wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:51 PM GMT

PDB ID	:	4V96
Title	:	The structure of a 1.8 MDa viral genome injection device suggests alternative infection mechanisms
Authors	:	Veesler, D.; Spinelli, S.; Mahony, J.; Lichiere, J.; Blangy, S.; Bricogne, G.; Legrand, P.; Ortiz-Lombardia, M.; Campanacci, V.; van Sinderen, D.; Cambillau, C.
Deposited on	:	2012-02-01
Resolution	:	3.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

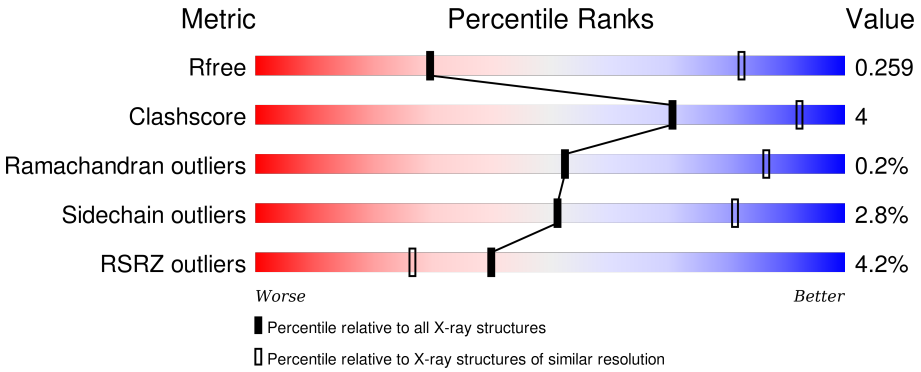
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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.



