B9BGY8
F	14	MET	-	expression tag	UNP A0A5B9BGY8
F	15	ALA	-	expression tag	UNP A0A5B9BGY8
F	16	SER	-	expression tag	UNP A0A5B9BGY8
F	17	MET	-	expression tag	UNP A0A5B9BGY8
F	18	THR	-	expression tag	UNP A0A5B9BGY8
F	19	GLY	-	expression tag	UNP A0A5B9BGY8
F	20	GLY	-	expression tag	UNP A0A5B9BGY8
F	21	GLN	-	expression tag	UNP A0A5B9BGY8
F	22	GLN	-	expression tag	UNP A0A5B9BGY8
F	23	MET	-	expression tag	UNP A0A5B9BGY8
F	24	GLY	-	expression tag	UNP A0A5B9BGY8
F	25	ARG	-	expression tag	UNP A0A5B9BGY8
F	26	GLY	-	expression tag	UNP A0A5B9BGY8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	27	SER	-	expression tag	UNP A0A5B9BGY8
F	28	GLU	-	expression tag	UNP A0A5B9BGY8
F	29	PHE	-	expression tag	UNP A0A5B9BGY8
F	113	ALA	SER	engineered mutation	UNP A0A5B9BGY8
G	-6	MET	-	initiating methionine	UNP A0A5B9BGY8
G	-5	GLY	-	expression tag	UNP A0A5B9BGY8
G	-4	SER	-	expression tag	UNP A0A5B9BGY8
G	-3	SER	-	expression tag	UNP A0A5B9BGY8
G	-2	HIS	-	expression tag	UNP A0A5B9BGY8
G	-1	HIS	-	expression tag	UNP A0A5B9BGY8
G	0	HIS	-	expression tag	UNP A0A5B9BGY8
G	1	HIS	-	expression tag	UNP A0A5B9BGY8
G	2	HIS	-	expression tag	UNP A0A5B9BGY8
G	3	HIS	-	expression tag	UNP A0A5B9BGY8
G	4	SER	-	expression tag	UNP A0A5B9BGY8
G	5	SER	-	expression tag	UNP A0A5B9BGY8
G	6	GLY	-	expression tag	UNP A0A5B9BGY8
G	7	LEU	-	expression tag	UNP A0A5B9BGY8
G	8	VAL	-	expression tag	UNP A0A5B9BGY8
G	9	PRO	-	expression tag	UNP A0A5B9BGY8
G	10	ARG	-	expression tag	UNP A0A5B9BGY8
G	11	GLY	-	expression tag	UNP A0A5B9BGY8
G	12	SER	-	expression tag	UNP A0A5B9BGY8
G	13	HIS	-	expression tag	UNP A0A5B9BGY8
G	14	MET	-	expression tag	UNP A0A5B9BGY8
G	15	ALA	-	expression tag	UNP A0A5B9BGY8
G	16	SER	-	expression tag	UNP A0A5B9BGY8
G	17	MET	-	expression tag	UNP A0A5B9BGY8
G	18	THR	-	expression tag	UNP A0A5B9BGY8
G	19	GLY	-	expression tag	UNP A0A5B9BGY8
G	20	GLY	-	expression tag	UNP A0A5B9BGY8
G	21	GLN	-	expression tag	UNP A0A5B9BGY8
G	22	GLN	-	expression tag	UNP A0A5B9BGY8
G	23	MET	-	expression tag	UNP A0A5B9BGY8
G	24	GLY	-	expression tag	UNP A0A5B9BGY8
G	25	ARG	-	expression tag	UNP A0A5B9BGY8
G	26	GLY	-	expression tag	UNP A0A5B9BGY8
G	27	SER	-	expression tag	UNP A0A5B9BGY8
G	28	GLU	-	expression tag	UNP A0A5B9BGY8
G	29	PHE	-	expression tag	UNP A0A5B9BGY8
G	113	ALA	SER	engineered mutation	UNP A0A5B9BGY8

- Molecule 4 is a protein called ATP-dependent Clp protease proteolytic subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	179	Total	C	N	O	S	0	0
			1371	855	233	273	10		
4	I	183	Total	C	N	O	S	0	0
			1399	871	238	280	10		
4	J	176	Total	C	N	O	S	0	0
			1346	840	229	268	9		
4	K	176	Total	C	N	O	S	0	0
			1346	840	229	268	9		
4	L	177	Total	C	N	O	S	0	0
			1355	846	231	269	9		
4	M	177	Total	C	N	O	S	0	0
			1355	846	231	269	9		
4	N	177	Total	C	N	O	S	0	0
			1355	846	231	269	9		

There are 154 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	29	MET	-	initiating methionine	UNP A0A5B9BIX9
H	30	GLY	-	expression tag	UNP A0A5B9BIX9
H	31	SER	-	expression tag	UNP A0A5B9BIX9
H	32	SER	-	expression tag	UNP A0A5B9BIX9
H	33	HIS	-	expression tag	UNP A0A5B9BIX9
H	34	HIS	-	expression tag	UNP A0A5B9BIX9
H	35	HIS	-	expression tag	UNP A0A5B9BIX9
H	36	HIS	-	expression tag	UNP A0A5B9BIX9
H	37	HIS	-	expression tag	UNP A0A5B9BIX9
H	38	HIS	-	expression tag	UNP A0A5B9BIX9
H	39	SER	-	expression tag	UNP A0A5B9BIX9
H	40	SER	-	expression tag	UNP A0A5B9BIX9
H	41	GLY	-	expression tag	UNP A0A5B9BIX9
H	42	LEU	-	expression tag	UNP A0A5B9BIX9
H	43	VAL	-	expression tag	UNP A0A5B9BIX9
H	44	PRO	-	expression tag	UNP A0A5B9BIX9
H	45	ARG	-	expression tag	UNP A0A5B9BIX9
H	46	GLY	-	expression tag	UNP A0A5B9BIX9
H	47	SER	-	expression tag	UNP A0A5B9BIX9
H	48	HIS	-	expression tag	UNP A0A5B9BIX9
H	49	MET	-	expression tag	UNP A0A5B9BIX9
H	131	ALA	SER	engineered mutation	UNP A0A5B9BIX9
I	29	MET	-	initiating methionine	UNP A0A5B9BIX9
I	30	GLY	-	expression tag	UNP A0A5B9BIX9
I	31	SER	-	expression tag	UNP A0A5B9BIX9
I	32	SER	-	expression tag	UNP A0A5B9BIX9

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Chain	Residue	Modelled	Actual	Comment	Reference
I	33	HIS	-	expression tag	UNP A0A5B9BIX9
I	34	HIS	-	expression tag	UNP A0A5B9BIX9
I	35	HIS	-	expression tag	UNP A0A5B9BIX9
I	36	HIS	-	expression tag	UNP A0A5B9BIX9
I	37	HIS	-	expression tag	UNP A0A5B9BIX9
I	38	HIS	-	expression tag	UNP A0A5B9BIX9
I	39	SER	-	expression tag	UNP A0A5B9BIX9
I	40	SER	-	expression tag	UNP A0A5B9BIX9
I	41	GLY	-	expression tag	UNP A0A5B9BIX9
I	42	LEU	-	expression tag	UNP A0A5B9BIX9
I	43	VAL	-	expression tag	UNP A0A5B9BIX9
I	44	PRO	-	expression tag	UNP A0A5B9BIX9
I	45	ARG	-	expression tag	UNP A0A5B9BIX9
I	46	GLY	-	expression tag	UNP A0A5B9BIX9
I	47	SER	-	expression tag	UNP A0A5B9BIX9
I	48	HIS	-	expression tag	UNP A0A5B9BIX9
I	49	MET	-	expression tag	UNP A0A5B9BIX9
I	131	ALA	SER	engineered mutation	UNP A0A5B9BIX9
J	29	MET	-	initiating methionine	UNP A0A5B9BIX9
J	30	GLY	-	expression tag	UNP A0A5B9BIX9
J	31	SER	-	expression tag	UNP A0A5B9BIX9
J	32	SER	-	expression tag	UNP A0A5B9BIX9
J	33	HIS	-	expression tag	UNP A0A5B9BIX9
J	34	HIS	-	expression tag	UNP A0A5B9BIX9
J	35	HIS	-	expression tag	UNP A0A5B9BIX9
J	36	HIS	-	expression tag	UNP A0A5B9BIX9
J	37	HIS	-	expression tag	UNP A0A5B9BIX9
J	38	HIS	-	expression tag	UNP A0A5B9BIX9
J	39	SER	-	expression tag	UNP A0A5B9BIX9
J	40	SER	-	expression tag	UNP A0A5B9BIX9
J	41	GLY	-	expression tag	UNP A0A5B9BIX9
J	42	LEU	-	expression tag	UNP A0A5B9BIX9
J	43	VAL	-	expression tag	UNP A0A5B9BIX9
J	44	PRO	-	expression tag	UNP A0A5B9BIX9
J	45	ARG	-	expression tag	UNP A0A5B9BIX9
J	46	GLY	-	expression tag	UNP A0A5B9BIX9
J	47	SER	-	expression tag	UNP A0A5B9BIX9
J	48	HIS	-	expression tag	UNP A0A5B9BIX9
J	49	MET	-	expression tag	UNP A0A5B9BIX9
J	131	ALA	SER	engineered mutation	UNP A0A5B9BIX9
K	29	MET	-	initiating methionine	UNP A0A5B9BIX9
K	30	GLY	-	expression tag	UNP A0A5B9BIX9

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Chain	Residue	Modelled	Actual	Comment	Reference
K	31	SER	-	expression tag	UNP A0A5B9BIX9
K	32	SER	-	expression tag	UNP A0A5B9BIX9
K	33	HIS	-	expression tag	UNP A0A5B9BIX9
K	34	HIS	-	expression tag	UNP A0A5B9BIX9
K	35	HIS	-	expression tag	UNP A0A5B9BIX9
K	36	HIS	-	expression tag	UNP A0A5B9BIX9
K	37	HIS	-	expression tag	UNP A0A5B9BIX9
K	38	HIS	-	expression tag	UNP A0A5B9BIX9
K	39	SER	-	expression tag	UNP A0A5B9BIX9
K	40	SER	-	expression tag	UNP A0A5B9BIX9
K	41	GLY	-	expression tag	UNP A0A5B9BIX9
K	42	LEU	-	expression tag	UNP A0A5B9BIX9
K	43	VAL	-	expression tag	UNP A0A5B9BIX9
K	44	PRO	-	expression tag	UNP A0A5B9BIX9
K	45	ARG	-	expression tag	UNP A0A5B9BIX9
K	46	GLY	-	expression tag	UNP A0A5B9BIX9
K	47	SER	-	expression tag	UNP A0A5B9BIX9
K	48	HIS	-	expression tag	UNP A0A5B9BIX9
K	49	MET	-	expression tag	UNP A0A5B9BIX9
K	131	ALA	SER	engineered mutation	UNP A0A5B9BIX9
L	29	MET	-	initiating methionine	UNP A0A5B9BIX9
L	30	GLY	-	expression tag	UNP A0A5B9BIX9
L	31	SER	-	expression tag	UNP A0A5B9BIX9
L	32	SER	-	expression tag	UNP A0A5B9BIX9
L	33	HIS	-	expression tag	UNP A0A5B9BIX9
L	34	HIS	-	expression tag	UNP A0A5B9BIX9
L	35	HIS	-	expression tag	UNP A0A5B9BIX9
L	36	HIS	-	expression tag	UNP A0A5B9BIX9
L	37	HIS	-	expression tag	UNP A0A5B9BIX9
L	38	HIS	-	expression tag	UNP A0A5B9BIX9
L	39	SER	-	expression tag	UNP A0A5B9BIX9
L	40	SER	-	expression tag	UNP A0A5B9BIX9
L	41	GLY	-	expression tag	UNP A0A5B9BIX9
L	42	LEU	-	expression tag	UNP A0A5B9BIX9
L	43	VAL	-	expression tag	UNP A0A5B9BIX9
L	44	PRO	-	expression tag	UNP A0A5B9BIX9
L	45	ARG	-	expression tag	UNP A0A5B9BIX9
L	46	GLY	-	expression tag	UNP A0A5B9BIX9
L	47	SER	-	expression tag	UNP A0A5B9BIX9
L	48	HIS	-	expression tag	UNP A0A5B9BIX9
L	49	MET	-	expression tag	UNP A0A5B9BIX9
L	131	ALA	SER	engineered mutation	UNP A0A5B9BIX9

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Chain	Residue	Modelled	Actual	Comment	Reference
M	29	MET	-	initiating methionine	UNP A0A5B9BIX9
M	30	GLY	-	expression tag	UNP A0A5B9BIX9
M	31	SER	-	expression tag	UNP A0A5B9BIX9
M	32	SER	-	expression tag	UNP A0A5B9BIX9
M	33	HIS	-	expression tag	UNP A0A5B9BIX9
M	34	HIS	-	expression tag	UNP A0A5B9BIX9
M	35	HIS	-	expression tag	UNP A0A5B9BIX9
M	36	HIS	-	expression tag	UNP A0A5B9BIX9
M	37	HIS	-	expression tag	UNP A0A5B9BIX9
M	38	HIS	-	expression tag	UNP A0A5B9BIX9
M	39	SER	-	expression tag	UNP A0A5B9BIX9
M	40	SER	-	expression tag	UNP A0A5B9BIX9
M	41	GLY	-	expression tag	UNP A0A5B9BIX9
M	42	LEU	-	expression tag	UNP A0A5B9BIX9
M	43	VAL	-	expression tag	UNP A0A5B9BIX9
M	44	PRO	-	expression tag	UNP A0A5B9BIX9
M	45	ARG	-	expression tag	UNP A0A5B9BIX9
M	46	GLY	-	expression tag	UNP A0A5B9BIX9
M	47	SER	-	expression tag	UNP A0A5B9BIX9
M	48	HIS	-	expression tag	UNP A0A5B9BIX9
M	49	MET	-	expression tag	UNP A0A5B9BIX9
M	131	ALA	SER	engineered mutation	UNP A0A5B9BIX9
N	29	MET	-	initiating methionine	UNP A0A5B9BIX9
N	30	GLY	-	expression tag	UNP A0A5B9BIX9
N	31	SER	-	expression tag	UNP A0A5B9BIX9
N	32	SER	-	expression tag	UNP A0A5B9BIX9
N	33	HIS	-	expression tag	UNP A0A5B9BIX9
N	34	HIS	-	expression tag	UNP A0A5B9BIX9
N	35	HIS	-	expression tag	UNP A0A5B9BIX9
N	36	HIS	-	expression tag	UNP A0A5B9BIX9
N	37	HIS	-	expression tag	UNP A0A5B9BIX9
N	38	HIS	-	expression tag	UNP A0A5B9BIX9
N	39	SER	-	expression tag	UNP A0A5B9BIX9
N	40	SER	-	expression tag	UNP A0A5B9BIX9
N	41	GLY	-	expression tag	UNP A0A5B9BIX9
N	42	LEU	-	expression tag	UNP A0A5B9BIX9
N	43	VAL	-	expression tag	UNP A0A5B9BIX9
N	44	PRO	-	expression tag	UNP A0A5B9BIX9
N	45	ARG	-	expression tag	UNP A0A5B9BIX9
N	46	GLY	-	expression tag	UNP A0A5B9BIX9
N	47	SER	-	expression tag	UNP A0A5B9BIX9
N	48	HIS	-	expression tag	UNP A0A5B9BIX9

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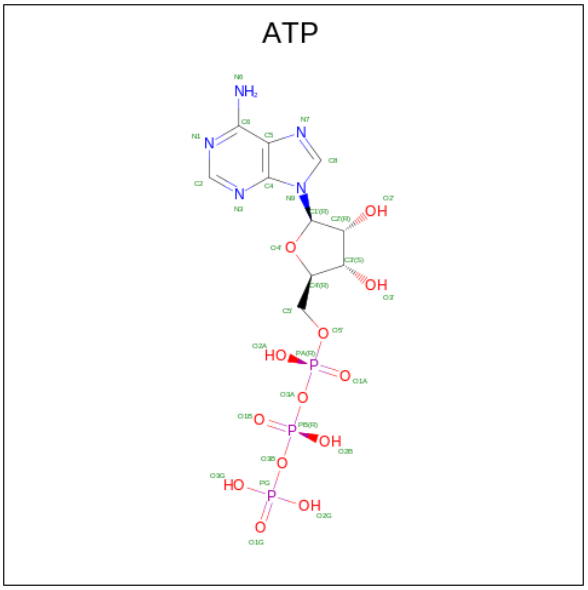
Chain	Residue	Modelled	Actual	Comment	Reference
N	49	MET	-	expression tag	UNP A0A5B9BIX9
N	131	ALA	SER	engineered mutation	UNP A0A5B9BIX9

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

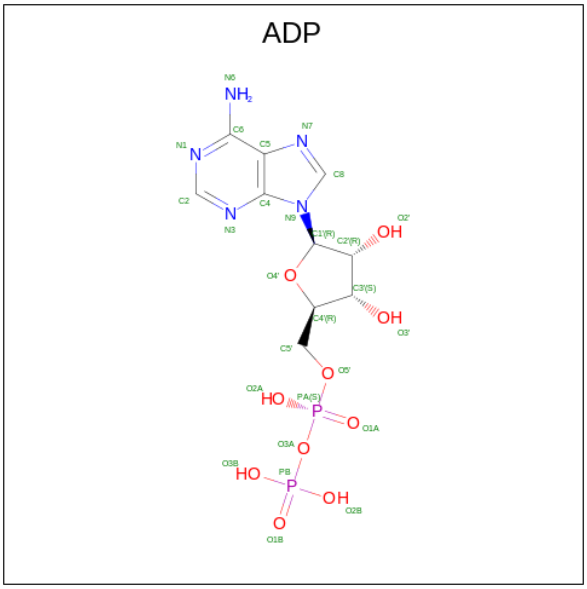


Mol	Chain	Residues	Atoms					AltConf
5	S	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	S	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	R	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	R	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	Q	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	P	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	O	1	Total	C	N	O	P	0
			31	10	5	13	3	
5	T	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
6	S	2	Total Mg 2 2	0
6	R	2	Total Mg 2 2	0
6	Q	1	Total Mg 1 1	0
6	P	1	Total Mg 1 1	0
6	T	1	Total Mg 1 1	0

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



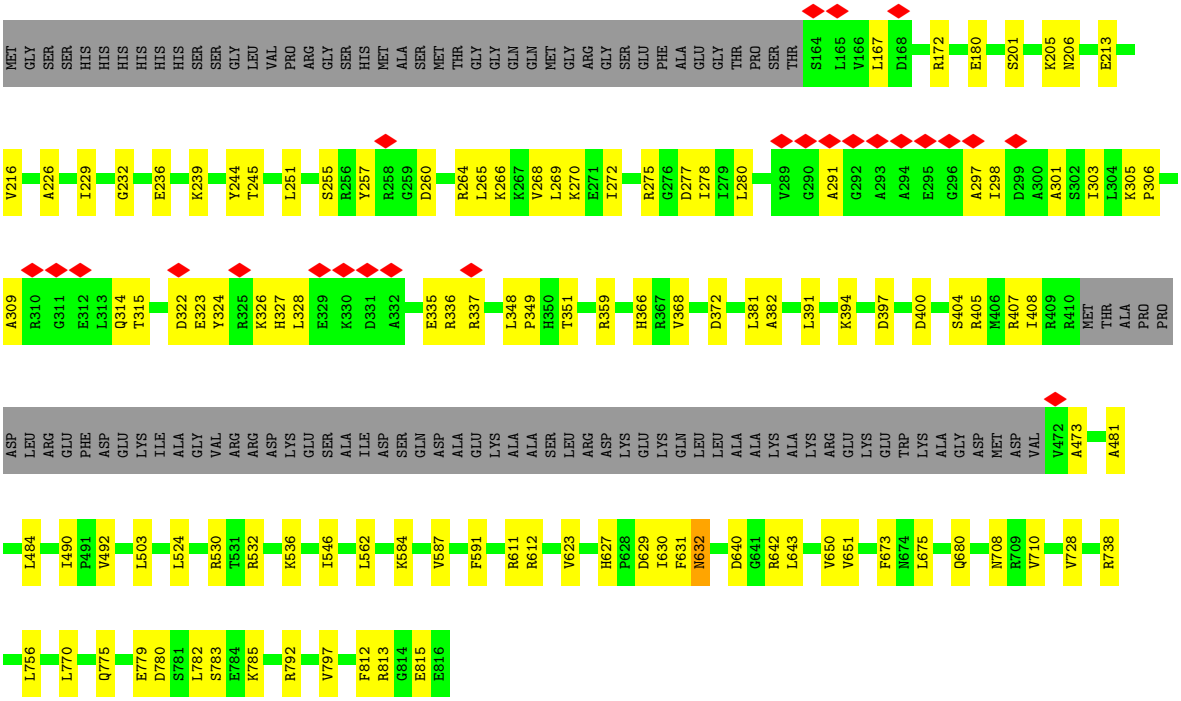
Mol	Chain	Residues	Atoms	AltConf
7	Q	1	Total C N O P 27 10 5 10 2	0
7	P	1	Total C N O P 27 10 5 10 2	0
7	O	1	Total C N O P 27 10 5 10 2	0
7	T	1	Total C N O P 27 10 5 10 2	0

3 Residue-property plots (i)

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

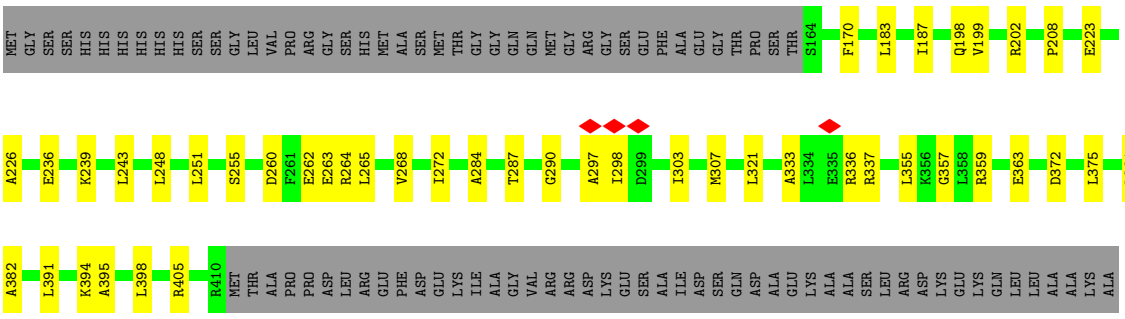
• Molecule 1: NDP-hexose 4-ketoreductase

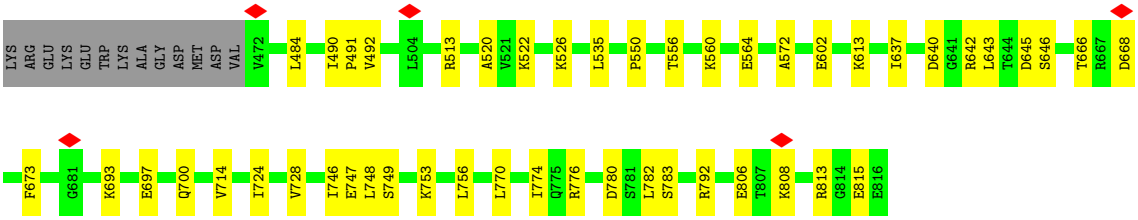
Chain S:



• Molecule 1: NDP-hexose 4-ketoreductase

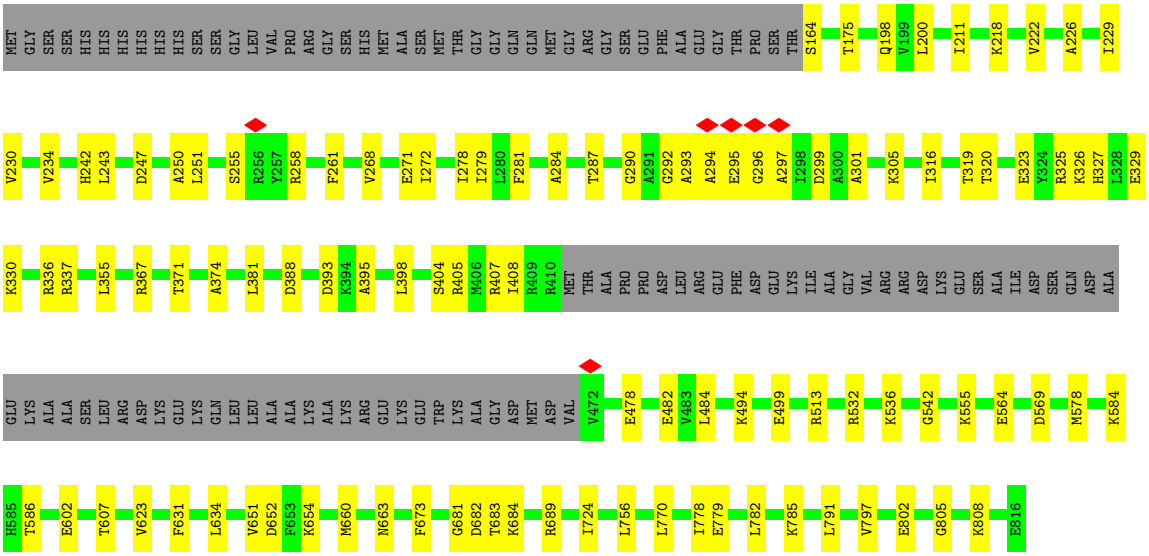
Chain R:





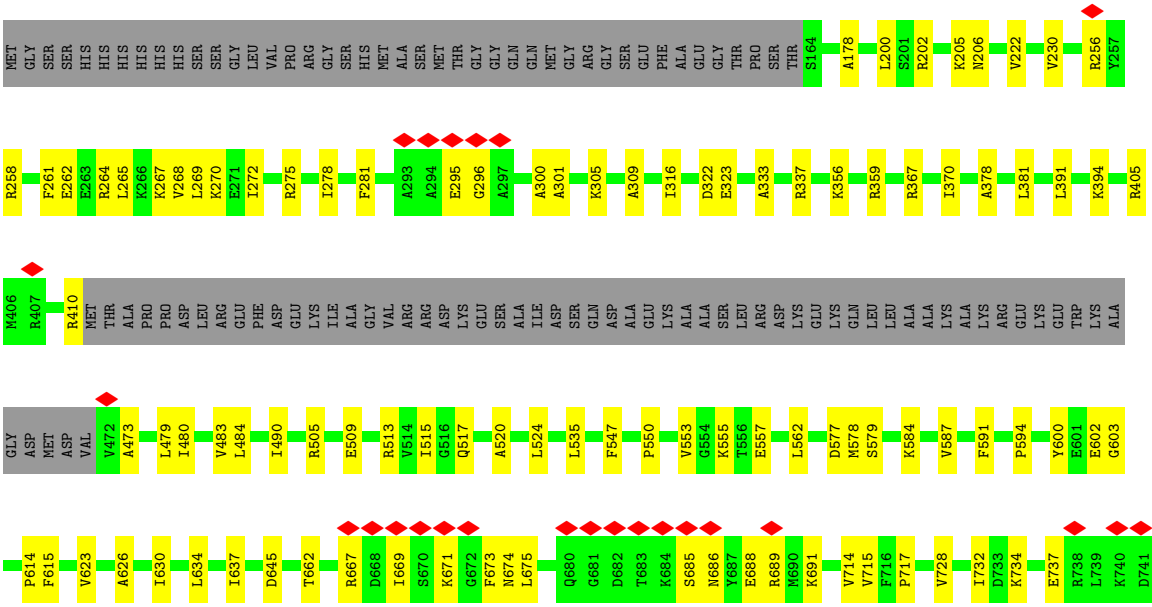
• Molecule 1: NDP-hexose 4-ketoreductase

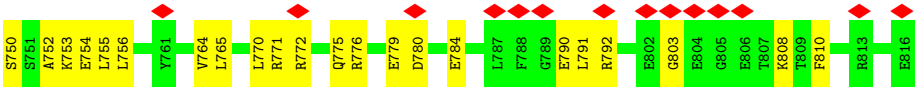
Chain Q:



• Molecule 1: NDP-hexose 4-ketoreductase

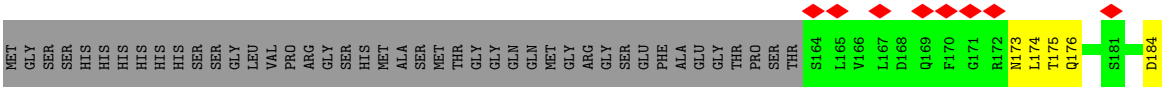
Chain P:

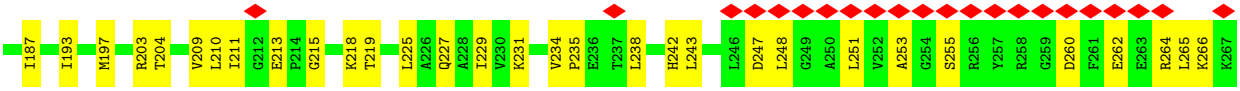


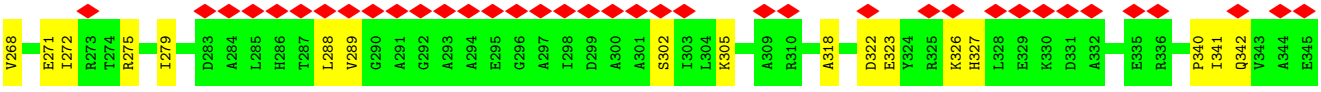


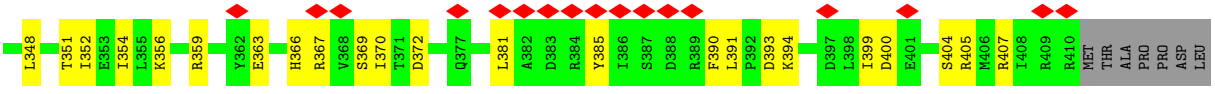
• Molecule 1: NDP-hexose 4-ketoreductase

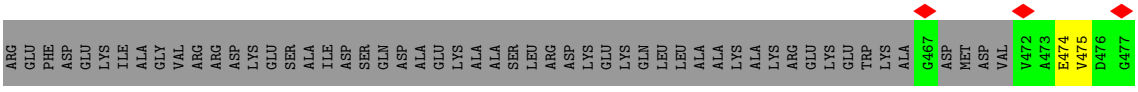
Chain O:

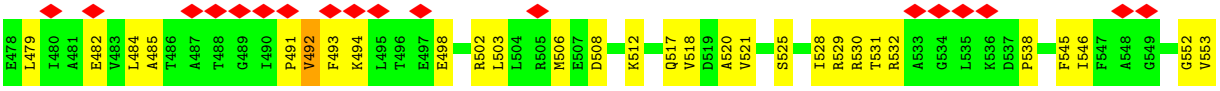


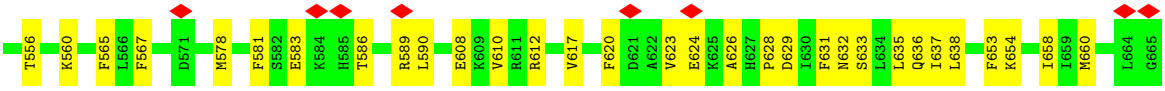


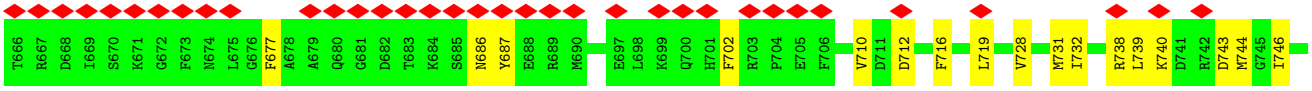


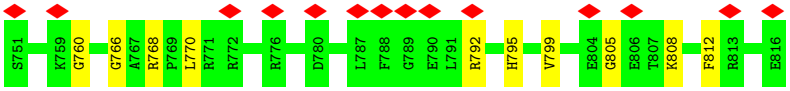






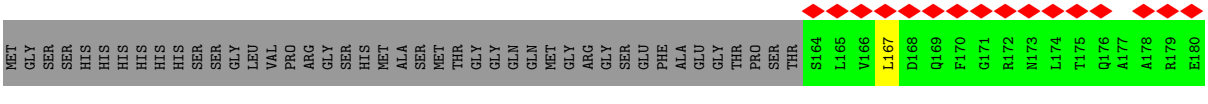


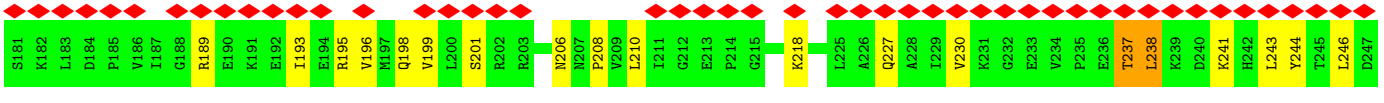


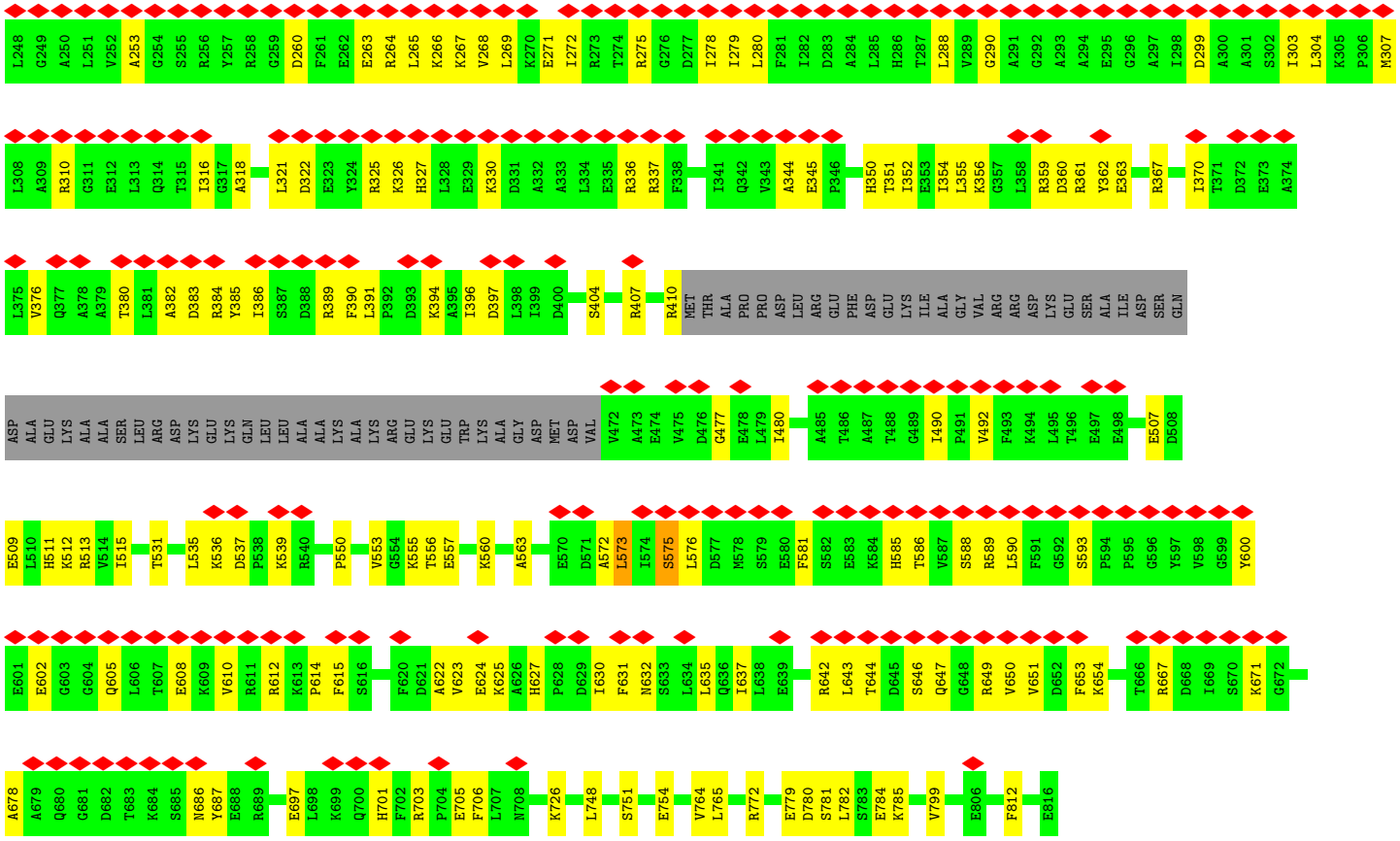


• Molecule 1: NDP-hexose 4-ketoreductase

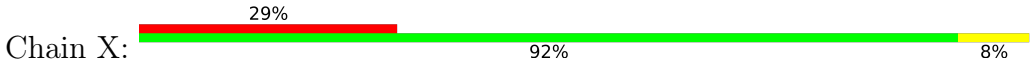
Chain T:

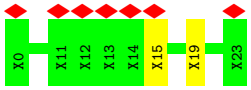




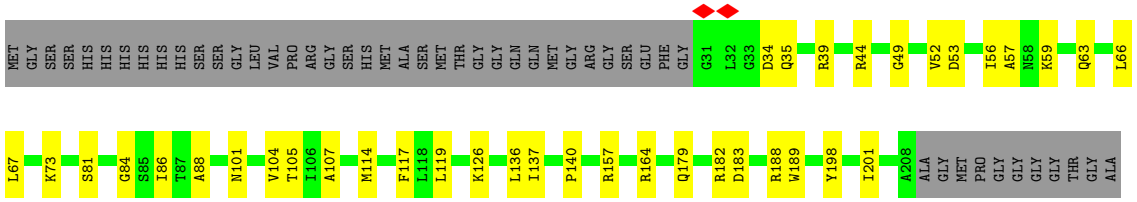


• Molecule 2: casein

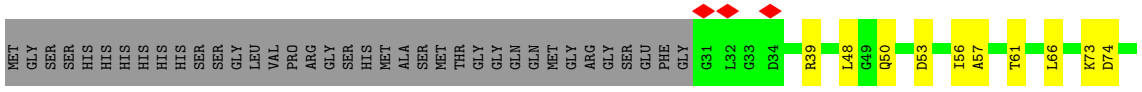


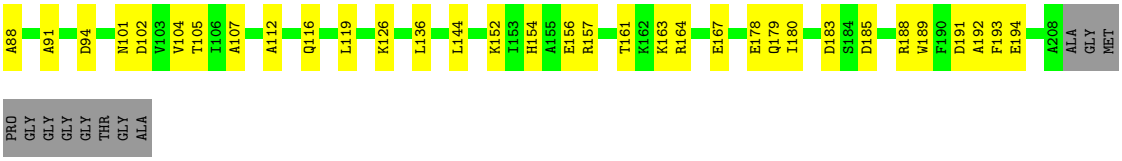


• Molecule 3: ATP-dependent Clp protease proteolytic subunit



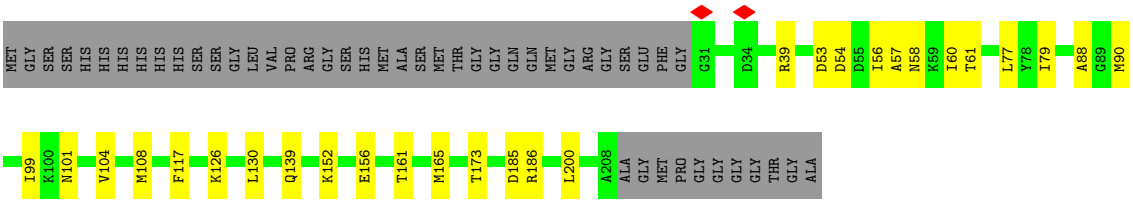
• Molecule 3: ATP-dependent Clp protease proteolytic subunit





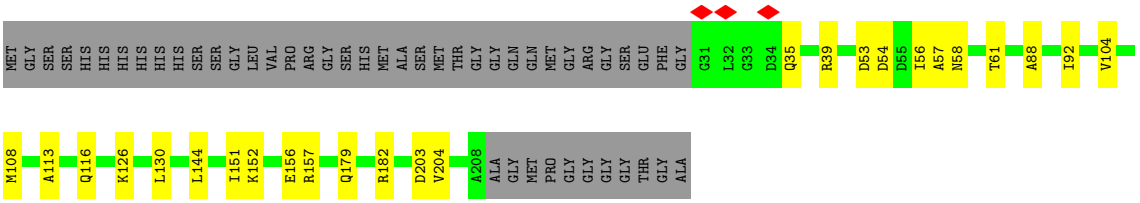
• Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain C:



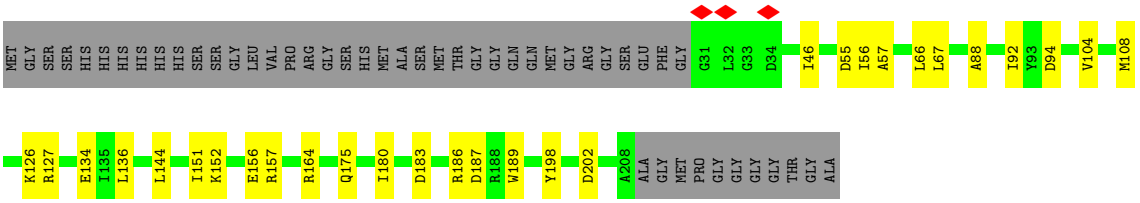
• Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain D:



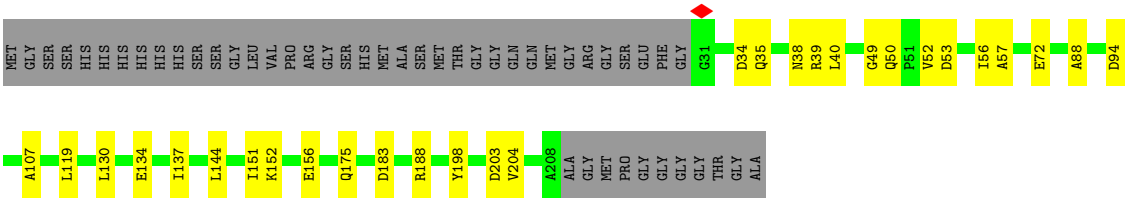
• Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain E:



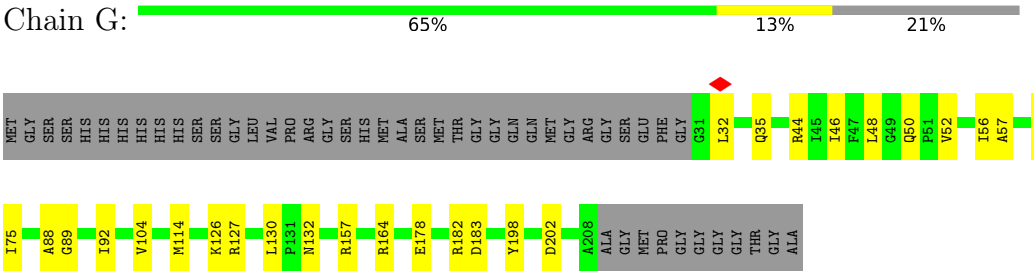
• Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain F:



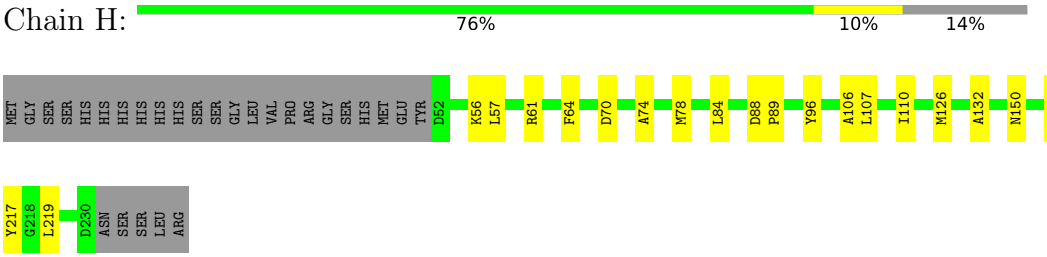
• Molecule 3: ATP-dependent Clp protease proteolytic subunit

Chain G:



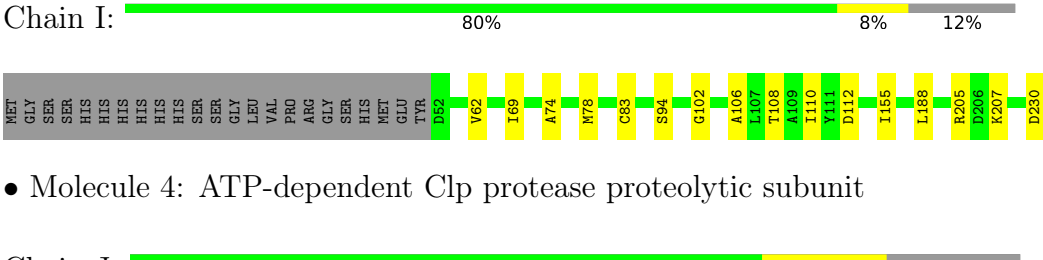
• Molecule 4: ATP-dependent Clp protease proteolytic subunit

Chain H:



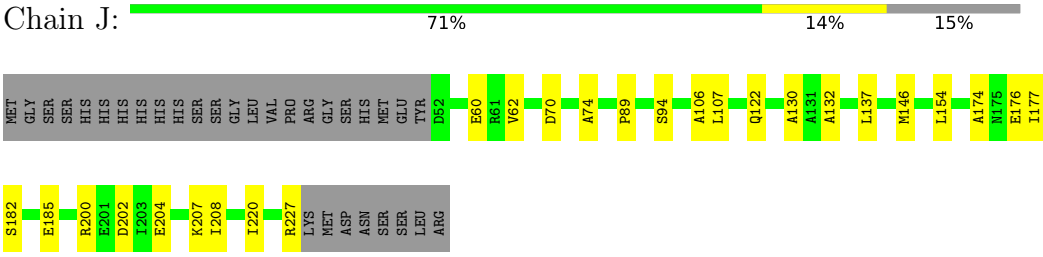
• Molecule 4: ATP-dependent Clp protease proteolytic subunit

Chain I:



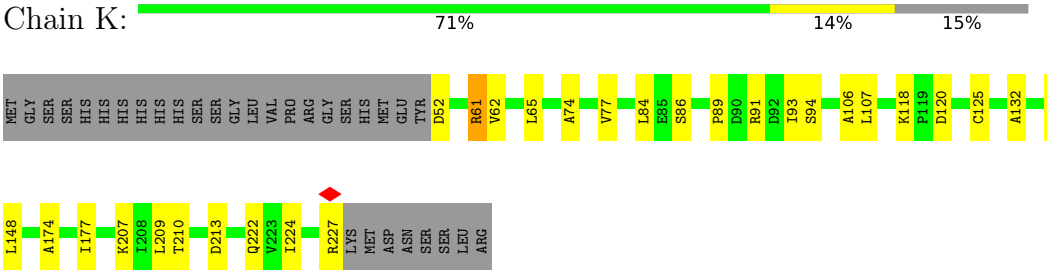
• Molecule 4: ATP-dependent Clp protease proteolytic subunit

Chain J:



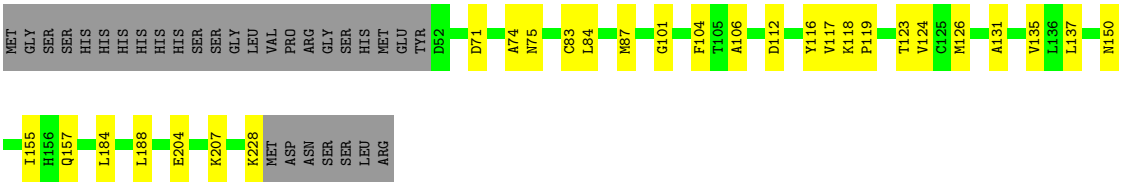
• Molecule 4: ATP-dependent Clp protease proteolytic subunit

Chain K:



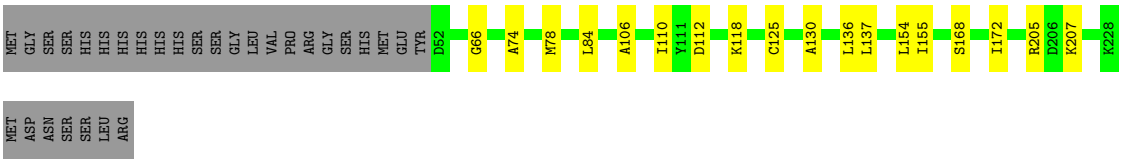
• Molecule 4: ATP-dependent Clp protease proteolytic subunit

Chain L:



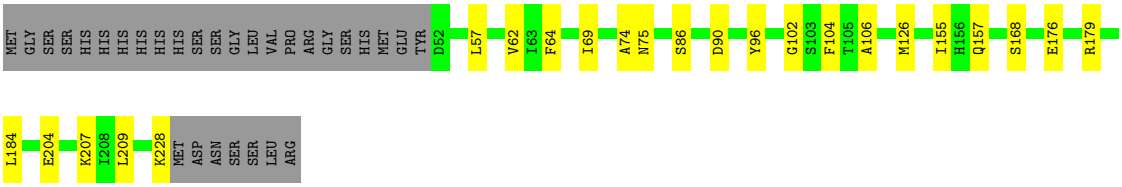
• Molecule 4: ATP-dependent Clp protease proteolytic subunit

Chain M:



• Molecule 4: ATP-dependent Clp protease proteolytic subunit

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	113281	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	46.329	Depositor
Minimum map value	-3.619	Depositor
Average map value	0.034	Depositor
Map value standard deviation	1.277	Depositor
Recommended contour level	3.9	Depositor
Map size (Å)	322.56, 322.56, 322.56	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	O	0.25	0/4703	0.52	0/6327
1	P	0.24	0/4700	0.50	0/6325
1	Q	0.25	0/4700	0.50	0/6325
1	R	0.25	0/4700	0.51	0/6325
1	S	0.25	0/4700	0.51	0/6325
1	T	0.24	0/4696	0.54	3/6321 (0.0%)
3	A	0.26	0/1391	0.52	0/1883
3	B	0.25	0/1391	0.51	0/1883
3	C	0.25	0/1391	0.48	0/1883
3	D	0.25	0/1391	0.49	0/1883
3	E	0.26	0/1391	0.51	0/1883
3	F	0.27	0/1391	0.49	0/1883
3	G	0.25	0/1391	0.49	0/1883
4	H	0.26	0/1389	0.47	0/1882
4	I	0.27	0/1417	0.50	0/1920
4	J	0.26	0/1364	0.48	0/1850
4	K	0.26	0/1364	0.49	0/1850
4	L	0.26	0/1373	0.49	0/1861
4	M	0.25	0/1373	0.48	0/1861
4	N	0.25	0/1373	0.48	0/1861
All	All	0.25	0/47589	0.51	3/64214 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	T	573	LEU	CA-CB-CG	6.70	130.71	115.30
1	T	238	LEU	CA-CB-CG	5.38	127.67	115.30
1	T	237	THR	C-N-CA	5.04	134.31	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	4640	0	4746	113	0
1	P	4636	0	4744	83	0
1	Q	4636	0	4743	72	0
1	R	4636	0	4742	59	0
1	S	4636	0	4743	75	0
1	T	4632	0	4733	117	0
2	X	120	0	32	2	0
3	A	1369	0	1368	27	0
3	B	1369	0	1368	33	0
3	C	1369	0	1368	19	0
3	D	1369	0	1368	16	0
3	E	1369	0	1368	20	0
3	F	1369	0	1368	21	0
3	G	1369	0	1368	22	0
4	H	1371	0	1374	16	0
4	I	1399	0	1401	13	0
4	J	1346	0	1348	18	0
4	K	1346	0	1348	20	0
4	L	1355	0	1361	21	0
4	M	1355	0	1361	14	0
4	N	1355	0	1361	16	0
5	O	31	0	12	2	0
5	P	31	0	12	1	0
5	Q	31	0	12	0	0
5	R	62	0	24	2	0
5	S	62	0	24	2	0
5	T	31	0	12	0	0
6	P	1	0	0	0	0
6	Q	1	0	0	0	0
6	R	2	0	0	0	0
6	S	2	0	0	0	0
6	T	1	0	0	0	0
7	O	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	P	27	0	12	0	0
7	Q	27	0	12	1	0
7	T	27	0	12	0	0
All	All	47409	0	47757	714	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (714) 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)
1:T:642:ARG:HH22	1:T:650:VAL:HA	1.46	0.80
1:O:302:SER:HA	1:O:305:LYS:HD3	1.64	0.80
1:S:257:TYR:HB2	1:S:260:ASP:HB2	1.63	0.79
3:A:49:GLY:HA2	3:A:81:SER:HB3	1.64	0.77
1:O:173:ASN:HB3	1:O:176:GLN:HE22	1.50	0.75
3:E:186:ARG:HG3	3:E:187:ASP:H	1.53	0.73
4:J:227:ARG:HB3	4:K:118:LYS:HE3	1.68	0.73
3:A:105:THR:HG21	3:A:119:LEU:HA	1.71	0.73
1:O:503:LEU:O	1:O:529:ARG:NH2	2.20	0.72
1:T:642:ARG:HH12	1:T:650:VAL:HG13	1.54	0.71
1:P:602:GLU:HG2	1:P:603:GLY:H	1.56	0.71
4:J:122:GLN:NE2	4:J:146:MET:SD	2.64	0.70
1:T:288:LEU:HD21	1:T:304:LEU:HD13	1.75	0.69
1:T:555:LYS:O	1:T:557:GLU:N	2.25	0.69
1:O:370:ILE:HD13	1:O:399:ILE:HD11	1.74	0.69
1:O:739:LEU:HD23	1:O:746:ILE:HD11	1.76	0.68
1:T:326:LYS:NZ	1:T:600:TYR:OH	2.26	0.68
3:B:66:LEU:HD21	3:C:39:ARG:HD2	1.75	0.68
1:R:602:GLU:HA	1:Q:325:ARG:HH12	1.59	0.68
3:B:105:THR:HG21	3:B:119:LEU:HA	1.76	0.67
1:T:686:ASN:OD1	1:T:687:TYR:N	2.28	0.67
1:Q:513:ARG:NH1	1:Q:564:GLU:OE1	2.28	0.67
1:Q:785:LYS:HB3	1:Q:791:LEU:HD23	1.77	0.67
1:O:268:VAL:O	1:O:272:ILE:HD12	1.96	0.66
3:A:44:ARG:NH2	3:A:67:LEU:O	2.29	0.66
1:P:275:ARG:HE	1:P:278:ILE:HD11	1.60	0.66
1:P:200:LEU:HD11	1:P:316:ILE:HD11	1.77	0.66
1:P:359:ARG:NH2	1:P:370:ILE:O	2.28	0.66
1:T:614:PRO:HB2	1:T:654:LYS:HE3	1.76	0.66
1:Q:802:GLU:O	1:Q:808:LYS:HA	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:589:ARG:O	1:T:605:GLN:NE2	2.28	0.65
1:S:255:SER:OG	1:S:264:ARG:NH2	2.29	0.65
1:P:378:ALA:HB2	1:P:480:ILE:HD13	1.78	0.65
3:B:102:ASP:OD2	3:B:126:LYS:NZ	2.30	0.65
1:R:513:ARG:NH1	1:R:564:GLU:OE1	2.29	0.65
1:T:779:GLU:HA	1:T:782:LEU:HB2	1.79	0.65
5:S:901:ATP:O1G	1:R:337:ARG:NH1	2.30	0.64
1:O:677:PHE:HD2	4:L:124:VAL:HG11	1.61	0.64
3:A:66:LEU:HD21	3:B:39:ARG:HD2	1.78	0.64
3:F:38:ASN:ND2	3:G:35:GLN:OE1	2.29	0.64
1:R:550:PRO:HA	1:R:666:THR:HG21	1.79	0.64
1:R:640:ASP:OD1	1:R:642:ARG:NH1	2.30	0.64
3:A:34:ASP:OD1	3:A:35:GLN:N	2.30	0.64
3:G:183:ASP:OD2	3:G:198:TYR:OH	2.15	0.64
3:D:179:GLN:OE1	3:D:182:ARG:NH2	2.30	0.64
1:O:323:GLU:OE2	1:O:327:HIS:ND1	2.31	0.64
1:S:708:ASN:O	1:T:772:ARG:NH2	2.30	0.63
1:R:170:PHE:HZ	1:R:264:ARG:HH11	1.46	0.63
3:A:179:GLN:OE1	3:A:182:ARG:NH2	2.31	0.63
4:L:126:MET:SD	4:M:78:MET:HE1	2.37	0.63
1:P:367:ARG:HH22	1:P:410:ARG:HD2	1.63	0.63
4:K:227:ARG:HG3	4:L:118:LYS:NZ	2.14	0.63
1:T:646:SER:OG	1:T:647:GLN:OE1	2.15	0.63
1:S:359:ARG:NH1	1:S:372:ASP:OD1	2.31	0.63
4:H:74:ALA:O	4:H:78:MET:HG2	1.98	0.63
1:Q:292:GLY:HA3	1:Q:299:ASP:HA	1.80	0.63
1:O:215:GLY:HA3	1:O:390:PHE:HB2	1.80	0.62
1:T:237:THR:O	1:T:238:LEU:HG	1.99	0.62
4:K:227:ARG:HG3	4:L:118:LYS:HZ3	1.63	0.62
1:R:382:ALA:HB1	1:R:394:LYS:HB2	1.81	0.62
1:Q:218:LYS:N	7:Q:901:ADP:O3B	2.32	0.62
1:O:578:MET:HB3	1:O:626:ALA:HB2	1.81	0.62
1:S:322:ASP:OD2	1:S:323:GLU:N	2.32	0.62
1:O:175:THR:HG21	1:O:242:HIS:HA	1.81	0.62
1:Q:405:ARG:NH1	1:Q:482:GLU:OE1	2.33	0.62
1:T:384:ARG:HG3	1:T:385:TYR:HD1	1.63	0.62
1:O:805:GLY:H	1:O:808:LYS:HE3	1.64	0.62
1:R:381:LEU:HB3	1:R:484:LEU:HD22	1.81	0.62
1:P:578:MET:HB3	1:P:626:ALA:HB2	1.81	0.62
1:S:381:LEU:HB3	1:S:484:LEU:HD22	1.81	0.62
1:R:265:LEU:HD23	1:R:303:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:553:VAL:HG11	1:O:716:PHE:HB3	1.82	0.62
4:K:120:ASP:HB3	4:K:141:THR:HG21	1.81	0.62
1:S:269:LEU:HA	1:S:272:ILE:HG12	1.82	0.61
1:O:738:ARG:NH1	1:T:535:LEU:O	2.32	0.61
3:A:119:LEU:HD21	3:A:201:ILE:HD11	1.82	0.61
1:Q:499:GLU:OE2	1:Q:532:ARG:NH1	2.33	0.61
1:T:325:ARG:HE	1:T:326:LYS:HE3	1.66	0.61
3:C:186:ARG:NH1	4:J:204:GLU:OE2	2.33	0.61
3:D:57:ALA:HB2	3:D:88:ALA:HB1	1.83	0.61
4:J:107:LEU:HD12	4:J:132:ALA:HB1	1.81	0.61
1:S:675:LEU:HD21	4:N:57:LEU:HG	1.83	0.61
4:L:71:ASP:O	4:L:75:ASN:ND2	2.33	0.61
4:N:207:LYS:HE3	4:N:209:LEU:HD21	1.83	0.61
1:P:688:GLU:HA	1:P:691:LYS:HE3	1.83	0.61
4:J:137:LEU:HD21	4:J:220:ILE:HD11	1.81	0.60
1:P:685:SER:HB3	1:P:688:GLU:HB2	1.82	0.60
1:S:530:ARG:NH1	1:T:780:ASP:OD1	2.34	0.60
1:O:393:ASP:OD1	1:O:394:LYS:N	2.34	0.60
1:P:750:SER:OG	1:P:754:GLU:OE2	2.18	0.60
3:F:203:ASP:OD1	3:F:204:VAL:N	2.34	0.60
1:S:640:ASP:OD2	1:S:642:ARG:NH1	2.34	0.60
1:Q:684:LYS:O	1:Q:689:ARG:NH1	2.34	0.60
1:Q:261:PHE:CE2	1:Q:292:GLY:HA2	2.37	0.59
1:O:738:ARG:NH2	1:T:536:LYS:O	2.34	0.59
1:S:351:THR:HG21	1:S:391:LEU:HG	1.84	0.59
1:O:322:ASP:OD1	1:O:323:GLU:N	2.35	0.59
1:O:517:GLN:HB3	1:O:520:ALA:HB3	1.85	0.59
1:S:298:ILE:HG12	1:R:297:ALA:HB3	1.83	0.59
1:O:326:LYS:HD2	1:O:327:HIS:CD2	2.37	0.59
1:O:359:ARG:NH1	1:O:372:ASP:OD1	2.36	0.59
1:T:383:ASP:HA	1:T:391:LEU:HD21	1.83	0.59
1:S:206:ASN:ND2	1:S:314:GLN:OE1	2.35	0.59
1:O:475:VAL:HG23	1:O:479:LEU:HD23	1.84	0.59
1:O:583:GLU:OE2	1:O:586:THR:N	2.36	0.59
1:T:359:ARG:NH2	1:T:363:GLU:OE2	2.36	0.59
1:R:262:GLU:HG2	1:R:298:ILE:HG13	1.85	0.58
1:Q:367:ARG:O	1:Q:407:ARG:NH2	2.36	0.58
1:R:355:LEU:HD11	1:R:395:ALA:HB1	1.84	0.58
1:R:359:ARG:O	1:R:363:GLU:HG2	2.03	0.58
1:P:381:LEU:HB3	1:P:484:LEU:HD13	1.85	0.58
4:I:155:ILE:HG13	4:I:207:LYS:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:326:LYS:O	1:Q:330:LYS:NZ	2.37	0.58
1:P:550:PRO:HD2	1:P:553:VAL:HG21	1.86	0.58
1:O:552:GLY:HA3	1:O:766:GLY:HA3	1.85	0.58
1:T:537:ASP:HB3	1:T:539:LYS:HG2	1.85	0.58
1:P:784:GLU:OE2	1:O:530:ARG:NH2	2.36	0.58
1:T:507:GLU:O	1:T:511:HIS:ND1	2.33	0.58
1:R:391:LEU:HA	1:R:394:LYS:HE2	1.86	0.58
1:Q:381:LEU:HB3	1:Q:484:LEU:HD13	1.84	0.58
1:T:384:ARG:HG3	1:T:385:TYR:CD1	2.39	0.58
1:S:785:LYS:HE2	1:S:812:PHE:HB2	1.86	0.57
1:T:189:ARG:NH2	1:T:344:ALA:O	2.34	0.57
1:O:187:ILE:O	7:O:901:ADP:N6	2.37	0.57
1:S:813:ARG:NE	1:S:815:GLU:OE2	2.36	0.57
1:R:359:ARG:NH1	1:R:372:ASP:OD1	2.32	0.57
3:G:89:GLY:HA3	3:G:114:MET:SD	2.44	0.57
5:R:901:ATP:O1G	1:Q:336:ARG:NH1	2.37	0.57
1:Q:295:GLU:OE1	1:Q:296:GLY:N	2.37	0.57
1:T:290:GLY:HA3	1:T:327:HIS:CD2	2.39	0.57
3:B:144:LEU:HD13	3:B:154:HIS:HB3	1.85	0.57
1:O:740:LYS:NZ	1:O:743:ASP:OD1	2.37	0.57
3:B:104:VAL:HG22	3:B:126:LYS:HB3	1.86	0.57
1:P:587:VAL:HG22	1:P:630:ILE:HD13	1.85	0.57
1:P:776:ARG:HA	1:P:780:ASP:OD1	2.04	0.57
1:P:669:ILE:O	1:P:689:ARG:NH2	2.38	0.57
1:P:790:GLU:O	1:P:792:ARG:NH1	2.37	0.57
1:O:351:THR:HG21	1:O:391:LEU:HG	1.86	0.57
4:I:62:VAL:HG22	4:I:94:SER:HB2	1.87	0.57
3:A:39:ARG:HH21	3:G:66:LEU:HD21	1.70	0.57
3:A:137:ILE:HG12	3:A:188:ARG:HB3	1.87	0.57
4:K:148:LEU:HD13	4:L:112:ASP:HB3	1.86	0.56
3:D:53:ASP:H	3:D:56:ILE:HG22	1.69	0.56
1:P:490:ILE:HD11	1:P:614:PRO:HB2	1.87	0.56
1:P:517:GLN:HG3	1:P:717:PRO:HD2	1.86	0.56
1:O:235:PRO:HG2	1:O:238:LEU:HD12	1.86	0.56
1:O:498:GLU:O	1:O:502:ARG:N	2.36	0.56
3:D:35:GLN:O	3:D:39:ARG:HG3	2.05	0.56
1:S:280:LEU:HB3	1:S:315:THR:HG22	1.86	0.56
1:O:219:THR:HG21	1:T:336:ARG:HH22	1.69	0.56
1:O:586:THR:O	1:O:589:ARG:HG2	2.06	0.56
1:O:628:PRO:O	1:O:631:PHE:HB2	2.06	0.56
1:T:359:ARG:NH2	1:T:370:ILE:O	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:205:LYS:NZ	1:S:335:GLU:O	2.39	0.56
1:S:524:LEU:HD21	1:S:562:LEU:HD22	1.88	0.56
1:P:261:PHE:HZ	1:P:300:ALA:HB2	1.71	0.56
1:O:624:GLU:HA	1:O:702:PHE:HZ	1.71	0.56
3:E:183:ASP:OD2	3:E:198:TYR:OH	2.20	0.56
1:T:386:ILE:O	1:T:394:LYS:NZ	2.38	0.56
1:Q:293:ALA:HB3	1:Q:297:ALA:HB3	1.88	0.55
1:S:407:ARG:NH2	1:R:236:GLU:OE2	2.39	0.55
3:E:127:ARG:NH2	3:E:202:ASP:OD1	2.34	0.55
1:S:275:ARG:HD2	1:S:278:ILE:HD11	1.88	0.55
1:O:173:ASN:ND2	1:O:176:GLN:OE1	2.39	0.55
1:T:208:PRO:HG2	1:T:316:ILE:HG22	1.88	0.55
1:T:351:THR:O	1:T:355:LEU:HG	2.07	0.55
1:T:643:LEU:HB2	1:T:651:VAL:HB	1.88	0.55
3:A:66:LEU:HD21	3:B:39:ARG:HH11	1.71	0.55
3:E:55:ASP:OD1	3:E:56:ILE:N	2.39	0.55
4:J:62:VAL:HG22	4:J:94:SER:HB2	1.89	0.55
1:Q:631:PHE:HA	1:Q:634:LEU:HD13	1.88	0.55
1:P:675:LEU:HD13	4:J:60:GLU:HG3	1.89	0.55
1:Q:243:LEU:HD23	1:Q:279:ILE:HB	1.88	0.55
3:F:53:ASP:H	3:F:56:ILE:HG22	1.72	0.55
3:C:77:LEU:HD23	3:C:79:ILE:HD11	1.88	0.54
1:O:633:SER:O	1:O:636:GLN:HG2	2.08	0.54
1:S:291:ALA:HA	1:S:297:ALA:HB3	1.90	0.54
3:A:86:ILE:HD11	3:A:140:PRO:HB3	1.89	0.54
4:K:61:ARG:NH2	4:K:91:ARG:O	2.40	0.54
4:L:157:GLN:NE2	4:L:204:GLU:O	2.39	0.54
1:R:484:LEU:HD23	1:R:492:VAL:HG21	1.90	0.54
4:H:61:ARG:HG2	4:H:84:LEU:HD22	1.90	0.54
1:Q:682:ASP:OD1	1:Q:689:ARG:NH1	2.40	0.54
3:B:107:ALA:HB2	3:B:119:LEU:HD13	1.89	0.54
1:O:404:SER:OG	1:T:198:GLN:O	2.25	0.54
1:Q:258:ARG:N	2:X:19:UNK:O	2.34	0.54
1:S:167:LEU:HB3	1:S:244:TYR:CE2	2.43	0.54
1:Q:294:ALA:N	1:P:295:GLU:OE1	2.35	0.53
4:M:74:ALA:HA	4:M:110:ILE:HD11	1.90	0.53
1:S:251:LEU:O	1:S:264:ARG:NH2	2.41	0.53
1:T:624:GLU:OE2	1:T:701:HIS:NE2	2.40	0.53
1:O:218:LYS:HD3	1:O:318:ALA:HB1	1.91	0.53
1:S:306:PRO:O	1:S:309:ALA:HB3	2.08	0.53
1:P:410:ARG:HH21	1:P:473:ALA:HB2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:363:GLU:O	1:O:367:ARG:NH1	2.42	0.53
1:O:686:ASN:OD1	1:O:687:TYR:N	2.41	0.53
1:T:321:LEU:HD23	1:T:649:ARG:HH22	1.73	0.53
1:T:671:LYS:NZ	4:N:86:SER:O	2.35	0.53
3:B:73:LYS:O	3:B:101:ASN:ND2	2.36	0.53
1:Q:325:ARG:HA	1:Q:329:GLU:HG3	1.90	0.53
1:T:632:ASN:HA	1:T:703:ARG:HH22	1.74	0.53
3:A:183:ASP:OD2	3:A:198:TYR:OH	2.26	0.53
4:K:62:VAL:HG22	4:K:94:SER:HB2	1.91	0.53
1:T:362:TYR:HE2	1:T:396:ILE:HD11	1.72	0.53
1:O:528:ILE:HA	1:O:531:THR:HG22	1.91	0.53
1:T:275:ARG:HH21	1:T:278:ILE:HG13	1.74	0.53
3:B:191:ASP:O	3:B:193:PHE:N	2.41	0.53
1:O:492:VAL:HG22	1:O:493:PHE:H	1.74	0.53
1:Q:268:VAL:O	1:Q:272:ILE:HG12	2.09	0.52
1:Q:327:HIS:HA	1:Q:330:LYS:NZ	2.24	0.52
1:T:586:THR:HG23	1:T:589:ARG:CZ	2.38	0.52
4:L:83:CYS:O	4:L:87:MET:HG2	2.08	0.52
3:F:175:GLN:NE2	3:F:198:TYR:O	2.42	0.52
4:H:150:ASN:ND2	4:I:112:ASP:OD1	2.41	0.52
4:M:168:SER:O	4:M:172:ILE:HD12	2.09	0.52
1:R:645:ASP:OD1	1:R:646:SER:N	2.42	0.52
1:R:668:ASP:OD2	1:R:693:LYS:NZ	2.26	0.52
1:P:265:LEU:HA	1:P:268:VAL:HG22	1.91	0.52
3:C:57:ALA:HB2	3:C:88:ALA:HB1	1.91	0.52
1:O:248:LEU:HD11	1:O:288:LEU:HD22	1.92	0.52
3:A:157:ARG:HD3	3:B:189:TRP:CD2	2.44	0.52
4:N:157:GLN:NE2	4:N:204:GLU:O	2.42	0.52
1:Q:398:LEU:HD11	1:Q:484:LEU:HD12	1.90	0.52
1:Q:478:GLU:OE1	1:Q:494:LYS:HB2	2.10	0.52
3:D:152:LYS:O	3:D:156:GLU:HG3	2.10	0.52
1:S:642:ARG:HD2	1:S:650:VAL:HG11	1.92	0.52
1:P:268:VAL:O	1:P:272:ILE:HG12	2.10	0.52
1:T:206:ASN:H	1:T:337:ARG:HH21	1.58	0.52
4:K:107:LEU:HD13	4:K:132:ALA:HB1	1.91	0.52
1:S:167:LEU:HD11	1:S:272:ILE:HG22	1.91	0.52
1:R:724:ILE:HG23	1:R:770:LEU:HD22	1.91	0.52
1:P:490:ILE:HD13	1:P:615:PHE:HB2	1.90	0.52
1:O:211:ILE:HD11	1:O:342:GLN:HG3	1.91	0.52
1:O:348:LEU:O	1:O:352:ILE:HG12	2.09	0.52
3:C:54:ASP:O	3:C:58:ASN:ND2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:203:ASP:OD1	3:D:204:VAL:N	2.43	0.52
3:G:178:GLU:OE1	3:G:182:ARG:NH2	2.43	0.51
1:O:366:HIS:HA	1:O:407:ARG:NH2	2.26	0.51
1:O:369:SER:HB3	1:O:474:GLU:HG3	1.91	0.51
1:T:513:ARG:NH2	1:T:557:GLU:OE2	2.43	0.51
1:Q:222:VAL:HG21	1:Q:281:PHE:CE1	2.44	0.51
1:O:404:SER:HA	1:O:407:ARG:HG2	1.92	0.51
4:L:155:ILE:HG13	4:L:207:LYS:HB3	1.92	0.51
1:O:567:PHE:HE2	1:O:617:VAL:HG23	1.76	0.51
1:T:246:LEU:HD22	1:T:280:LEU:HD21	1.92	0.51
3:B:116:GLN:HA	3:B:119:LEU:HB3	1.92	0.51
3:E:144:LEU:HB3	3:E:151:ILE:HD12	1.91	0.51
1:S:265:LEU:HA	1:S:268:VAL:HG12	1.93	0.51
1:O:485:ALA:HB1	1:O:491:PRO:HA	1.93	0.51
1:S:336:ARG:HH22	1:T:389:ARG:HH22	1.58	0.51
1:Q:602:GLU:OE2	1:P:600:TYR:OH	2.28	0.51
1:P:577:ASP:OD2	1:P:579:SER:OG	2.27	0.51
1:T:585:HIS:O	1:T:588:SER:HB3	2.11	0.51
3:A:104:VAL:HG22	3:A:126:LYS:HD3	1.92	0.51
1:Q:652:ASP:OD2	1:Q:654:LYS:NZ	2.34	0.51
1:P:524:LEU:HD11	1:P:547:PHE:HZ	1.76	0.51
3:E:57:ALA:HB2	3:E:88:ALA:HB1	1.92	0.51
4:M:155:ILE:HG13	4:M:207:LYS:HB3	1.92	0.51
1:S:180:GLU:OE1	1:S:180:GLU:N	2.44	0.51
3:A:114:MET:HE3	3:A:117:PHE:CD2	2.45	0.51
3:F:57:ALA:HB2	3:F:88:ALA:HB1	1.91	0.50
1:P:295:GLU:H	2:X:15:UNK:HA	1.76	0.50
1:P:688:GLU:OE1	1:P:688:GLU:N	2.45	0.50
1:P:673:PHE:HZ	4:K:89:PRO:HB3	1.76	0.50
3:A:73:LYS:O	3:A:101:ASN:ND2	2.44	0.50
1:T:490:ILE:O	1:T:492:VAL:N	2.42	0.50
1:P:513:ARG:NE	1:P:557:GLU:OE2	2.42	0.50
1:T:269:LEU:HA	1:T:272:ILE:HG12	1.93	0.50
3:B:185:ASP:OD1	4:I:205:ARG:NH2	2.42	0.50
1:T:764:VAL:HG13	1:T:765:LEU:HD22	1.94	0.50
4:L:74:ALA:HB2	4:L:106:ALA:HB1	1.93	0.50
1:R:236:GLU:HA	1:R:239:LYS:HG2	1.92	0.50
1:T:238:LEU:HB2	1:T:241:LYS:HD3	1.94	0.50
1:T:360:ASP:OD1	1:T:361:ARG:N	2.43	0.50
1:S:629:ASP:O	1:S:632:ASN:HB3	2.12	0.50
1:S:782:LEU:HD21	1:S:797:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:813:ARG:NH1	1:R:815:GLU:OE1	2.45	0.50
1:T:253:ALA:O	1:T:264:ARG:NH2	2.45	0.50
1:Q:756:LEU:HD21	1:Q:778:ILE:HD11	1.94	0.49
4:K:52:ASP:N	4:K:52:ASP:OD1	2.45	0.49
1:S:272:ILE:HA	1:S:278:ILE:HD12	1.94	0.49
1:S:324:TYR:CE1	1:S:328:LEU:HD22	2.46	0.49
1:Q:555:LYS:NZ	1:Q:663:ASN:OD1	2.46	0.49
1:O:637:ILE:HG22	1:O:638:LEU:HD22	1.94	0.49
1:T:748:LEU:HG	1:T:799:VAL:HB	1.93	0.49
4:H:57:LEU:HD22	4:H:64:PHE:CE2	2.48	0.49
1:T:218:LYS:HD3	1:T:318:ALA:HB1	1.93	0.49
4:M:125:CYS:HB2	4:M:137:LEU:HD13	1.93	0.49
1:Q:261:PHE:HE2	1:Q:292:GLY:HA2	1.77	0.49
3:C:152:LYS:O	3:C:156:GLU:HG3	2.13	0.49
4:N:57:LEU:HD23	4:N:62:VAL:HG11	1.94	0.49
1:R:724:ILE:O	1:R:728:VAL:HG13	2.12	0.49
3:D:61:THR:HG21	3:E:108:MET:SD	2.53	0.49
4:M:110:ILE:HG21	4:M:136:LEU:HD21	1.95	0.49
3:B:66:LEU:HD21	3:C:39:ARG:HH11	1.78	0.49
1:P:309:ALA:HB2	1:P:337:ARG:HG2	1.95	0.49
1:O:262:GLU:HB3	1:O:266:LYS:HZ2	1.78	0.49
1:R:359:ARG:HD3	1:R:375:LEU:HD11	1.95	0.49
1:P:728:VAL:HG12	1:P:770:LEU:HD21	1.95	0.49
1:T:350:HIS:O	1:T:354:ILE:HG12	2.13	0.49
4:H:107:LEU:HD13	4:H:132:ALA:HB1	1.94	0.49
3:A:189:TRP:HB2	3:G:157:ARG:HH21	1.78	0.49
4:J:185:GLU:OE1	4:J:200:ARG:HG2	2.13	0.49
4:N:90:ASP:OD1	4:N:90:ASP:N	2.46	0.49
1:S:205:LYS:HA	1:S:337:ARG:HA	1.94	0.48
1:Q:683:THR:O	4:I:231:ASN:ND2	2.46	0.48
1:P:505:ARG:NH1	1:P:509:GLU:OE2	2.45	0.48
1:P:591:PHE:HB2	1:P:645:ASP:HA	1.95	0.48
3:B:50:GLN:NE2	3:B:56:ILE:HD13	2.28	0.48
3:B:183:ASP:OD2	3:B:188:ARG:NH1	2.46	0.48
1:O:405:ARG:NH1	1:O:482:GLU:OE2	2.46	0.48
3:F:94:ASP:OD1	3:G:132:ASN:HB2	2.12	0.48
1:R:522:LYS:HG3	1:R:526:LYS:HE2	1.94	0.48
1:Q:284:ALA:O	1:Q:287:THR:HG22	2.13	0.48
1:T:608:GLU:O	1:T:612:ARG:HG2	2.12	0.48
3:D:104:VAL:HG22	3:D:126:LYS:HB3	1.95	0.48
1:P:803:GLY:HA3	1:P:808:LYS:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:366:HIS:NE2	1:O:400:ASP:OD1	2.45	0.48
1:S:481:ALA:HB1	1:S:492:VAL:O	2.13	0.48
1:S:623:VAL:HG22	1:S:631:PHE:HE1	1.78	0.48
1:P:520:ALA:HB2	1:P:714:VAL:HG11	1.96	0.48
1:T:477:GLY:HA2	1:T:480:ILE:HG22	1.96	0.48
1:T:550:PRO:HG2	1:T:553:VAL:HG21	1.95	0.48
1:P:267:LYS:O	1:P:270:LYS:HG2	2.13	0.48
3:A:136:LEU:HD13	3:A:189:TRP:CE2	2.48	0.48
1:S:266:LYS:NZ	1:S:270:LYS:HB2	2.28	0.48
1:P:333:ALA:O	1:P:337:ARG:NH1	2.45	0.48
1:T:356:LYS:O	1:T:359:ARG:HG2	2.13	0.48
1:T:667:ARG:HH22	1:T:697:GLU:HB2	1.78	0.48
4:H:96:TYR:HB3	4:H:126:MET:CE	2.43	0.48
4:K:207:LYS:HE3	4:K:209:LEU:HD21	1.95	0.48
1:O:739:LEU:HG	1:O:744:MET:HB2	1.95	0.48
1:T:244:TYR:CE1	1:T:278:ILE:HD12	2.48	0.48
3:F:35:GLN:O	3:F:39:ARG:HG3	2.12	0.48
1:R:260:ASP:O	1:R:263:GLU:HG3	2.14	0.48
1:Q:301:ALA:O	1:Q:305:LYS:HG3	2.14	0.48
1:O:610:VAL:HG21	1:O:653:PHE:HE1	1.79	0.48
1:T:509:GLU:HG3	1:T:512:LYS:HE2	1.95	0.48
1:T:563:ALA:HB1	1:T:572:ALA:HB3	1.95	0.48
3:D:108:MET:HA	3:D:130:LEU:HD12	1.95	0.48
3:F:34:ASP:OD1	3:G:32:LEU:N	2.47	0.48
4:M:74:ALA:HB2	4:M:106:ALA:HB1	1.95	0.48
3:C:104:VAL:HG22	3:C:126:LYS:HB3	1.96	0.47
3:F:72:GLU:O	3:F:72:GLU:HG2	2.13	0.47
4:N:96:TYR:HB3	4:N:126:MET:CE	2.44	0.47
1:S:232:GLY:HA2	1:S:239:LYS:HZ3	1.79	0.47
1:S:591:PHE:HE2	1:S:643:LEU:HD21	1.79	0.47
1:P:734:LYS:O	1:P:737:GLU:HG3	2.14	0.47
1:O:581:PHE:CE1	1:O:590:LEU:HB2	2.49	0.47
3:C:139:GLN:NE2	3:C:185:ASP:O	2.45	0.47
1:T:385:TYR:HA	1:T:615:PHE:HZ	1.80	0.47
3:B:94:ASP:HB3	3:C:130:LEU:HD13	1.96	0.47
4:K:224:ILE:HD12	4:L:116:TYR:CE1	2.50	0.47
1:S:779:GLU:HG2	1:R:535:LEU:HD12	1.96	0.47
1:T:272:ILE:HG22	1:T:275:ARG:HH22	1.79	0.47
1:T:623:VAL:HB	1:T:631:PHE:HZ	1.79	0.47
3:D:144:LEU:HB3	3:D:151:ILE:HD12	1.96	0.47
1:P:524:LEU:HD23	1:P:562:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:ILE:HD12	3:C:101:ASN:HB2	1.96	0.47
1:Q:724:ILE:HG23	1:Q:770:LEU:HD22	1.97	0.47
1:P:602:GLU:HG2	1:P:603:GLY:N	2.28	0.47
3:A:164:ARG:HA	3:A:164:ARG:HD2	1.69	0.47
4:I:74:ALA:HB2	4:I:106:ALA:HB1	1.96	0.47
1:T:751:SER:O	1:T:754:GLU:HG3	2.15	0.47
1:P:550:PRO:O	1:P:555:LYS:NZ	2.48	0.47
1:O:381:LEU:HB3	1:O:484:LEU:HD22	1.96	0.47
1:T:195:ARG:HE	1:T:199:VAL:HG23	1.79	0.47
1:T:271:GLU:HB3	1:T:275:ARG:HH12	1.79	0.47
1:T:575:SER:O	1:T:576:LEU:HD22	2.15	0.47
3:F:183:ASP:OD2	3:F:198:TYR:OH	2.25	0.47
4:N:74:ALA:HB2	4:N:106:ALA:HB1	1.97	0.47
1:R:183:LEU:HD13	1:R:223:GLU:OE1	2.14	0.47
1:O:553:VAL:HA	1:O:719:LEU:HD21	1.95	0.47
1:O:677:PHE:CD2	4:L:124:VAL:HG11	2.47	0.47
1:T:195:ARG:O	1:T:199:VAL:HG23	2.16	0.47
3:G:50:GLN:HG3	3:G:56:ILE:HD13	1.97	0.47
1:S:397:ASP:OD1	1:R:202:ARG:NH2	2.36	0.46
3:F:107:ALA:HB2	3:F:119:LEU:HD13	1.98	0.46
1:S:587:VAL:HG12	1:S:630:ILE:HD13	1.96	0.46
1:O:262:GLU:HA	1:O:265:LEU:HB3	1.97	0.46
1:O:728:VAL:O	1:O:732:ILE:HG12	2.14	0.46
1:T:246:LEU:HB2	1:T:280:LEU:HD11	1.96	0.46
3:C:173:THR:HG21	3:C:200:LEU:HD23	1.97	0.46
1:S:612:ARG:HE	1:R:321:LEU:HD22	1.79	0.46
1:T:390:PHE:O	1:T:394:LYS:N	2.48	0.46
3:C:56:ILE:O	3:C:60:ILE:HG12	2.15	0.46
3:E:104:VAL:HG22	3:E:126:LYS:HD3	1.96	0.46
4:K:222:GLN:HE22	4:K:224:ILE:HG23	1.80	0.46
4:N:69:ILE:HB	4:N:102:GLY:HA3	1.96	0.46
1:R:268:VAL:O	1:R:272:ILE:HG12	2.15	0.46
1:R:806:GLU:HG2	1:R:808:LYS:H	1.79	0.46
1:Q:175:THR:HG23	1:Q:243:LEU:H	1.78	0.46
1:Q:255:SER:HB2	1:P:258:ARG:HH21	1.80	0.46
1:O:243:LEU:HA	1:O:279:ILE:O	2.15	0.46
1:O:288:LEU:HD23	1:O:288:LEU:H	1.80	0.46
1:O:608:GLU:O	1:O:612:ARG:HG2	2.16	0.46
3:A:59:LYS:HG2	3:A:63:GLN:NE2	2.30	0.46
5:S:901:ATP:O1G	1:R:336:ARG:NH1	2.43	0.46
1:R:187:ILE:HD11	1:R:357:GLY:HA3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:157:ARG:HD3	3:B:189:TRP:CE2	2.51	0.46
1:S:490:ILE:HG22	1:S:492:VAL:HG13	1.98	0.46
1:O:210:LEU:HD23	1:O:341:ILE:HB	1.97	0.46
1:O:760:GLY:HA3	1:O:770:LEU:HD23	1.97	0.46
3:E:157:ARG:NH1	3:F:134:GLU:OE1	2.48	0.46
1:T:703:ARG:HD2	1:T:705:GLU:OE2	2.16	0.46
3:A:52:VAL:HB	3:A:84:GLY:HA3	1.98	0.46
4:K:74:ALA:HB2	4:K:106:ALA:HB1	1.98	0.46
1:T:785:LYS:HE3	1:T:812:PHE:HB2	1.97	0.46
3:E:104:VAL:HG22	3:E:126:LYS:HB3	1.98	0.46
4:J:202:ASP:HB3	4:J:207:LYS:HD2	1.98	0.46
4:L:117:VAL:HB	4:L:119:PRO:HD2	1.97	0.46
1:S:680:GLN:OE1	4:N:228:LYS:NZ	2.46	0.46
1:Q:578:MET:HG3	1:Q:623:VAL:HA	1.97	0.46
1:O:632:ASN:O	1:O:635:LEU:HB3	2.15	0.46
1:T:509:GLU:HA	1:T:512:LYS:HE2	1.97	0.46
4:H:150:ASN:HB2	4:I:108:THR:HG23	1.97	0.46
1:S:546:ILE:HD11	1:S:710:VAL:HG21	1.98	0.46
1:P:748:LEU:HD11	1:P:753:LYS:HE2	1.98	0.46
1:T:380:THR:O	1:T:384:ARG:HG2	2.16	0.46
4:J:176:GLU:OE1	4:J:179:ARG:NH2	2.42	0.46
1:S:213:GLU:O	1:S:216:VAL:HG22	2.16	0.45
1:R:602:GLU:HA	1:Q:325:ARG:NH1	2.27	0.45
1:R:756:LEU:HD21	1:R:774:ILE:HG12	1.98	0.45
3:B:164:ARG:HD2	3:B:164:ARG:HA	1.71	0.45
1:R:697:GLU:OE2	1:R:700:GLN:NE2	2.49	0.45
1:O:193:ILE:HG22	1:O:197:MET:HE1	1.98	0.45
1:T:345:GLU:OE1	1:T:391:LEU:HD12	2.16	0.45
1:T:352:ILE:HD13	1:T:376:VAL:HG12	1.98	0.45
1:T:590:LEU:HD23	1:T:630:ILE:HD11	1.99	0.45
3:A:53:ASP:H	3:A:56:ILE:HG22	1.82	0.45
3:F:49:GLY:O	3:F:50:GLN:HG2	2.16	0.45
1:S:236:GLU:HA	1:S:239:LYS:HG2	1.98	0.45
1:S:303:ILE:HD12	1:S:303:ILE:H	1.82	0.45
1:T:196:VAL:HG11	1:T:210:LEU:HD21	1.98	0.45
1:P:322:ASP:OD1	1:P:323:GLU:N	2.50	0.45
1:O:503:LEU:HD13	1:O:529:ARG:HG3	1.99	0.45
3:A:39:ARG:NH2	3:G:66:LEU:HD21	2.31	0.45
3:B:91:ALA:HB1	3:C:108:MET:HG2	1.98	0.45
1:O:545:PHE:HD1	1:O:712:ASP:HB3	1.82	0.45
3:C:61:THR:HG21	3:D:108:MET:SD	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:54:ASP:O	3:D:58:ASN:ND2	2.50	0.45
4:H:96:TYR:HB3	4:H:126:MET:HE1	1.98	0.45
1:S:201:SER:OG	1:T:404:SER:OG	2.31	0.45
1:S:405:ARG:HB2	1:R:198:GLN:NE2	2.32	0.45
1:O:517:GLN:HB2	1:O:521:VAL:HG23	1.99	0.45
1:T:227:GLN:HA	1:T:230:VAL:HG22	1.99	0.45
3:G:44:ARG:HD2	3:G:75:ILE:HG12	1.97	0.45
4:N:57:LEU:HD22	4:N:64:PHE:CE2	2.52	0.45
1:S:301:ALA:O	1:S:305:LYS:HG2	2.16	0.45
1:R:382:ALA:HB2	1:R:398:LEU:HD12	1.99	0.45
1:P:772:ARG:HD2	1:P:772:ARG:HA	1.75	0.45
1:O:629:ASP:OD2	1:O:629:ASP:N	2.46	0.45
1:S:326:LYS:HD2	1:S:327:HIS:HB2	1.99	0.45
1:S:611:ARG:HD3	1:S:651:VAL:HG22	1.97	0.45
1:O:255:SER:HB3	1:O:264:ARG:HH22	1.82	0.45
4:K:210:THR:HG23	4:K:213:ASP:H	1.82	0.45
1:S:738:ARG:NH1	1:S:779:GLU:OE2	2.49	0.45
1:R:405:ARG:HD3	1:Q:198:GLN:OE1	2.17	0.45
1:Q:164:SER:OG	1:Q:271:GLU:OE2	2.35	0.45
1:Q:623:VAL:HG11	1:Q:660:MET:HB3	1.99	0.45
1:P:691:LYS:HG2	1:P:715:VAL:HG21	1.98	0.45
3:F:52:VAL:HA	3:F:56:ILE:HG21	1.98	0.45
4:L:135:VAL:HG21	4:L:184:LEU:HD11	1.98	0.45
1:O:275:ARG:O	1:O:275:ARG:NH1	2.50	0.45
3:A:57:ALA:HB2	3:A:88:ALA:HB1	1.99	0.45
3:B:48:LEU:HD23	3:B:48:LEU:O	2.17	0.45
4:H:173:ALA:O	4:H:177:ILE:HG12	2.17	0.45
1:R:226:ALA:HB2	1:R:243:LEU:HD23	1.99	0.44
3:E:94:ASP:HB3	3:F:130:LEU:HD13	1.98	0.44
1:S:336:ARG:NH2	1:T:389:ARG:HH22	2.14	0.44
1:S:366:HIS:NE2	1:S:400:ASP:OD1	2.33	0.44
1:S:368:VAL:HG12	1:S:473:ALA:HB3	2.00	0.44
1:S:382:ALA:HB1	1:S:394:LYS:HG3	1.99	0.44
1:O:799:VAL:HG22	1:O:812:PHE:CE1	2.52	0.44
1:T:167:LEU:HD11	1:T:275:ARG:NH2	2.32	0.44
1:O:288:LEU:HG	1:O:289:VAL:HG13	1.97	0.44
1:O:352:ILE:HG22	1:O:356:LYS:NZ	2.32	0.44
1:T:593:SER:HB2	1:T:602:GLU:O	2.18	0.44
3:C:53:ASP:H	3:C:56:ILE:HG22	1.82	0.44
3:F:94:ASP:HB3	3:G:130:LEU:HD13	1.99	0.44
4:H:74:ALA:HA	4:H:110:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:326:LYS:HE3	1:Q:326:LYS:HB2	1.81	0.44
1:P:686:ASN:O	1:P:689:ARG:HG3	2.17	0.44
1:O:556:THR:N	5:O:902:ATP:O1B	2.35	0.44
1:T:326:LYS:HA	1:T:330:LYS:NZ	2.32	0.44
1:T:560:LYS:HG2	1:T:573:LEU:HD21	1.98	0.44
3:G:44:ARG:HG2	3:G:74:ASP:O	2.17	0.44
1:Q:226:ALA:HA	1:Q:229:ILE:HG12	2.00	0.44
1:Q:607:THR:HB	1:Q:651:VAL:HG21	1.98	0.44
1:T:573:LEU:HD12	1:T:573:LEU:O	2.18	0.44
3:G:104:VAL:HG22	3:G:126:LYS:HB3	2.00	0.44
4:K:125:CYS:HB2	4:K:137:LEU:HD13	1.98	0.44
1:S:275:ARG:HG2	1:S:277:ASP:OD1	2.18	0.44
1:R:747:GLU:OE1	1:R:749:SER:N	2.50	0.44
1:O:184:ASP:O	1:O:227:GLN:NE2	2.38	0.44
1:O:792:ARG:O	1:O:795:HIS:ND1	2.44	0.44
3:C:90:MET:HE1	3:C:117:PHE:CZ	2.53	0.44
1:S:226:ALA:O	1:S:229:ILE:HG22	2.18	0.44
1:R:746:ILE:HD12	1:R:782:LEU:HD11	1.99	0.44
1:Q:564:GLU:HG3	1:Q:569:ASP:HA	1.99	0.44
1:O:174:LEU:HD22	1:O:243:LEU:HD22	1.99	0.44
1:O:253:ALA:HA	1:T:299:ASP:O	2.18	0.44
1:O:556:THR:HG22	1:O:560:LYS:HE3	1.98	0.44
3:C:161:THR:O	3:C:165:MET:HG2	2.17	0.44
4:H:74:ALA:HB2	4:H:106:ALA:HB1	1.98	0.44
1:O:528:ILE:O	1:O:532:ARG:HG2	2.17	0.44
4:I:69:ILE:HB	4:I:102:GLY:HA3	2.00	0.44
1:Q:211:ILE:HA	1:Q:319:THR:O	2.18	0.44
1:P:356:LYS:O	1:P:359:ARG:HG2	2.18	0.44
4:I:188:LEU:HD23	4:I:188:LEU:HA	1.85	0.44
4:M:130:ALA:HA	4:M:154:LEU:HB2	1.99	0.44
1:P:202:ARG:HB2	1:P:206:ASN:HB3	1.99	0.43
1:T:269:LEU:HD21	1:T:307:MET:HG3	2.00	0.43
1:T:610:VAL:HG21	1:T:653:PHE:CZ	2.53	0.43
3:B:57:ALA:HB2	3:B:88:ALA:HB1	1.98	0.43
3:E:136:LEU:HD13	3:E:189:TRP:CE2	2.53	0.43
3:G:46:ILE:HD11	3:G:67:LEU:HD12	1.99	0.43
1:Q:673:PHE:HZ	4:J:89:PRO:HB3	1.83	0.43
1:P:752:ALA:HA	1:P:810:PHE:HE1	1.84	0.43
1:O:731:MET:HE1	1:O:770:LEU:HD13	2.00	0.43
1:T:781:SER:HA	1:T:784:GLU:HG2	2.00	0.43
3:A:107:ALA:HB2	3:A:119:LEU:HD13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:65:LEU:HD13	4:K:77:VAL:HG21	1.99	0.43
1:R:290:GLY:O	1:Q:296:GLY:HA2	2.18	0.43
1:Q:327:HIS:HA	1:Q:330:LYS:HZ1	1.83	0.43
1:P:584:LYS:HE3	1:P:584:LYS:HB3	1.88	0.43
1:P:623:VAL:HG12	1:P:662:THR:HB	2.01	0.43
1:O:359:ARG:HD2	1:O:370:ILE:HB	2.00	0.43
3:E:57:ALA:HA	3:E:92:ILE:HD11	2.01	0.43
3:F:137:ILE:HG13	3:F:188:ARG:HB3	2.01	0.43
3:G:57:ALA:HB2	3:G:88:ALA:HB1	2.00	0.43
4:L:150:ASN:HB2	4:M:112:ASP:OD2	2.18	0.43
1:P:775:GLN:NE2	1:P:780:ASP:OD2	2.51	0.43
1:Q:404:SER:O	1:Q:408:ILE:HG12	2.18	0.43
1:P:728:VAL:O	1:P:732:ILE:HG12	2.18	0.43
1:S:205:LYS:HG2	1:S:336:ARG:O	2.18	0.43
1:P:391:LEU:HA	1:P:394:LYS:HE2	2.01	0.43
1:O:229:ILE:HA	1:O:234:VAL:HG21	1.99	0.43
1:O:385:TYR:HB2	1:O:484:LEU:HD21	1.99	0.43
1:T:267:LYS:O	1:T:271:GLU:HG2	2.19	0.43
1:R:262:GLU:CG	1:R:298:ILE:HG13	2.47	0.43
1:P:756:LEU:HD23	1:P:756:LEU:HA	1.88	0.43
1:T:275:ARG:HE	1:T:278:ILE:HG13	1.83	0.43
3:B:61:THR:HG21	3:C:108:MET:SD	2.59	0.43
4:J:74:ALA:HB2	4:J:106:ALA:HB1	2.00	0.43
4:L:101:GLY:HA3	4:L:131:ALA:HB3	2.01	0.43
5:R:901:ATP:O1G	1:Q:337:ARG:NH1	2.50	0.43
1:Q:388:ASP:N	1:Q:388:ASP:OD1	2.50	0.43
1:Q:536:LYS:HD2	1:Q:542:GLY:HA2	2.01	0.43
1:Q:681:GLY:O	4:I:230:ASP:HA	2.19	0.43
1:P:755:LEU:HD22	1:P:808:LYS:HG2	1.99	0.43
1:O:251:LEU:O	1:O:264:ARG:NE	2.40	0.43
3:B:53:ASP:H	3:B:56:ILE:HG22	1.83	0.43
1:Q:782:LEU:HD21	1:Q:797:VAL:HG21	2.01	0.43
1:P:405:ARG:HD3	1:P:483:VAL:HG22	2.01	0.43
1:P:479:LEU:O	1:P:483:VAL:HG23	2.19	0.43
1:P:584:LYS:O	1:P:587:VAL:HG23	2.18	0.43
1:O:506:MET:HG3	1:O:565:PHE:CE2	2.54	0.43
4:L:123:THR:HB	4:L:137:LEU:HD12	2.01	0.43
4:N:155:ILE:HG13	4:N:207:LYS:HB3	2.00	0.43
1:S:532:ARG:HA	1:S:532:ARG:HD2	1.86	0.43
1:S:611:ARG:NH2	1:S:612:ARG:HH12	2.17	0.43
1:R:303:ILE:O	1:R:307:MET:HE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:780:ASP:O	1:R:783:SER:OG	2.21	0.43
1:Q:200:LEU:HD11	1:Q:316:ILE:HD11	2.00	0.43
1:T:193:ILE:HA	1:T:196:VAL:HG22	2.01	0.43
1:T:243:LEU:HD12	1:T:279:ILE:O	2.19	0.43
1:T:637:ILE:HD11	1:T:643:LEU:HD11	1.99	0.43
3:F:152:LYS:O	3:F:156:GLU:OE1	2.37	0.43
1:S:780:ASP:O	1:S:783:SER:OG	2.19	0.42
1:P:262:GLU:C	1:P:264:ARG:H	2.23	0.42
1:T:167:LEU:HD13	1:T:244:TYR:CE1	2.54	0.42
4:H:70:ASP:N	4:H:70:ASP:OD1	2.52	0.42
4:H:88:ASP:HA	4:H:89:PRO:HD3	1.90	0.42
4:I:74:ALA:HA	4:I:110:ILE:HD11	2.01	0.42
1:Q:355:LEU:HD11	1:Q:395:ALA:HB1	2.01	0.42
1:O:187:ILE:HB	1:O:354:ILE:HG12	2.01	0.42
3:G:127:ARG:NH2	3:G:202:ASP:OD1	2.38	0.42
4:K:84:LEU:HD13	4:K:93:ILE:HG12	2.01	0.42
4:M:66:GLY:HA3	4:N:75:ASN:HD21	1.83	0.42
1:S:728:VAL:HG22	1:S:770:LEU:HD11	2.00	0.42
1:R:572:ALA:HB1	1:R:613:LYS:NZ	2.34	0.42
1:T:307:MET:HA	1:T:310:ARG:HB2	1.99	0.42
1:T:390:PHE:CE1	1:T:650:VAL:HG21	2.55	0.42
1:R:248:LEU:HD23	1:R:251:LEU:HD12	2.00	0.42
1:Q:229:ILE:HG22	1:Q:234:VAL:HG11	2.00	0.42
1:Q:290:GLY:O	1:P:296:GLY:HA3	2.19	0.42
1:P:268:VAL:HG23	1:P:269:LEU:HD12	2.02	0.42
1:O:768:ARG:NH2	5:O:902:ATP:O2G	2.52	0.42
1:T:622:ALA:HB1	1:T:625:LYS:HE2	2.01	0.42
1:T:627:HIS:O	1:T:630:ILE:HG22	2.18	0.42
3:B:112:ALA:HB1	3:B:136:LEU:HD23	1.99	0.42
3:F:40:LEU:HD23	3:F:40:LEU:HA	1.81	0.42
1:P:222:VAL:HG21	1:P:281:PHE:CE1	2.54	0.42
1:O:545:PHE:CD1	1:O:712:ASP:HB3	2.55	0.42
1:T:265:LEU:HB3	1:T:303:ILE:HG21	2.01	0.42
3:D:108:MET:O	3:D:108:MET:HG2	2.18	0.42
3:G:164:ARG:HD2	3:G:164:ARG:HA	1.79	0.42
1:R:748:LEU:O	1:R:753:LYS:HE2	2.20	0.42
1:P:178:ALA:HB3	1:P:230:VAL:HG21	2.01	0.42
1:O:407:ARG:NH1	1:T:237:THR:HG21	2.35	0.42
1:T:642:ARG:HH21	1:T:644:THR:HA	1.84	0.42
4:H:56:LYS:HE3	4:I:83:CYS:SG	2.60	0.42
1:P:515:ILE:H	5:P:902:ATP:HN62	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:515:ILE:HG21	1:T:726:LYS:HB2	2.01	0.42
1:T:581:PHE:HA	1:T:586:THR:HG21	2.01	0.42
1:S:348:LEU:HB3	1:S:349:PRO:HD3	2.02	0.42
1:S:584:LYS:HB3	1:S:627:HIS:CE1	2.54	0.42
1:O:492:VAL:HG13	1:O:493:PHE:N	2.35	0.42
1:T:531:THR:HA	1:T:536:LYS:HB2	2.01	0.42
4:J:154:LEU:HD13	4:J:208:ILE:HG13	2.01	0.42
4:L:188:LEU:HD23	4:L:188:LEU:HA	1.87	0.42
1:S:205:LYS:HD3	1:T:397:ASP:OD2	2.20	0.42
1:T:367:ARG:HB3	1:T:410:ARG:NH2	2.35	0.42
3:D:57:ALA:HA	3:D:92:ILE:HD11	2.02	0.42
1:Q:586:THR:HG22	1:P:594:PRO:HG3	2.02	0.42
1:P:775:GLN:HG2	1:P:779:GLU:OE2	2.20	0.42
1:O:508:ASP:O	1:O:512:LYS:N	2.53	0.42
3:E:175:GLN:HB2	3:E:180:ILE:HD11	2.02	0.42
4:M:155:ILE:HD11	4:M:207:LYS:HD3	2.02	0.42
1:R:637:ILE:HD11	1:R:643:LEU:HD22	2.02	0.41
1:Q:247:ASP:OD2	1:Q:250:ALA:N	2.46	0.41
1:O:620:PHE:HB3	1:O:623:VAL:HG22	2.02	0.41
3:E:66:LEU:HD21	3:F:39:ARG:NE	2.35	0.41
3:G:44:ARG:NH2	3:G:73:LYS:HE2	2.35	0.41
4:J:130:ALA:HB1	4:J:154:LEU:HD23	2.02	0.41
4:L:84:LEU:HD23	4:L:84:LEU:HA	1.87	0.41
4:L:104:PHE:HE1	4:L:184:LEU:HD13	1.84	0.41
4:L:228:LYS:NZ	4:M:118:LYS:HA	2.35	0.41
1:R:255:SER:OG	1:R:255:SER:O	2.35	0.41
1:Q:218:LYS:HB2	1:Q:218:LYS:HE3	1.84	0.41
1:T:359:ARG:HB2	1:T:370:ILE:HD11	2.03	0.41
1:O:225:LEU:O	1:O:229:ILE:HG12	2.20	0.41
3:E:152:LYS:O	3:E:156:GLU:OE1	2.38	0.41
1:R:520:ALA:HB2	1:R:714:VAL:HG11	2.01	0.41
1:Q:393:ASP:OD2	1:P:205:LYS:NZ	2.51	0.41
1:P:634:LEU:HD23	1:P:637:ILE:HD12	2.02	0.41
1:O:546:ILE:HG13	1:O:710:VAL:HG21	2.02	0.41
3:D:113:ALA:O	3:D:116:GLN:HG3	2.20	0.41
3:E:46:ILE:HD11	3:E:67:LEU:HD12	2.02	0.41
4:J:176:GLU:O	4:J:180:MET:HG3	2.21	0.41
1:R:333:ALA:O	1:R:337:ARG:HG2	2.21	0.41
1:Q:226:ALA:O	1:Q:230:VAL:HG12	2.20	0.41
1:O:525:SER:O	1:O:529:ARG:HD3	2.20	0.41
1:T:268:VAL:O	1:T:272:ILE:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:152:LYS:O	3:B:156:GLU:HG3	2.21	0.41
3:B:163:LYS:O	3:B:167:GLU:HG3	2.21	0.41
4:J:70:ASP:OD1	4:J:70:ASP:N	2.52	0.41
1:S:172:ARG:HB3	1:S:245:THR:HG22	2.02	0.41
1:S:404:SER:O	1:S:408:ILE:HG12	2.20	0.41
1:S:775:GLN:HA	1:S:779:GLU:HB2	2.02	0.41
1:Q:371:THR:HG23	1:Q:374:ALA:H	1.85	0.41
3:B:178:GLU:HG2	3:B:179:GLN:N	2.36	0.41
3:D:157:ARG:HD2	3:E:134:GLU:OE2	2.20	0.41
4:H:217:TYR:HD2	4:H:219:LEU:HG	1.85	0.41
4:M:84:LEU:HD23	4:M:84:LEU:HA	1.90	0.41
1:Q:320:THR:OG1	1:Q:323:GLU:HG2	2.20	0.41
1:Q:805:GLY:O	1:Q:808:LYS:HG3	2.21	0.41
1:P:301:ALA:O	1:P:305:LYS:HG3	2.21	0.41
1:P:791:LEU:HD23	1:P:791:LEU:H	1.85	0.41
1:O:247:ASP:OD1	1:O:247:ASP:N	2.47	0.41
1:O:268:VAL:O	1:O:271:GLU:HB3	2.21	0.41
1:T:244:TYR:HE1	1:T:278:ILE:HD12	1.86	0.41
1:R:556:THR:HG22	1:R:560:LYS:HE3	2.02	0.41
3:B:136:LEU:HD13	3:B:189:TRP:CE2	2.56	0.41
3:B:191:ASP:OD1	3:B:194:GLU:HG3	2.20	0.41
3:F:144:LEU:HD13	3:F:151:ILE:HG23	2.02	0.41
3:G:57:ALA:HA	3:G:92:ILE:HD11	2.02	0.41
4:H:126:MET:SD	4:I:78:MET:HE1	2.61	0.41
4:J:174:ALA:HA	4:J:177:ILE:HG22	2.03	0.41
1:S:503:LEU:HD11	1:S:532:ARG:HG2	2.03	0.41
1:R:490:ILE:HA	1:R:491:PRO:HD3	1.97	0.41
1:R:776:ARG:HA	1:R:780:ASP:OD2	2.21	0.41
1:P:671:LYS:NZ	1:P:674:ASN:HA	2.36	0.41
1:O:209:VAL:HG13	1:O:340:PRO:HA	2.03	0.41
1:T:322:ASP:OD1	1:T:325:ARG:NH2	2.53	0.41
1:T:382:ALA:HB1	1:T:394:LYS:HD2	2.02	0.41
3:G:130:LEU:HD23	3:G:130:LEU:HA	1.94	0.41
1:R:199:VAL:HG11	1:R:208:PRO:HB3	2.03	0.41
1:R:284:ALA:O	1:R:287:THR:OG1	2.32	0.40
1:Q:779:GLU:HG3	1:P:535:LEU:HD13	2.03	0.40
1:T:321:LEU:HD23	1:T:321:LEU:H	1.86	0.40
3:B:157:ARG:O	3:B:161:THR:HG23	2.21	0.40
3:E:164:ARG:HA	3:E:164:ARG:HD2	1.74	0.40
4:J:182:SER:HA	4:J:185:GLU:HG2	2.02	0.40
4:K:174:ALA:O	4:K:177:ILE:HG22	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:205:ARG:NH1	4:N:168:SER:HB2	2.36	0.40
1:P:205:LYS:HD2	1:P:337:ARG:HA	2.02	0.40
1:P:675:LEU:HG	4:K:86:SER:HB2	2.04	0.40
1:O:173:ASN:HB3	1:O:176:GLN:NE2	2.28	0.40
1:O:359:ARG:HG3	1:O:370:ILE:HD12	2.02	0.40
1:O:538:PRO:HB3	1:O:654:LYS:HE3	2.03	0.40
3:B:180:ILE:HD13	3:B:180:ILE:HA	1.98	0.40
4:N:176:GLU:OE2	4:N:179:ARG:NH2	2.42	0.40
1:Q:251:LEU:HB3	1:Q:261:PHE:HE1	1.87	0.40
1:O:407:ARG:HD2	1:T:201:SER:HB2	2.04	0.40
1:O:610:VAL:HG21	1:O:653:PHE:CE1	2.55	0.40
1:O:658:ILE:HG22	1:O:660:MET:SD	2.61	0.40
3:G:48:LEU:HD11	3:G:52:VAL:HG22	2.03	0.40
4:N:104:PHE:HE1	4:N:184:LEU:HD12	1.86	0.40
1:S:756:LEU:HD23	1:S:756:LEU:HA	1.89	0.40
1:Q:242:HIS:HB2	1:Q:278:ILE:HD13	2.02	0.40
1:P:256:ARG:HH12	1:O:260:ASP:HB2	1.86	0.40
1:P:764:VAL:HG13	1:P:765:LEU:HD22	2.04	0.40
1:T:260:ASP:O	1:T:263:GLU:HG3	2.22	0.40
3:E:186:ARG:HG3	3:E:187:ASP:N	2.30	0.40
1:S:490:ILE:H	1:S:490:ILE:HD12	1.86	0.40
1:P:623:VAL:CG1	1:P:662:THR:HB	2.52	0.40
1:O:203:ARG:HG2	1:O:204:THR:HG23	2.04	0.40
1:O:213:GLU:HG2	1:O:390:PHE:CZ	2.57	0.40
1:O:494:LYS:HA	1:O:498:GLU:OE2	2.22	0.40
1:T:635:LEU:HD21	1:T:706:PHE:HB2	2.03	0.40
3:A:179:GLN:NE2	3:A:183:ASP:OD2	2.44	0.40
3:B:74:ASP:OD1	3:B:74:ASP:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	O	588/696 (84%)	558 (95%)	28 (5%)	2 (0%)	41	30
1	P	588/696 (84%)	561 (95%)	27 (5%)	0	100	100
1	Q	588/696 (84%)	562 (96%)	26 (4%)	0	100	100
1	R	588/696 (84%)	557 (95%)	30 (5%)	1 (0%)	47	38
1	S	588/696 (84%)	568 (97%)	19 (3%)	1 (0%)	47	38
1	T	588/696 (84%)	552 (94%)	33 (6%)	3 (0%)	29	17
3	A	176/226 (78%)	171 (97%)	5 (3%)	0	100	100
3	B	176/226 (78%)	170 (97%)	5 (3%)	1 (1%)	25	14
3	C	176/226 (78%)	168 (96%)	8 (4%)	0	100	100
3	D	176/226 (78%)	171 (97%)	5 (3%)	0	100	100
3	E	176/226 (78%)	168 (96%)	8 (4%)	0	100	100
3	F	176/226 (78%)	171 (97%)	5 (3%)	0	100	100
3	G	176/226 (78%)	169 (96%)	7 (4%)	0	100	100
4	H	177/207 (86%)	171 (97%)	6 (3%)	0	100	100
4	I	181/207 (87%)	174 (96%)	7 (4%)	0	100	100
4	J	174/207 (84%)	169 (97%)	5 (3%)	0	100	100
4	K	174/207 (84%)	166 (95%)	7 (4%)	1 (1%)	25	14
4	L	175/207 (84%)	169 (97%)	6 (3%)	0	100	100
4	M	175/207 (84%)	172 (98%)	3 (2%)	0	100	100
4	N	175/207 (84%)	169 (97%)	6 (3%)	0	100	100
All	All	5991/7207 (83%)	5736 (96%)	246 (4%)	9 (0%)	50	38

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	R	673	PHE
1	T	556	THR
3	B	192	ALA
4	K	61	ARG
1	O	518	VAL
1	S	673	PHE
1	O	492	VAL
1	T	575	SER
1	T	678	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	500/582 (86%)	499 (100%)	1 (0%)	93	93
1	P	500/582 (86%)	498 (100%)	2 (0%)	91	90
1	Q	500/582 (86%)	499 (100%)	1 (0%)	93	93
1	R	500/582 (86%)	499 (100%)	1 (0%)	93	93
1	S	500/582 (86%)	497 (99%)	3 (1%)	86	85
1	T	499/582 (86%)	497 (100%)	2 (0%)	91	90
3	A	144/175 (82%)	144 (100%)	0	100	100
3	B	144/175 (82%)	144 (100%)	0	100	100
3	C	144/175 (82%)	144 (100%)	0	100	100
3	D	144/175 (82%)	144 (100%)	0	100	100
3	E	144/175 (82%)	144 (100%)	0	100	100
3	F	144/175 (82%)	144 (100%)	0	100	100
3	G	144/175 (82%)	144 (100%)	0	100	100
4	H	149/174 (86%)	149 (100%)	0	100	100
4	I	153/174 (88%)	153 (100%)	0	100	100
4	J	146/174 (84%)	146 (100%)	0	100	100
4	K	146/174 (84%)	146 (100%)	0	100	100
4	L	147/174 (84%)	147 (100%)	0	100	100
4	M	147/174 (84%)	147 (100%)	0	100	100
4	N	147/174 (84%)	147 (100%)	0	100	100
All	All	5042/5935 (85%)	5032 (100%)	10 (0%)	93	93

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	536	LYS
1	S	632	ASN
1	S	792	ARG

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Mol	Chain	Res	Type
1	R	792	ARG
1	Q	584	LYS
1	P	667	ARG
1	P	771	ARG
1	O	231	LYS
1	T	266	LYS
1	T	407	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	206	ASN
1	R	700	GLN
1	T	198	GLN
4	I	122	GLN
4	K	222	GLN
4	L	122	GLN
4	M	122	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 7 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ATP	O	902	-	26,33,33	0.61	0	31,52,52	0.76	2 (6%)
5	ATP	S	901	6	26,33,33	0.60	0	31,52,52	0.75	2 (6%)
5	ATP	P	902	6	26,33,33	0.60	0	31,52,52	0.75	2 (6%)
5	ATP	R	901	6	26,33,33	0.60	0	31,52,52	0.74	2 (6%)
5	ATP	T	902	6	26,33,33	0.60	0	31,52,52	0.74	2 (6%)
7	ADP	T	901	-	24,29,29	0.95	1 (4%)	29,45,45	1.46	4 (13%)
7	ADP	O	901	-	24,29,29	0.95	1 (4%)	29,45,45	1.47	4 (13%)
7	ADP	P	901	-	24,29,29	0.95	1 (4%)	29,45,45	1.45	4 (13%)
5	ATP	Q	902	6	26,33,33	0.63	0	31,52,52	0.76	2 (6%)
7	ADP	Q	901	-	24,29,29	0.96	1 (4%)	29,45,45	1.47	4 (13%)
5	ATP	S	902	6	26,33,33	0.61	0	31,52,52	0.74	2 (6%)
5	ATP	R	902	6	26,33,33	0.62	0	31,52,52	0.75	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	O	902	-	-	8/18/38/38	0/3/3/3
5	ATP	S	901	6	-	0/18/38/38	0/3/3/3
5	ATP	P	902	6	-	3/18/38/38	0/3/3/3
5	ATP	R	901	6	-	4/18/38/38	0/3/3/3
5	ATP	T	902	6	-	2/18/38/38	0/3/3/3
7	ADP	T	901	-	-	2/12/32/32	0/3/3/3
7	ADP	O	901	-	-	3/12/32/32	0/3/3/3
7	ADP	P	901	-	-	3/12/32/32	0/3/3/3
5	ATP	Q	902	6	-	7/18/38/38	0/3/3/3
7	ADP	Q	901	-	-	1/12/32/32	0/3/3/3
5	ATP	S	902	6	-	7/18/38/38	0/3/3/3
5	ATP	R	902	6	-	8/18/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	T	901	ADP	C5-C4	2.52	1.47	1.40
7	O	901	ADP	C5-C4	2.43	1.47	1.40
7	P	901	ADP	C5-C4	2.42	1.47	1.40
7	Q	901	ADP	C5-C4	2.41	1.47	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	O	901	ADP	PA-O3A-PB	-3.84	119.64	132.83
7	Q	901	ADP	PA-O3A-PB	-3.79	119.81	132.83
7	T	901	ADP	PA-O3A-PB	-3.57	120.56	132.83
7	P	901	ADP	PA-O3A-PB	-3.51	120.77	132.83
7	T	901	ADP	C3'-C2'-C1'	3.28	105.91	100.98
7	P	901	ADP	N3-C2-N1	-3.16	123.73	128.68
7	O	901	ADP	C3'-C2'-C1'	3.15	105.73	100.98
7	O	901	ADP	N3-C2-N1	-3.12	123.80	128.68
7	T	901	ADP	N3-C2-N1	-3.11	123.81	128.68
7	Q	901	ADP	C3'-C2'-C1'	3.09	105.63	100.98
7	Q	901	ADP	N3-C2-N1	-3.08	123.87	128.68
7	P	901	ADP	C3'-C2'-C1'	3.03	105.54	100.98
7	O	901	ADP	C4-C5-N7	-2.74	106.55	109.40
7	P	901	ADP	C4-C5-N7	-2.68	106.60	109.40
7	Q	901	ADP	C4-C5-N7	-2.67	106.62	109.40
7	T	901	ADP	C4-C5-N7	-2.66	106.62	109.40
5	P	902	ATP	C5-C6-N6	2.31	123.86	120.35
5	S	901	ATP	C5-C6-N6	2.30	123.85	120.35
5	R	902	ATP	C5-C6-N6	2.30	123.85	120.35
5	S	902	ATP	C5-C6-N6	2.28	123.82	120.35
5	T	902	ATP	C5-C6-N6	2.28	123.82	120.35
5	R	901	ATP	C5-C6-N6	2.27	123.80	120.35
5	Q	902	ATP	C5-C6-N6	2.27	123.80	120.35
5	O	902	ATP	C5-C6-N6	2.26	123.78	120.35
5	P	902	ATP	PB-O3B-PG	2.05	139.85	132.83
5	O	902	ATP	PB-O3B-PG	2.04	139.82	132.83
5	R	901	ATP	PB-O3B-PG	2.02	139.77	132.83
5	S	901	ATP	PB-O3B-PG	2.02	139.76	132.83
5	S	902	ATP	PB-O3B-PG	2.02	139.75	132.83
5	R	902	ATP	PB-O3B-PG	2.01	139.74	132.83
5	Q	902	ATP	PB-O3B-PG	2.01	139.74	132.83
5	T	902	ATP	PB-O3B-PG	2.01	139.74	132.83

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	S	902	ATP	C5'-O5'-PA-O1A
5	R	901	ATP	PB-O3B-PG-O2G
5	R	902	ATP	PB-O3B-PG-O2G
5	R	902	ATP	C5'-O5'-PA-O1A
5	Q	902	ATP	PB-O3B-PG-O2G
5	Q	902	ATP	C5'-O5'-PA-O2A
5	Q	902	ATP	C5'-O5'-PA-O3A
5	Q	902	ATP	O4'-C4'-C5'-O5'
5	Q	902	ATP	C3'-C4'-C5'-O5'
5	P	902	ATP	C5'-O5'-PA-O1A
5	O	902	ATP	PB-O3B-PG-O3G
5	O	902	ATP	C5'-O5'-PA-O1A
5	O	902	ATP	C3'-C4'-C5'-O5'
5	T	902	ATP	PB-O3B-PG-O2G
7	P	901	ADP	C5'-O5'-PA-O1A
7	P	901	ADP	C5'-O5'-PA-O2A
7	O	901	ADP	C5'-O5'-PA-O1A
7	O	901	ADP	C5'-O5'-PA-O2A
7	T	901	ADP	C5'-O5'-PA-O2A
7	T	901	ADP	C5'-O5'-PA-O3A
5	S	902	ATP	O4'-C4'-C5'-O5'
5	O	902	ATP	O4'-C4'-C5'-O5'
5	S	902	ATP	C3'-C4'-C5'-O5'
5	R	902	ATP	O4'-C4'-C5'-O5'
5	R	902	ATP	C3'-C4'-C5'-O5'
5	R	901	ATP	C5'-O5'-PA-O3A
5	R	902	ATP	C5'-O5'-PA-O3A
5	P	902	ATP	C5'-O5'-PA-O3A
5	O	902	ATP	C5'-O5'-PA-O3A
5	R	901	ATP	PG-O3B-PB-O1B
5	R	902	ATP	PG-O3B-PB-O1B
5	S	902	ATP	C5'-O5'-PA-O2A
5	R	902	ATP	C5'-O5'-PA-O2A
5	P	902	ATP	C5'-O5'-PA-O2A
5	O	902	ATP	C5'-O5'-PA-O2A
5	S	902	ATP	PA-O3A-PB-O2B
5	O	902	ATP	C4'-C5'-O5'-PA
5	S	902	ATP	PB-O3B-PG-O1G
5	R	902	ATP	PB-O3B-PG-O1G
5	O	902	ATP	PB-O3B-PG-O1G
5	R	901	ATP	PA-O3A-PB-O1B
5	Q	902	ATP	PB-O3B-PG-O1G
5	T	902	ATP	PB-O3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
5	Q	902	ATP	PB-O3B-PG-O3G
5	S	902	ATP	C5'-O5'-PA-O3A
7	P	901	ADP	C5'-O5'-PA-O3A
7	O	901	ADP	C5'-O5'-PA-O3A
7	Q	901	ADP	O4'-C4'-C5'-O5'

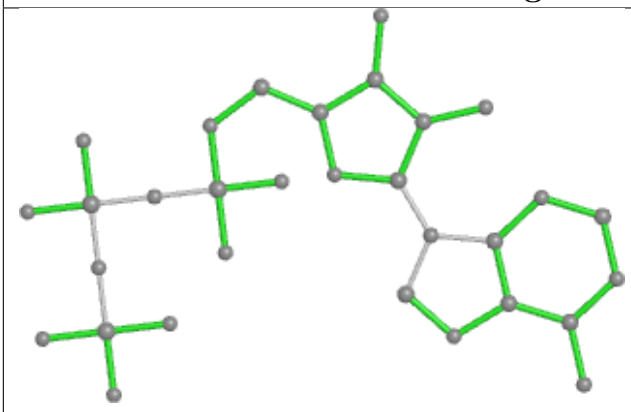
There are no ring outliers.

6 monomers are involved in 9 short contacts:

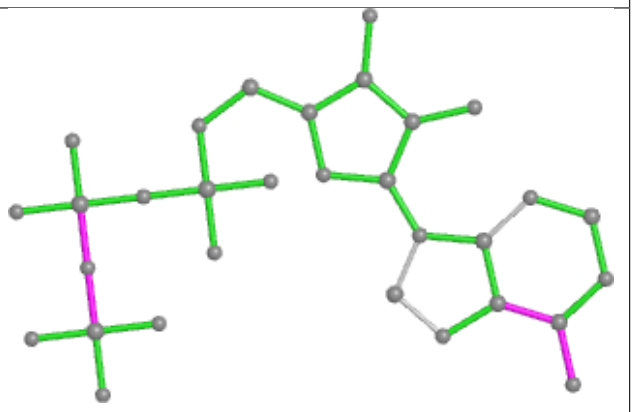
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	902	ATP	2	0
5	S	901	ATP	2	0
5	P	902	ATP	1	0
5	R	901	ATP	2	0
7	O	901	ADP	1	0
7	Q	901	ADP	1	0

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

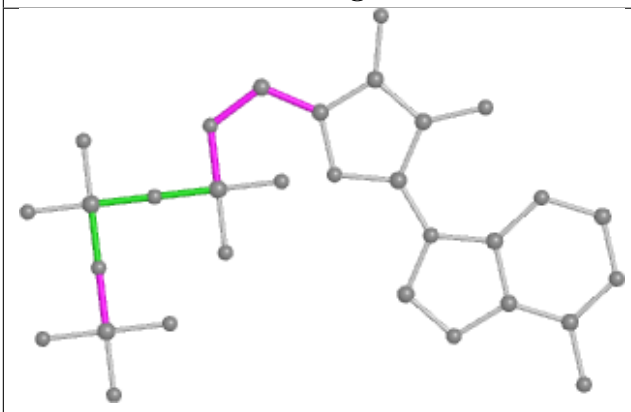
Ligand ATP O 902



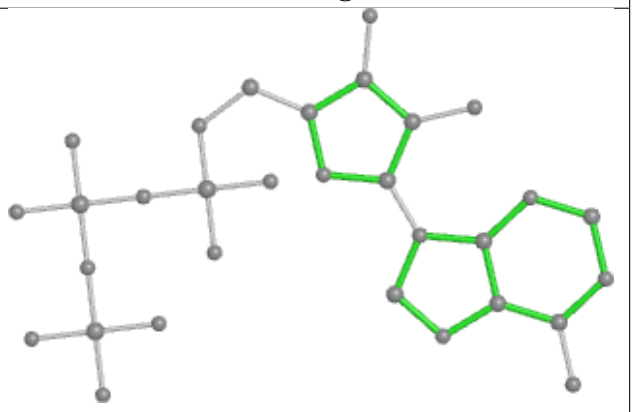
Bond lengths



Bond angles

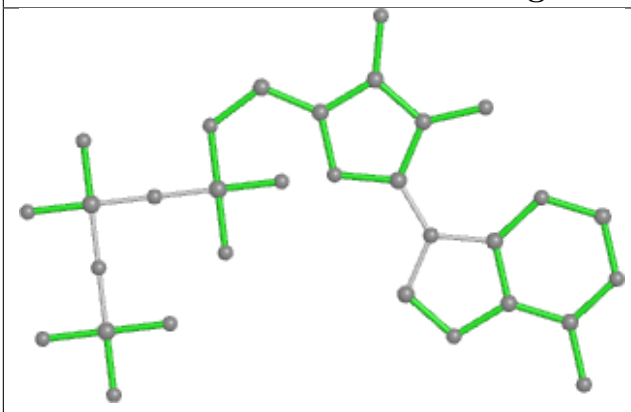


Torsions

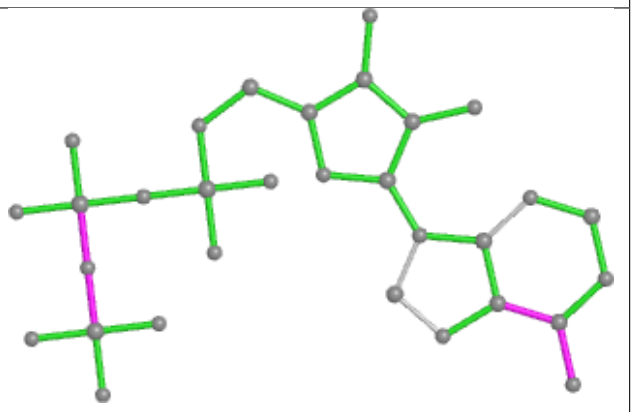


Rings

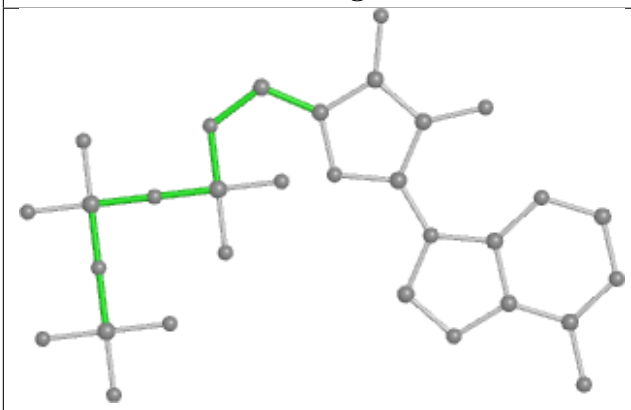
Ligand ATP S 901



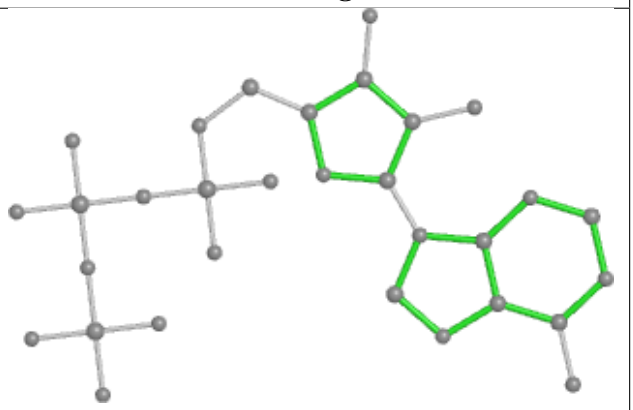
Bond lengths



Bond angles

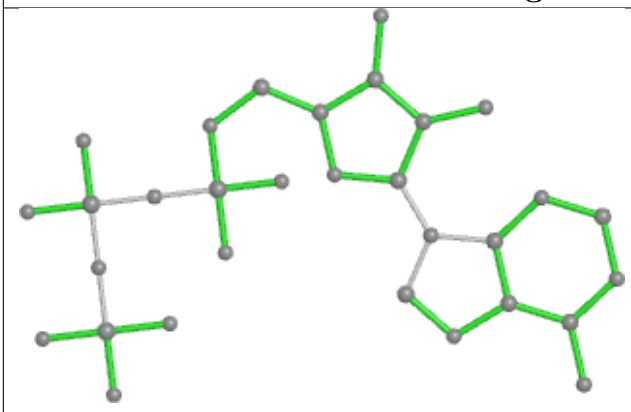


Torsions

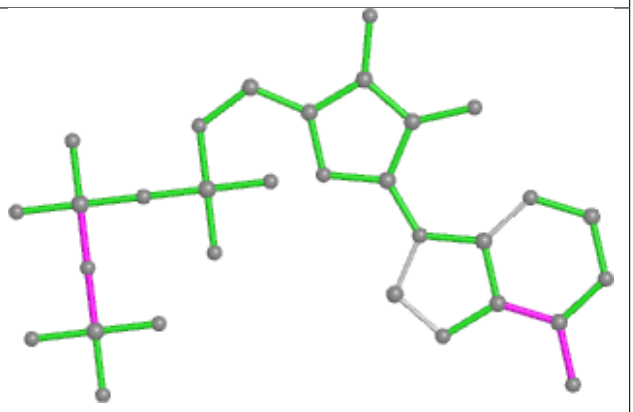


Rings

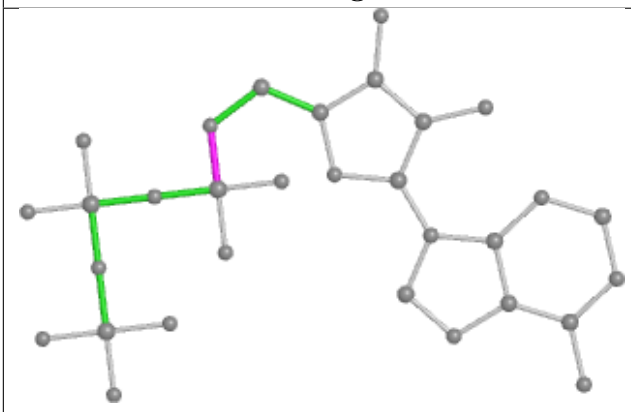
Ligand ATP P 902



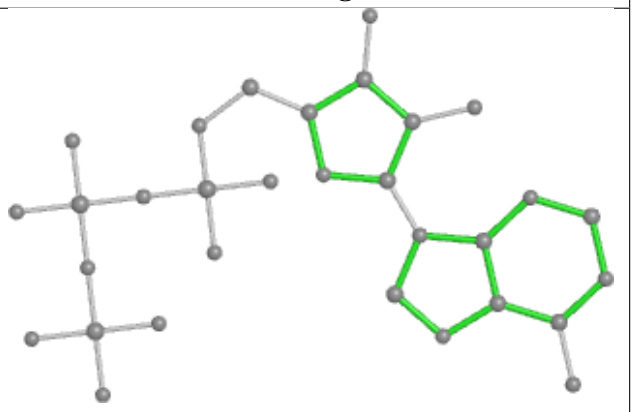
Bond lengths



Bond angles

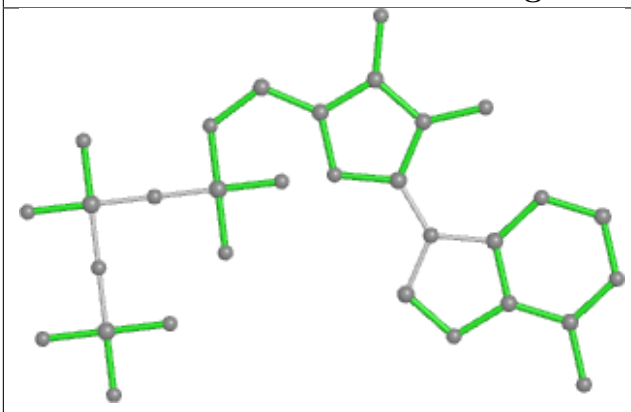


Torsions

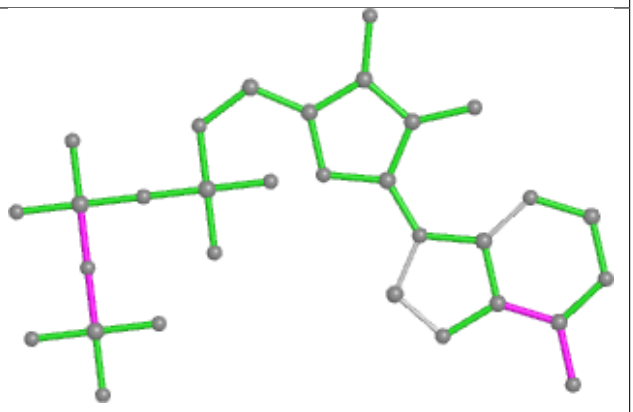


Rings

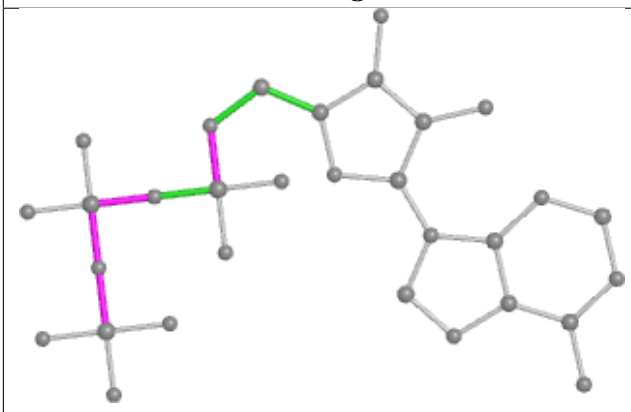
Ligand ATP R 901



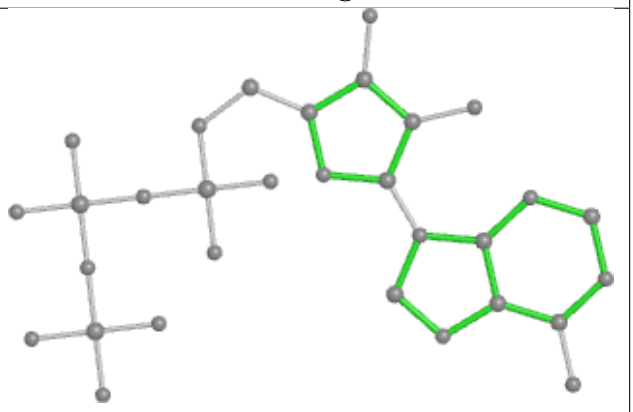
Bond lengths



Bond angles

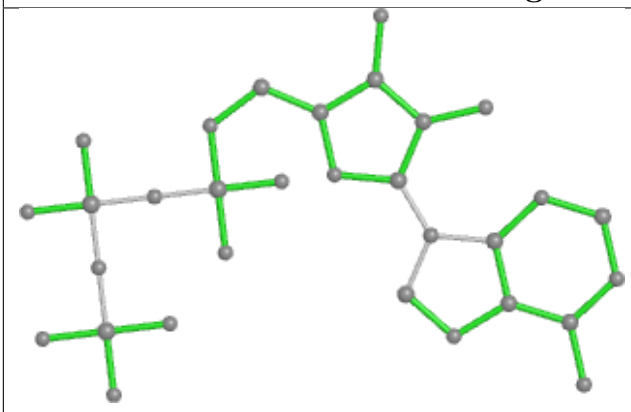


Torsions

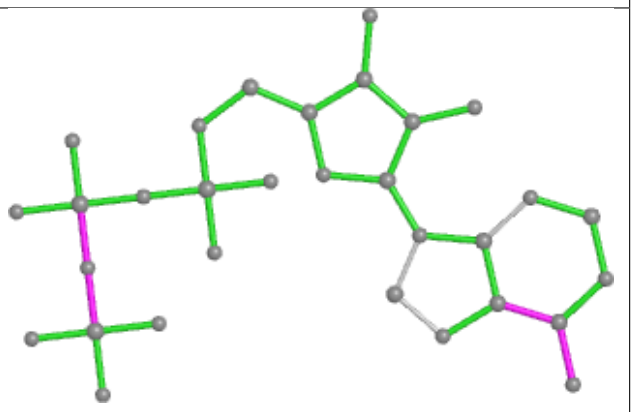


Rings

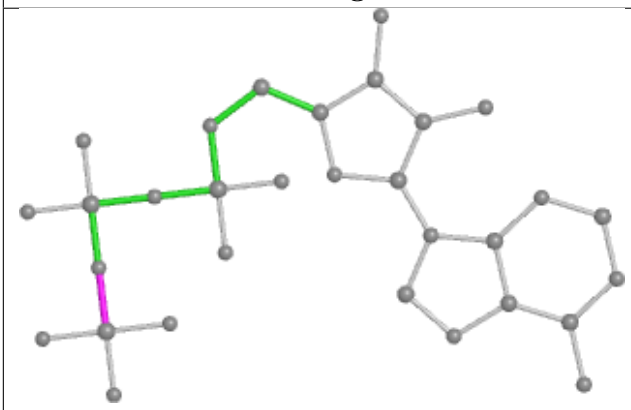
Ligand ATP T 902



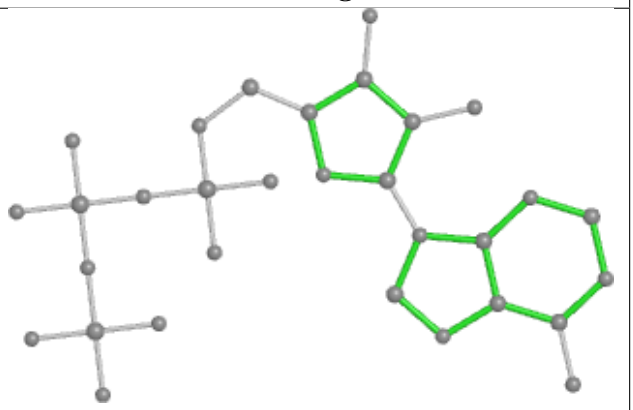
Bond lengths



Bond angles

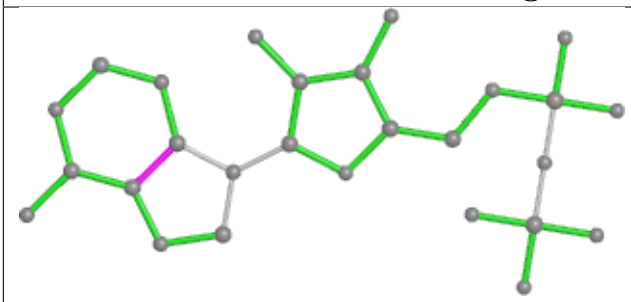


Torsions

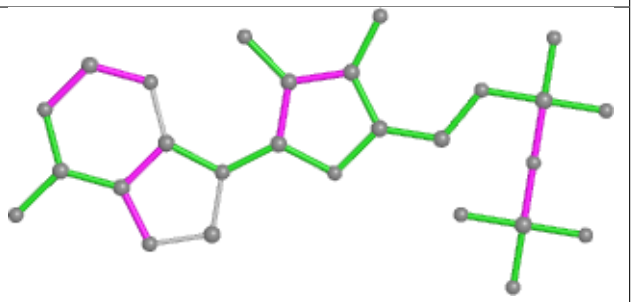


Rings

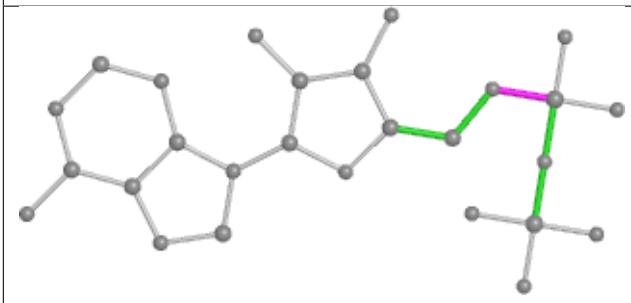
Ligand ADP T 901



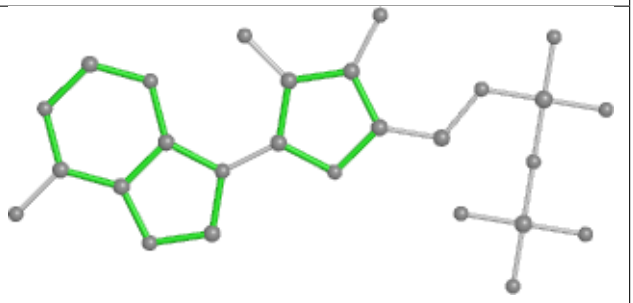
Bond lengths



Bond angles

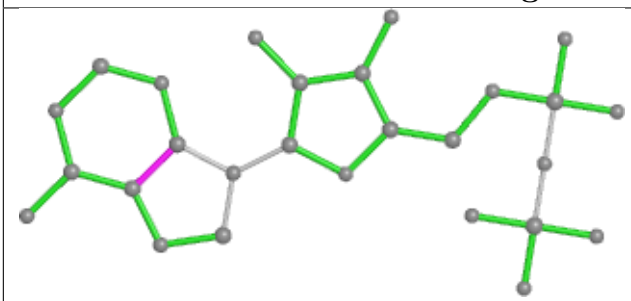


Torsions

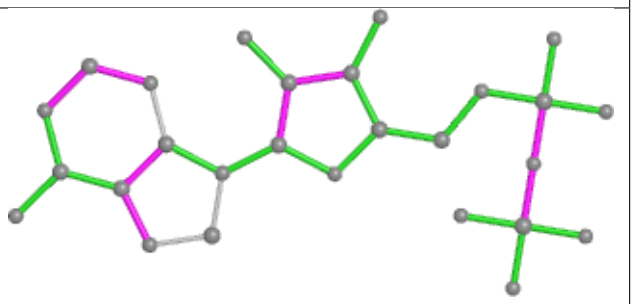


Rings

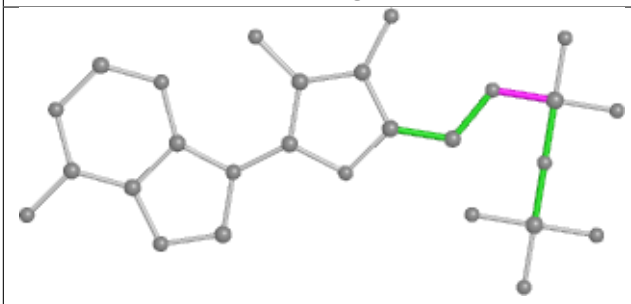
Ligand ADP O 901



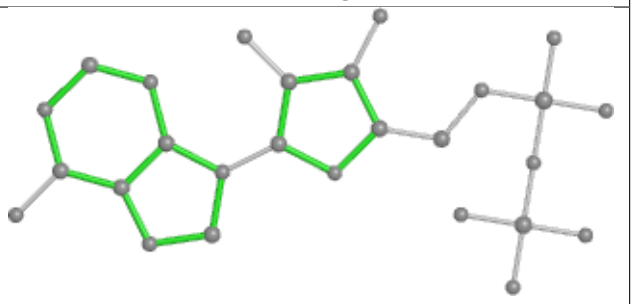
Bond lengths



Bond angles

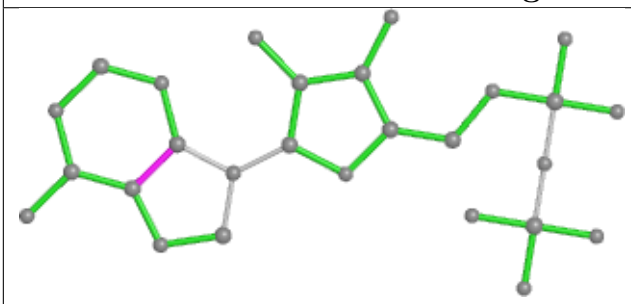


Torsions

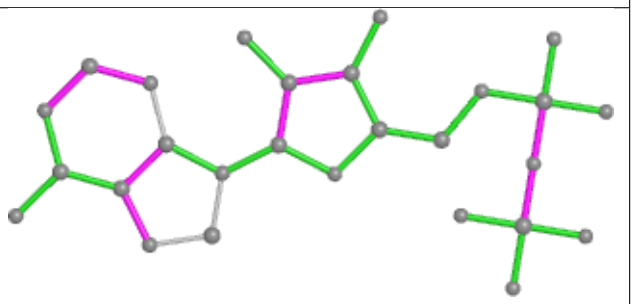


Rings

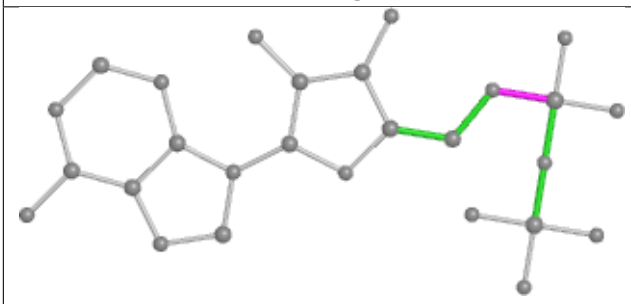
Ligand ADP P 901



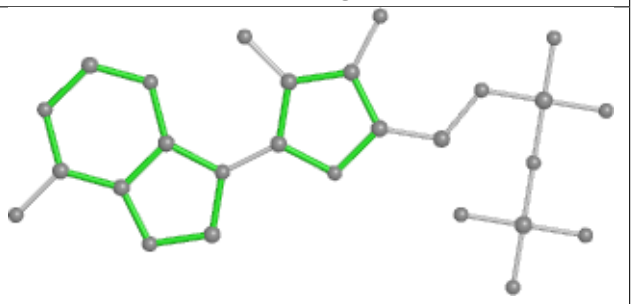
Bond lengths



Bond angles

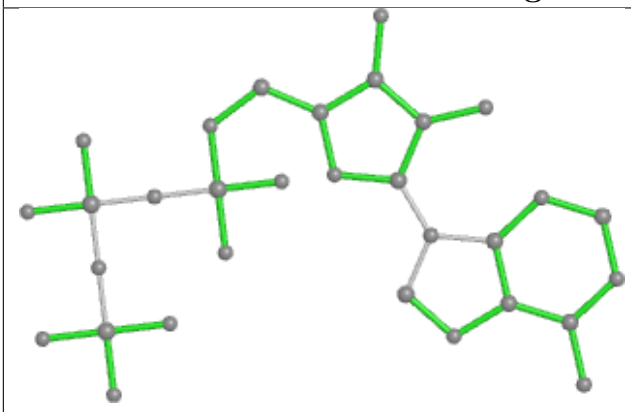


Torsions

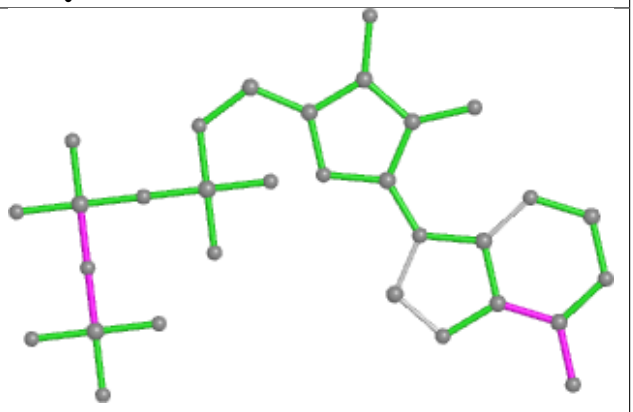


Rings

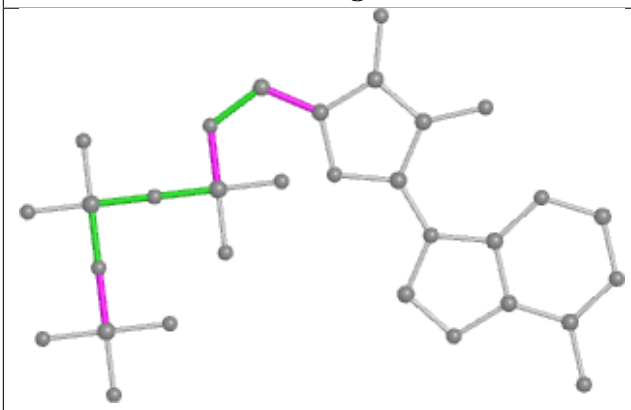
Ligand ATP Q 902



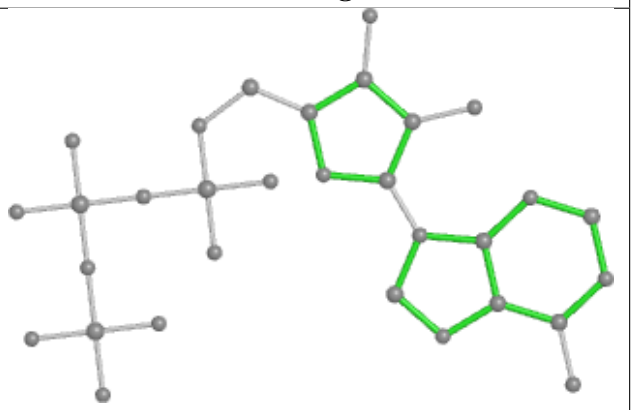
Bond lengths



Bond angles

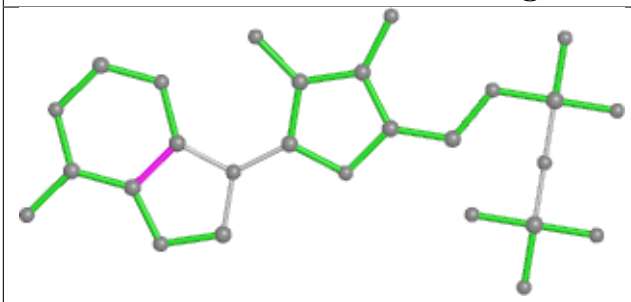


Torsions

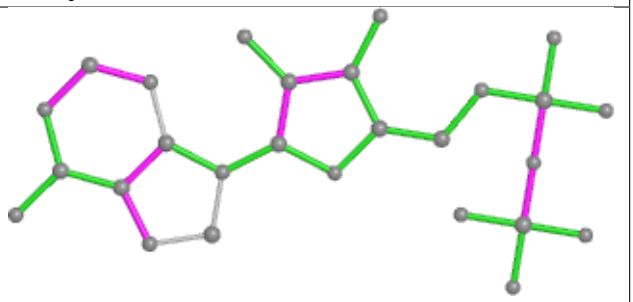


Rings

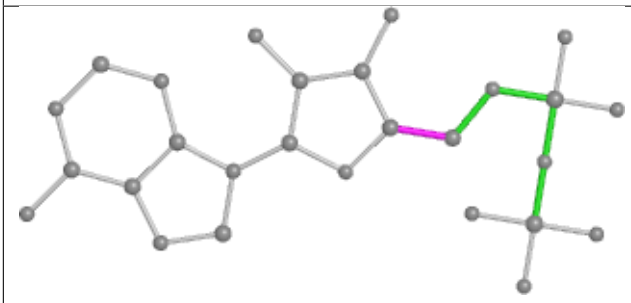
Ligand ADP Q 901



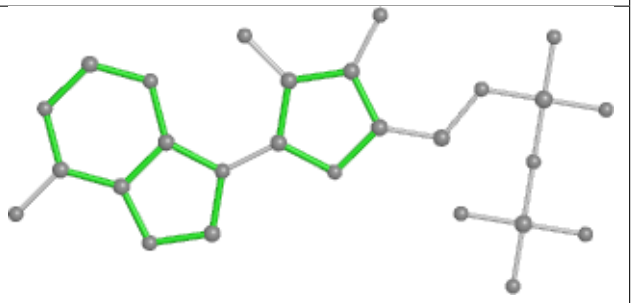
Bond lengths



Bond angles

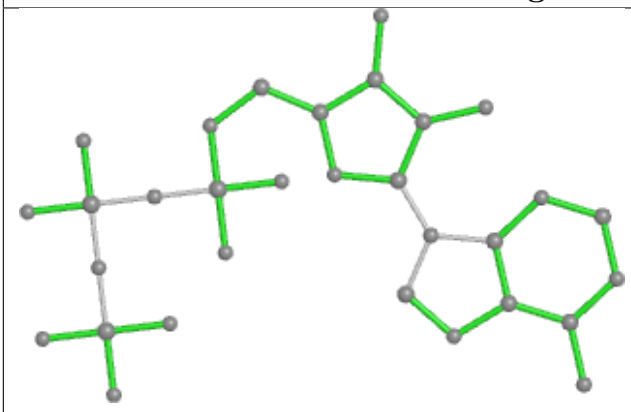


Torsions

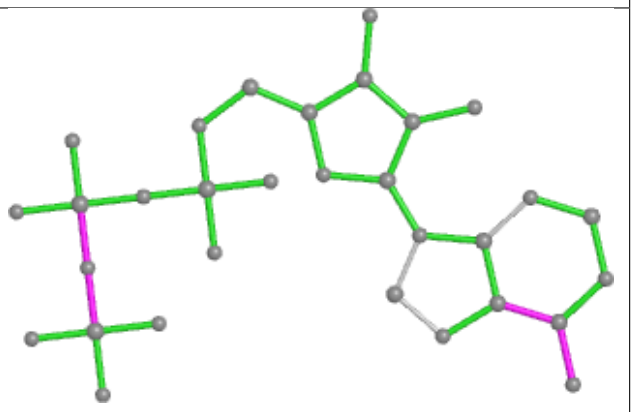


Rings

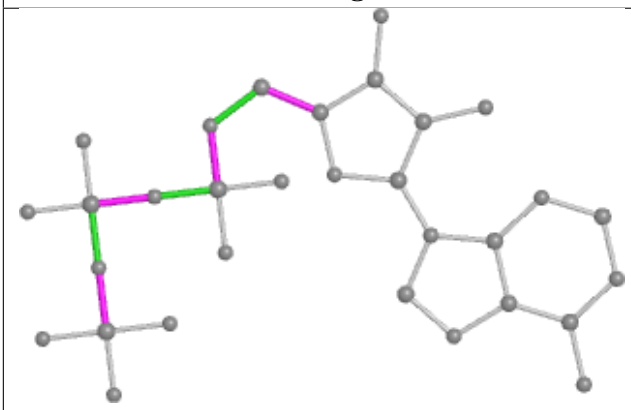
Ligand ATP S 902



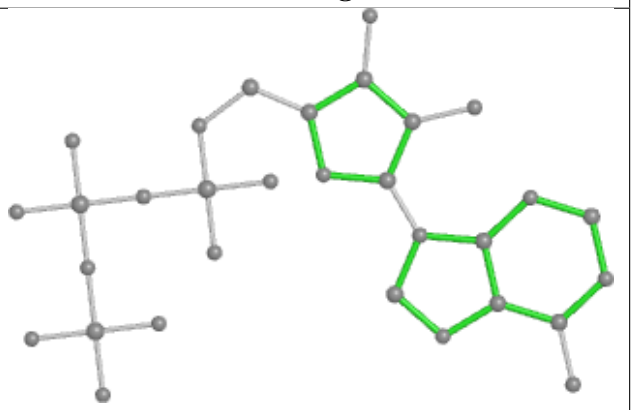
Bond lengths



Bond angles

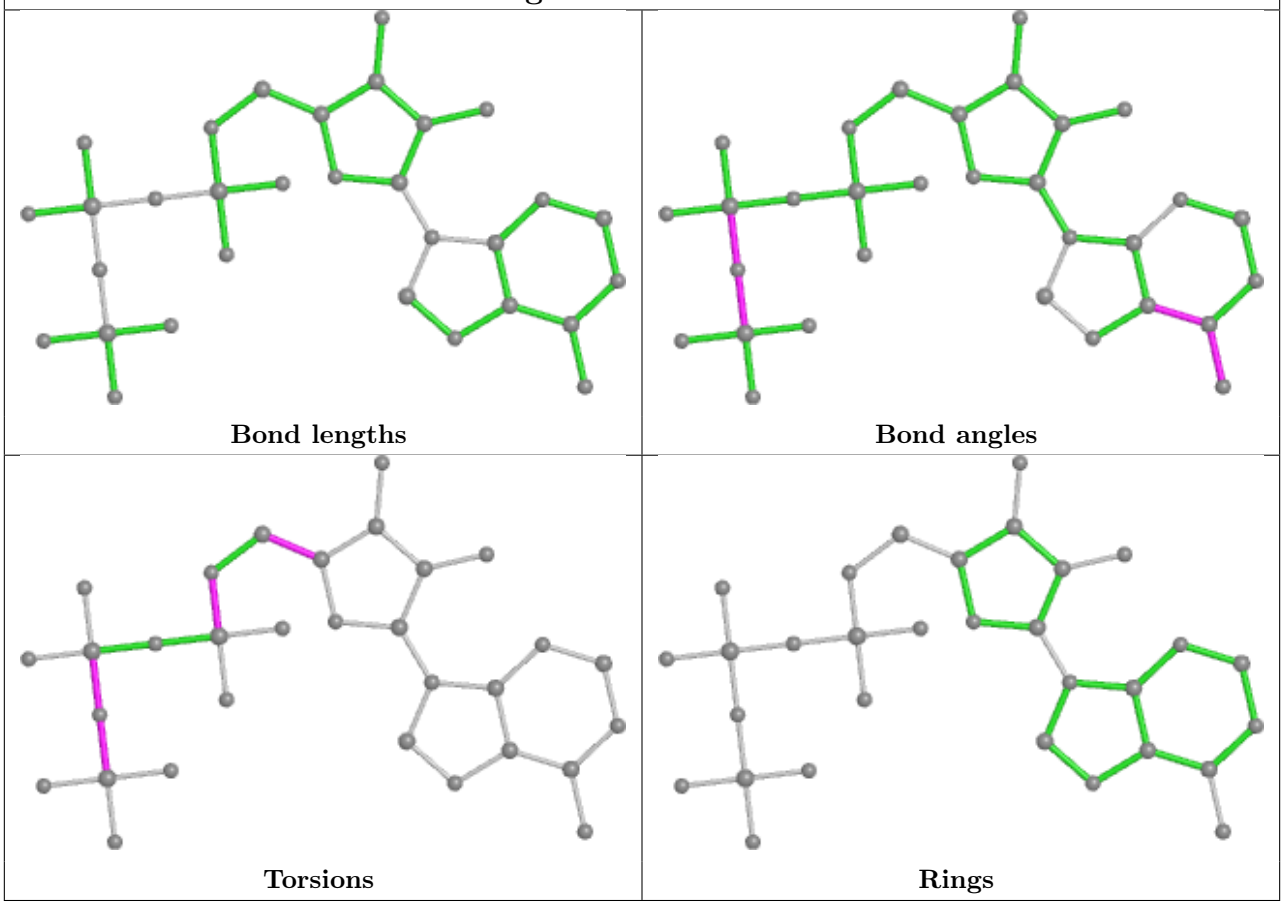


Torsions



Rings

Ligand ATP R 902



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

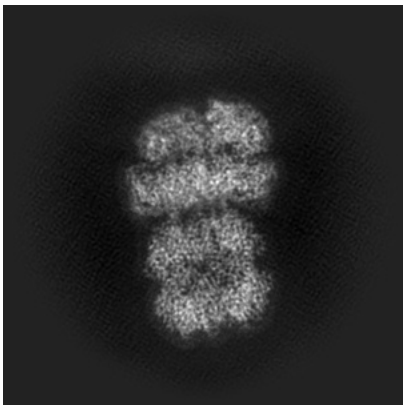
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38535. These allow visual inspection of the internal detail of the map and identification of artifacts.

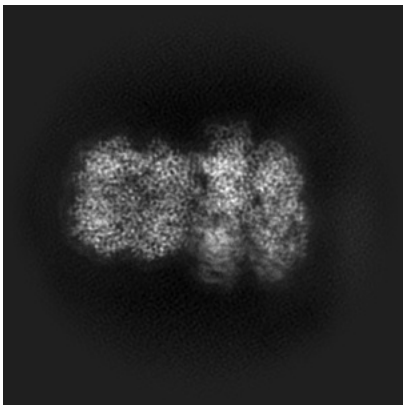
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

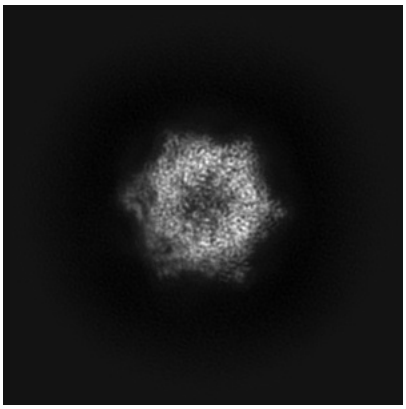
6.1.1 Primary map



X

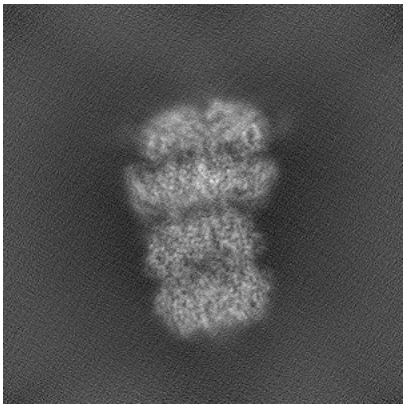


Y

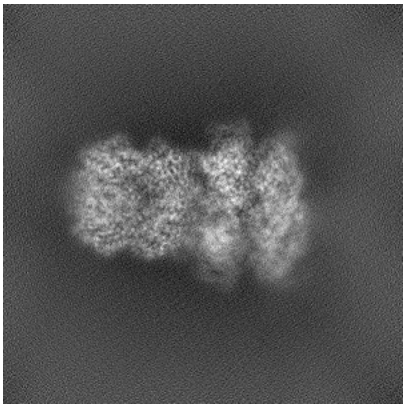


Z

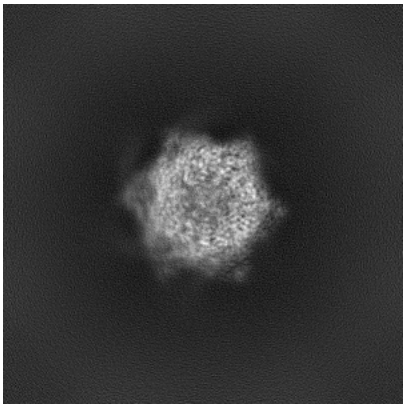
6.1.2 Raw map



X



Y

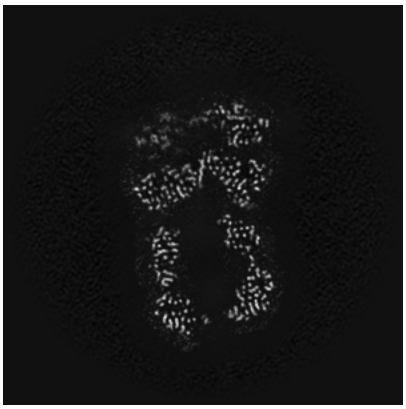


Z

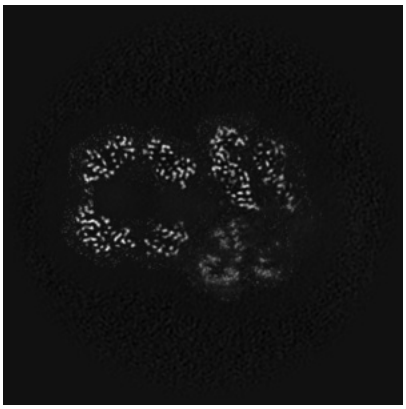
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

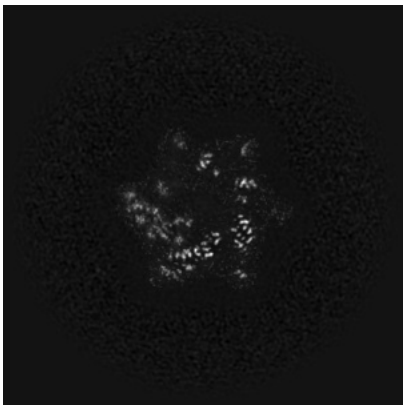
6.2.1 Primary map



X Index: 192

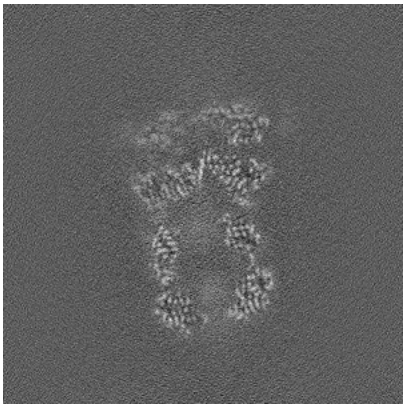


Y Index: 192



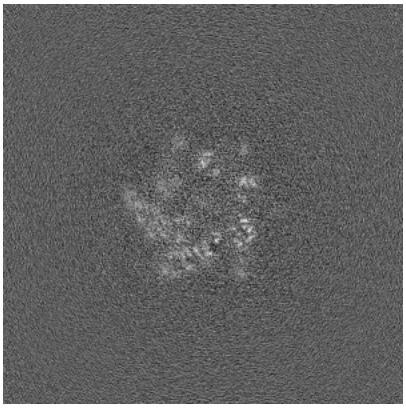
Z Index: 192

6.2.2 Raw map



X Index: 192

Y Index: 192

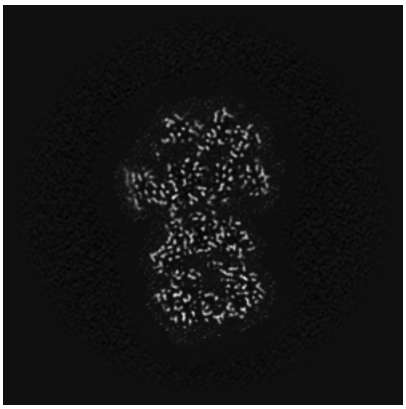


Z Index: 192

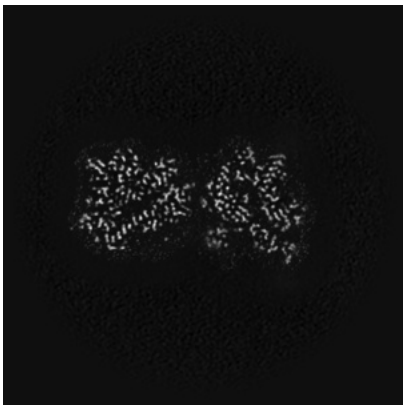
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

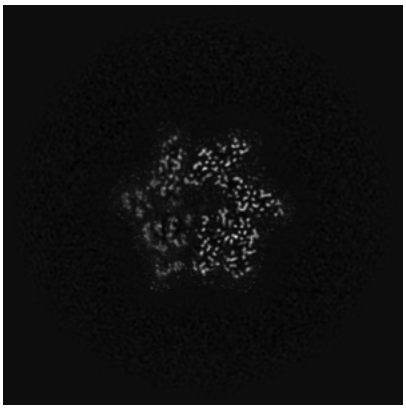
6.3.1 Primary map



X Index: 226

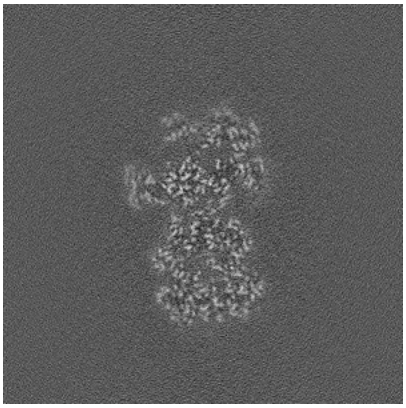


Y Index: 232

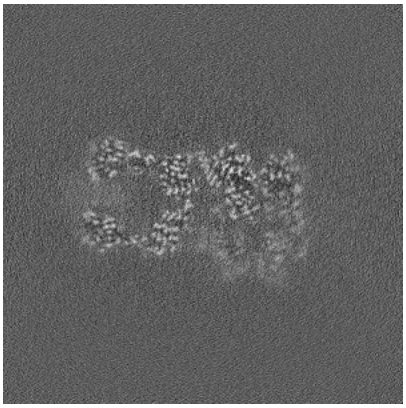


Z Index: 207

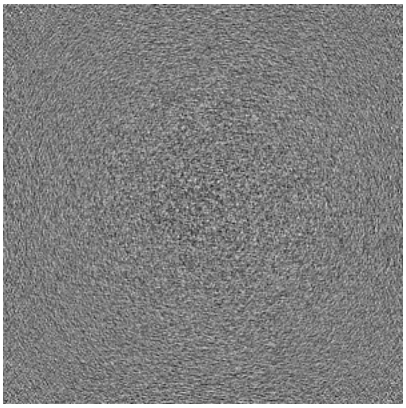
6.3.2 Raw map



X Index: 228



Y Index: 211

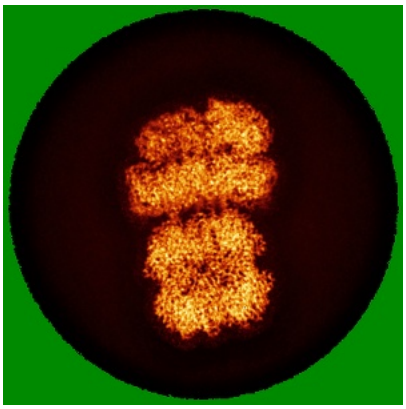


Z Index: 0

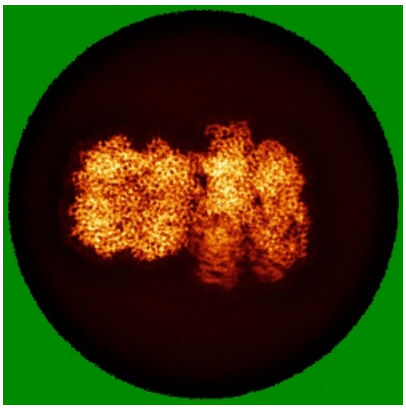
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

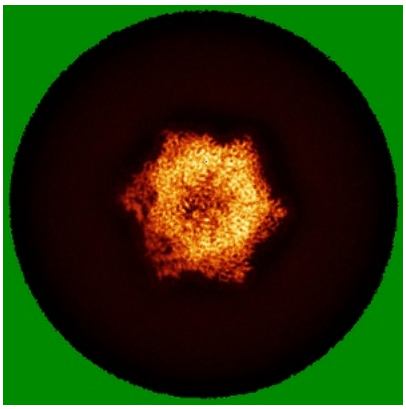
6.4.1 Primary map



X

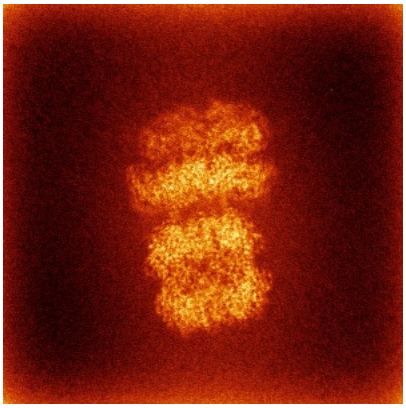


Y

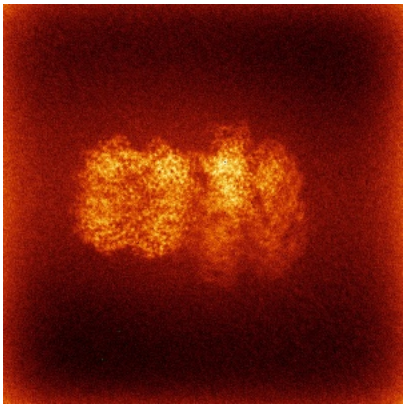


Z

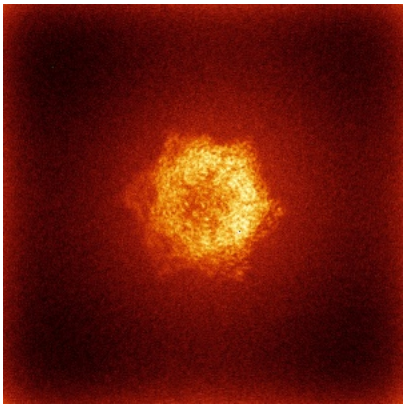
6.4.2 Raw map



X



Y

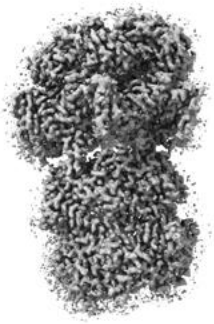


Z

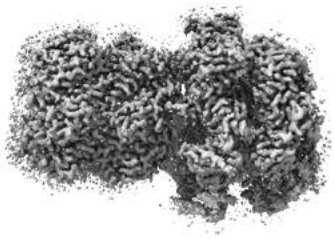
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

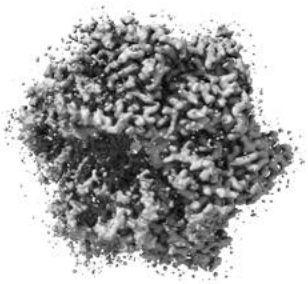
6.5.1 Primary map



X



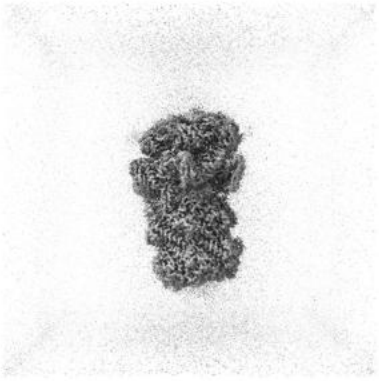
Y



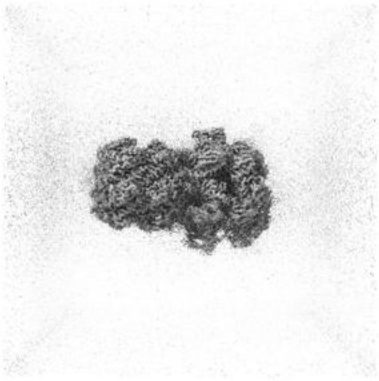
Z

The images above show the 3D surface view of the map at the recommended contour level 3.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

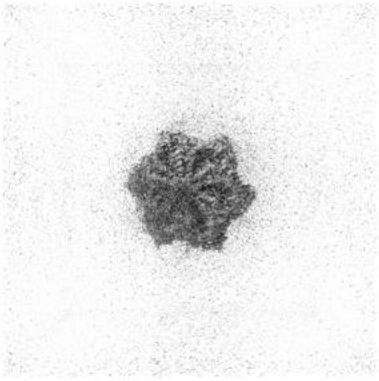
6.5.2 Raw map



X



Y



Z

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

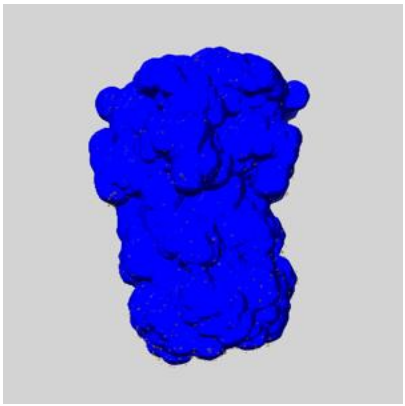
6.6 Mask visualisation (i)

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

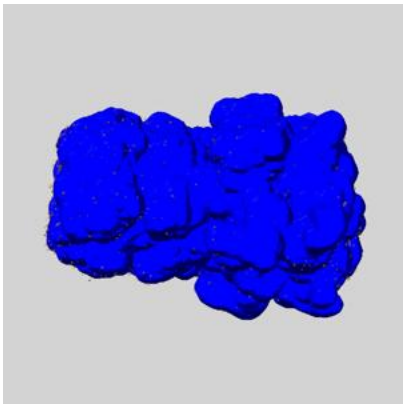
A mask typically either:

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

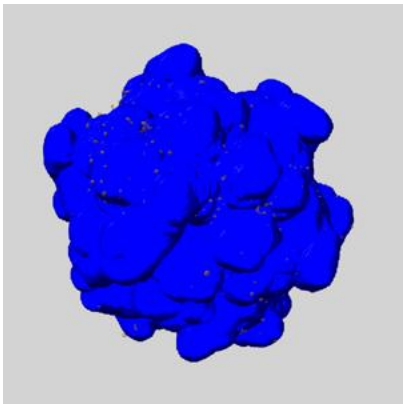
6.6.1 emd_38535_msk_1.map (i)



X



Y

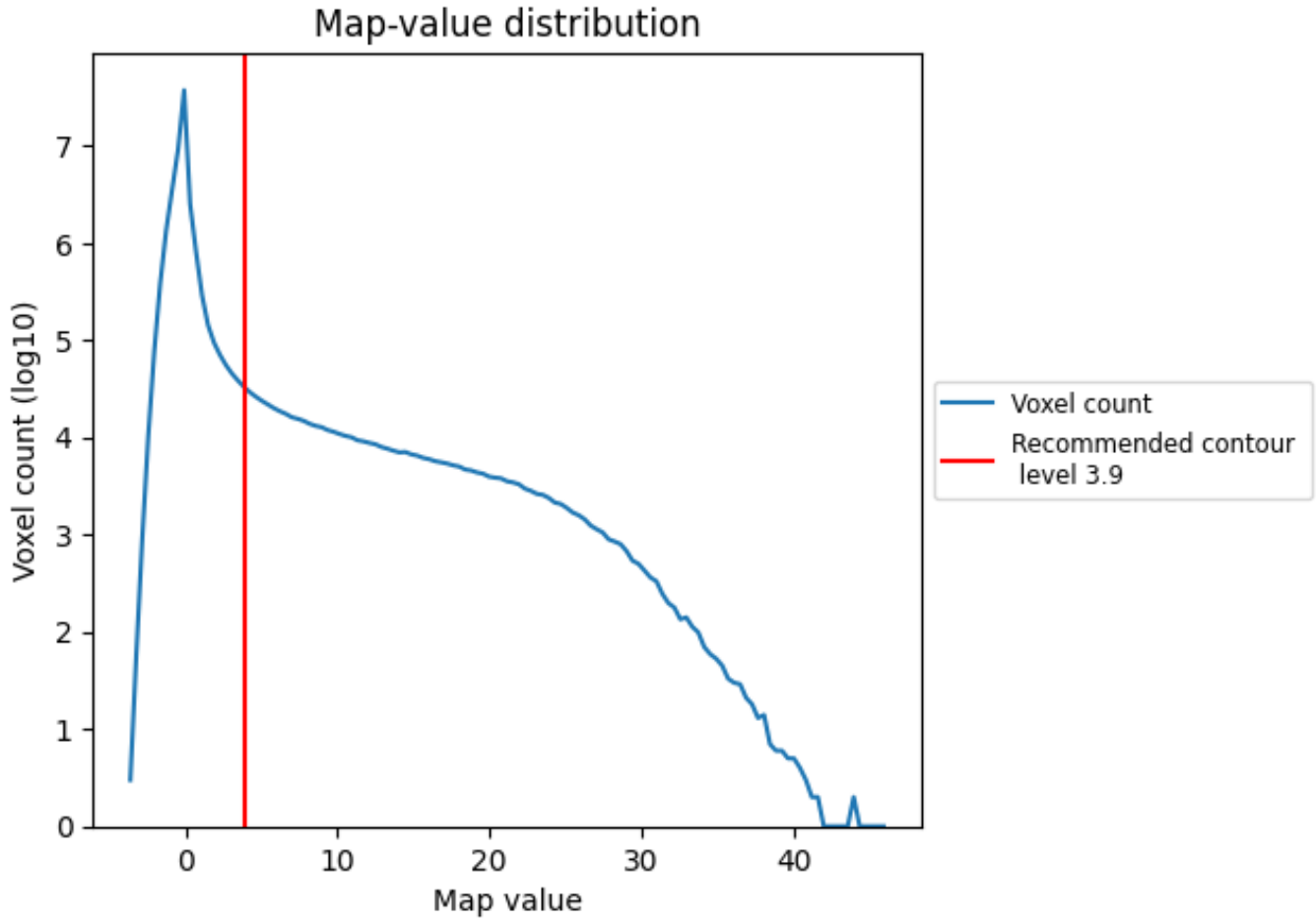


Z

7 Map analysis

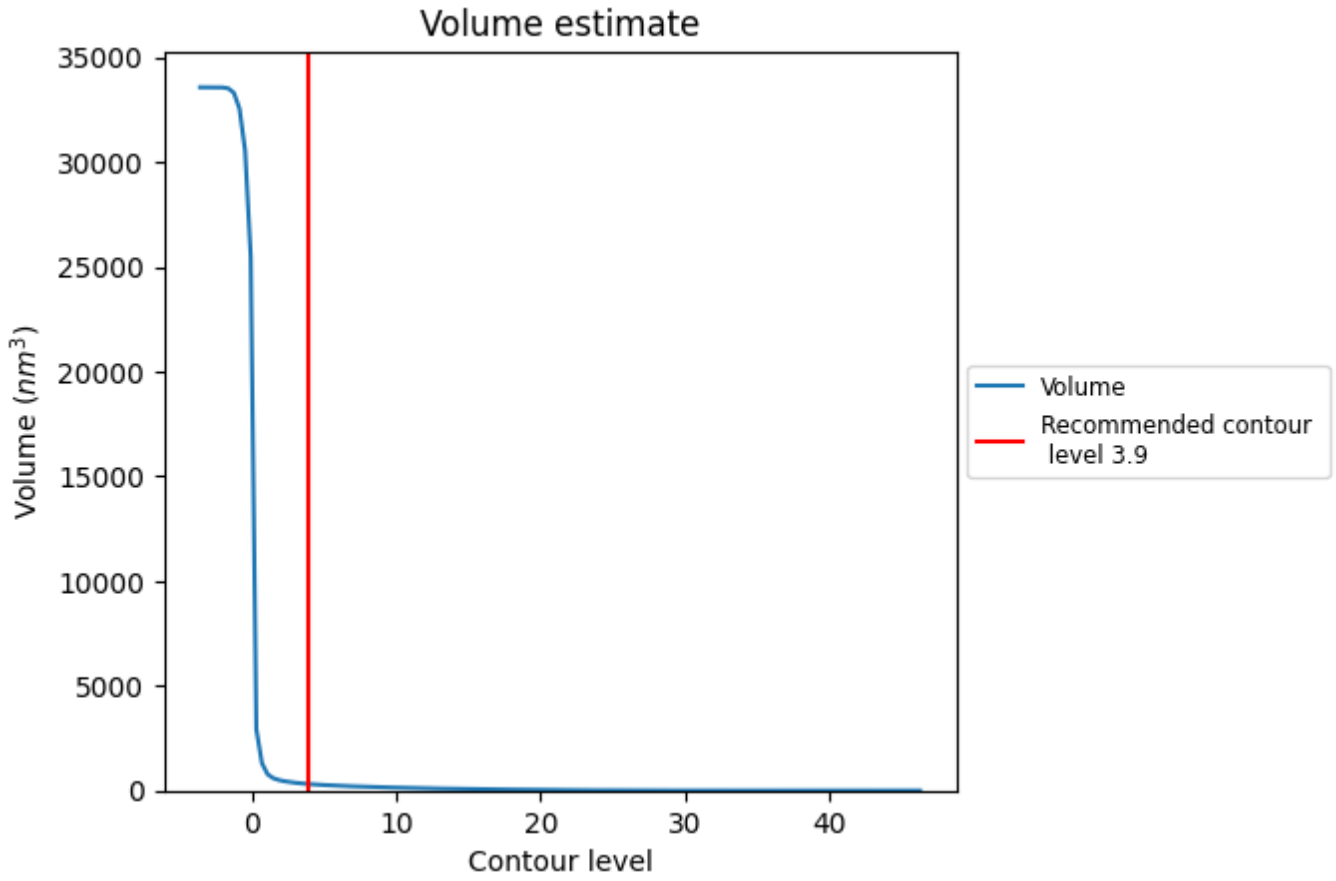
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

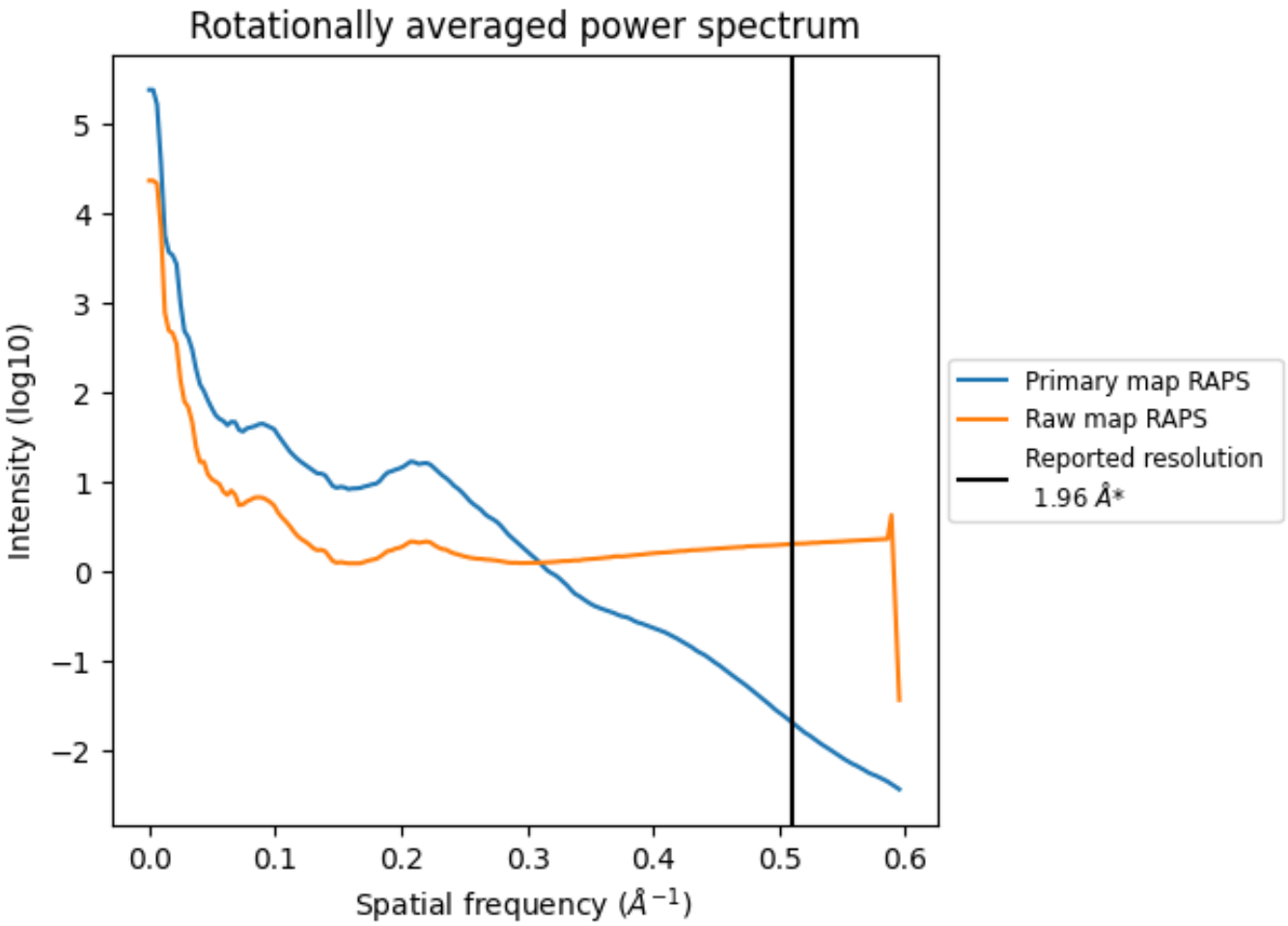
7.2 Volume estimate



The volume at the recommended contour level is 312 nm^3; this corresponds to an approximate mass of 282 kDa.

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

7.3 Rotationally averaged power spectrum (i)

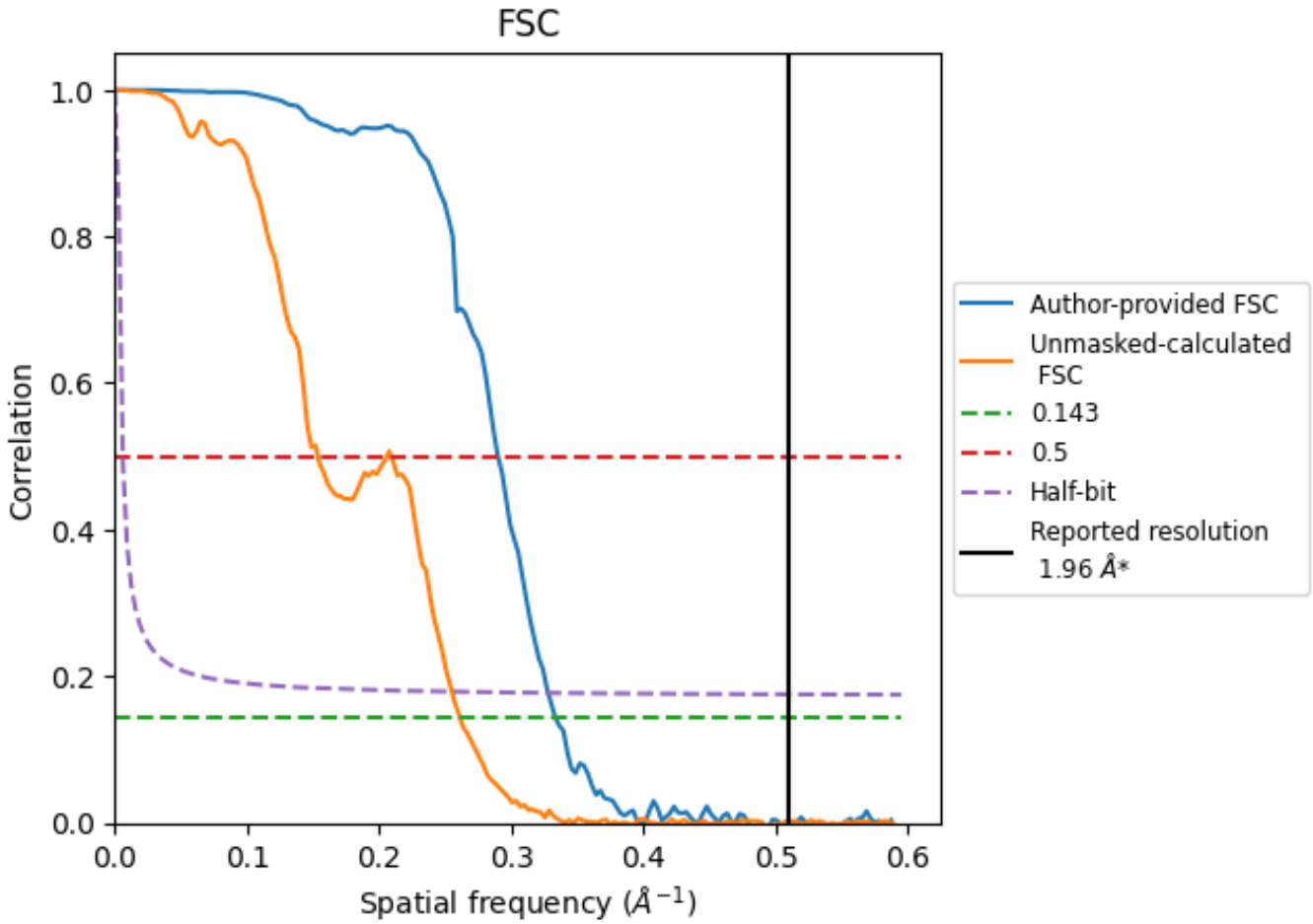


*Reported resolution corresponds to spatial frequency of 0.510 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.510 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.96	-	-
Author-provided FSC curve	3.00	3.45	3.05
Unmasked-calculated*	3.83	6.51	3.92

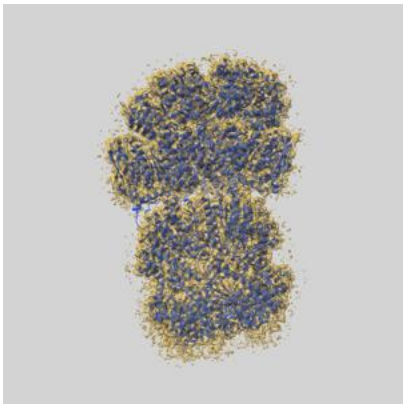
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.00 differs from the reported value 1.96 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.83 differs from the reported value 1.96 by more than 10 %

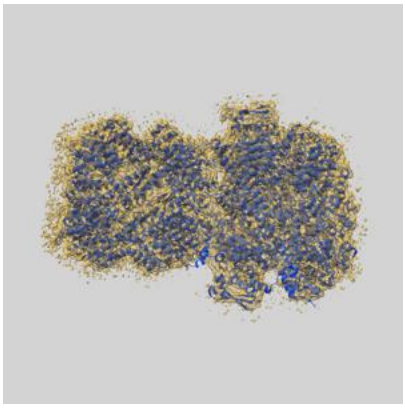
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38535 and PDB model 8XON. Per-residue inclusion information can be found in section 3 on page 23.

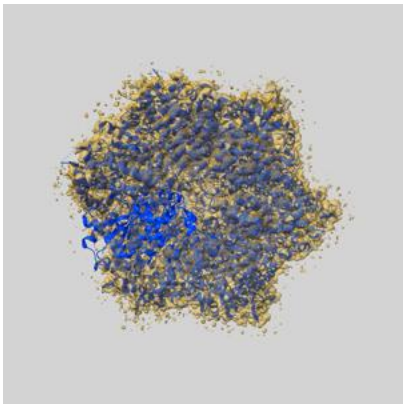
9.1 Map-model overlay



X



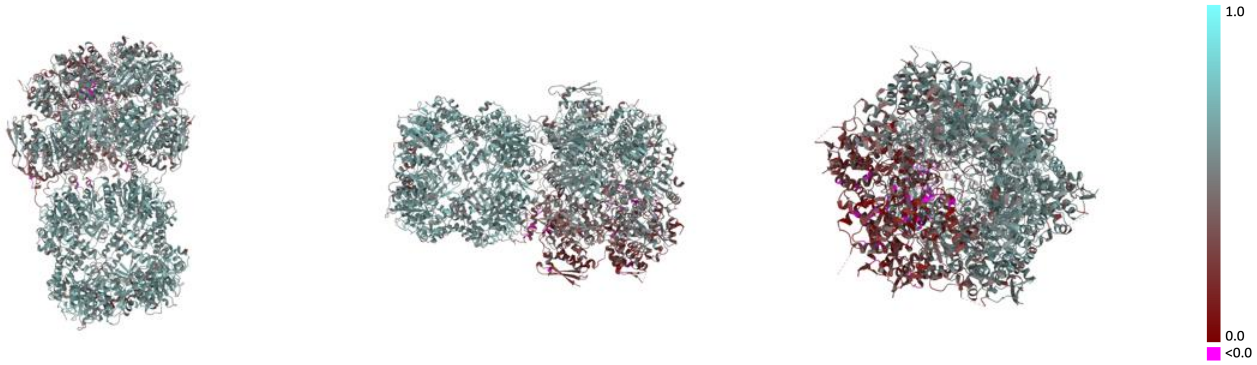
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.9 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.

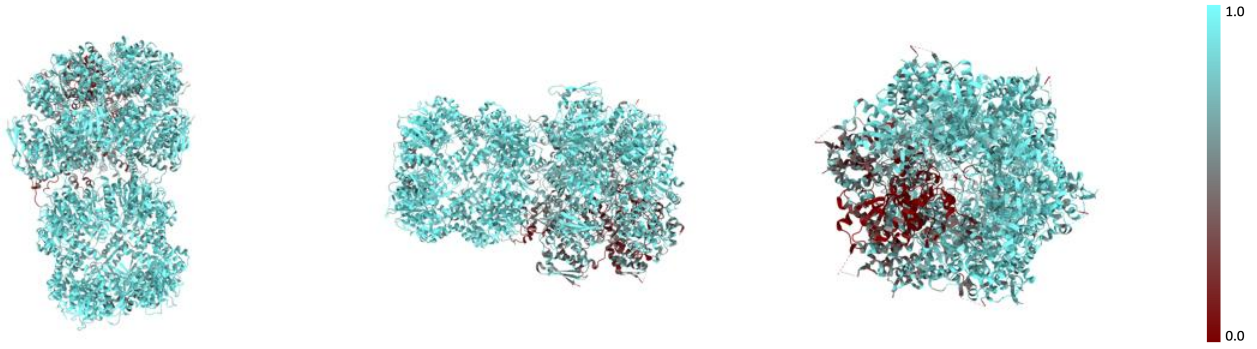
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

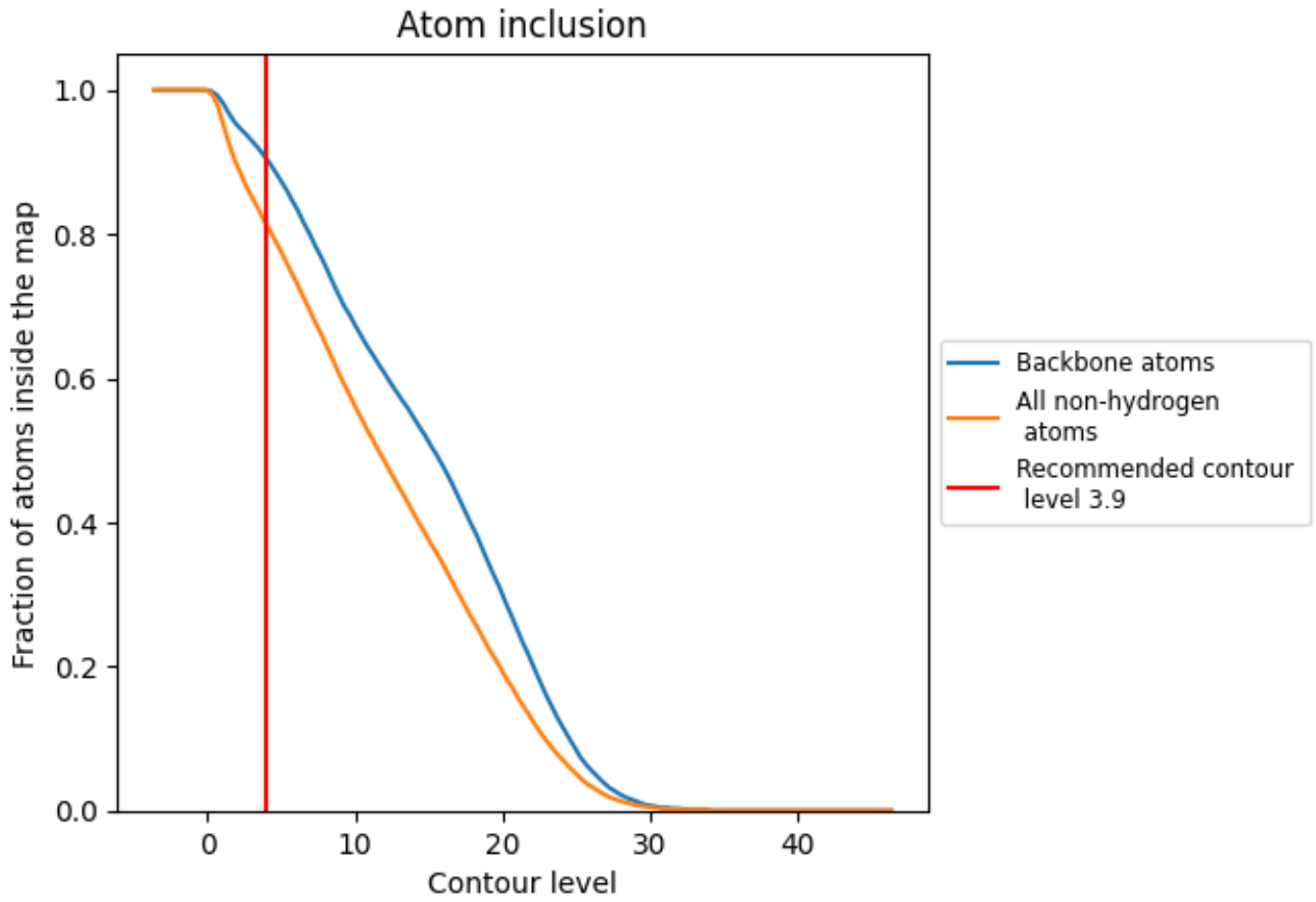
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.9).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8160	0.5030
A	0.9170	0.5830
B	0.9130	0.5760
C	0.9230	0.5720
D	0.9210	0.5670
E	0.9330	0.5730
F	0.9310	0.5870
G	0.9290	0.5870
H	0.9380	0.6090
I	0.9370	0.6000
J	0.9280	0.5950
K	0.9230	0.5820
L	0.9190	0.5780
M	0.9230	0.5850
N	0.9290	0.6020
O	0.5780	0.3050
P	0.8170	0.4780
Q	0.8980	0.5600
R	0.8960	0.5530
S	0.8340	0.4970
T	0.4290	0.2880
X	0.6830	0.4270