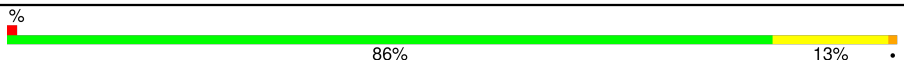
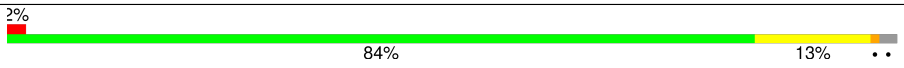
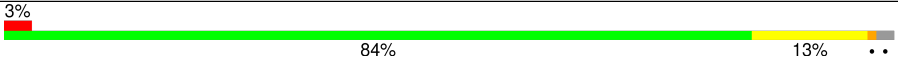
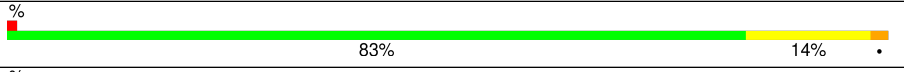
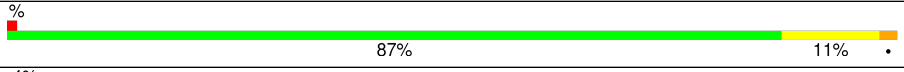
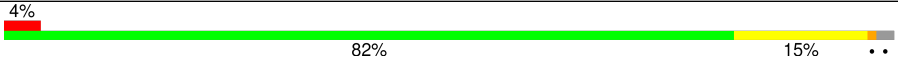
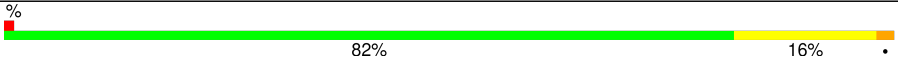
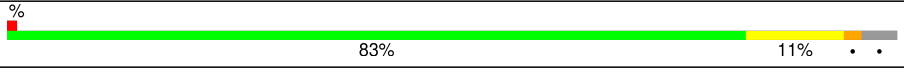
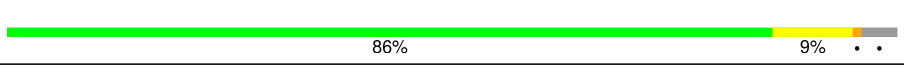
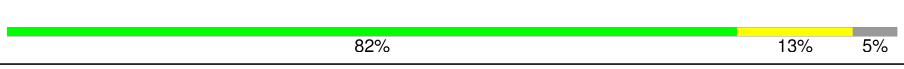
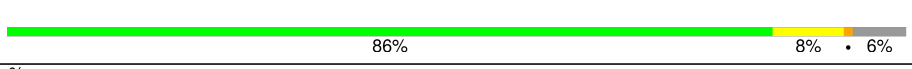
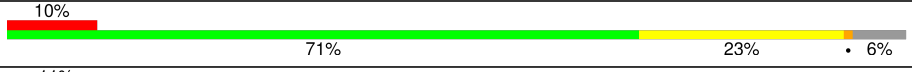
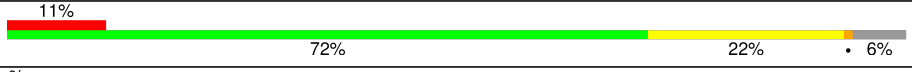
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	299	76% 21% •
1	AB	299	3% 81% 16% • •
1	AC	299	79% 20% •
1	AD	299	84% 14% •
1	AE	299	2% 85% 12% • •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	AF	299	
1	AG	299	
1	AH	299	
1	AI	299	
1	AJ	299	
1	AK	299	
1	AL	299	
1	AM	299	
1	AN	299	
1	AO	299	
1	AP	299	
1	AQ	299	
1	AR	299	
2	AS	253	
2	AT	253	
2	AU	253	
2	AV	253	
2	AW	253	
2	AX	253	
3	B1	173	
3	B2	173	
3	BA	173	
3	BB	173	
3	BC	173	
3	BD	173	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	BE	173	79% 15% • 5%
3	BF	173	3% 80% 14% 6%
3	BG	173	3% 79% 16% 5%
3	BH	173	2% 81% 13% • 5%
3	BI	173	3% 79% 16% 6%
3	BJ	173	% 79% 16% 5%
3	BK	173	2% 82% 12% • 6%
3	BL	173	2% 82% 13% 6%
3	BM	173	20% 80% 14% 6%
3	BN	173	20% 82% 10% • 6%
3	BO	173	20% 77% 16% 6%
3	BP	173	17% 76% 18% 6%
3	BQ	173	16% 79% 14% • 6%
3	BR	173	18% 81% 13% 6%
3	BS	173	% 78% 16% 6%
3	BT	173	% 82% 12% • 5%
3	BU	173	5% 82% 13% • 5%
3	BV	173	% 78% 16% • 6%
3	BW	173	% 81% 13% • 5%
3	BX	173	% 78% 15% • 6%
3	BY	173	79% 16% 6%
3	BZ	173	% 81% 13% • 6%
3	Ba	173	93% • 6%
3	Bb	173	2% 93% • 6%
3	Bc	173	% 94% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	Bd	173	2% 94% • 5%
3	Be	173	13% 93% • 6%
3	Bf	173	12% 94% • 5%
3	Bg	173	7% 94% • 6%
3	Bh	173	22% 92% • 7%
3	Bi	173	12% 93% • 6%
3	Bj	173	19% 92% • 6%
3	Bk	173	3% 93% • 6%
3	Bl	173	% 94% • 6%
3	Bm	173	93% • 6%
3	Bn	173	5% 92% • 6%
3	Bo	173	9% 93% • 6%
3	Bp	173	7% 94% • 5%
3	Bq	173	2% 93% • 6%
3	Br	173	% 94% • 6%
3	Bs	173	% 94% • 6%
3	Bt	173	5% 92% • 6%
3	Bu	173	16% 93% • 6%
3	Bv	173	9% 94% • 5%
3	Bw	173	6% 93% • 6%
3	Bx	173	12% 93% • 6%
3	By	173	17% 92% • 6%
3	Bz	173	2% 92% • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 118740 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 ORF48.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	299	Total	C	N	O	S	0	0	0
			2389	1537	386	460	6			
1	AB	294	Total	C	N	O	S	0	0	0
			2345	1511	379	449	6			
1	AC	299	Total	C	N	O	S	0	0	0
			2389	1538	387	458	6			
1	AD	299	Total	C	N	O	S	0	0	0
			2393	1540	387	460	6			
1	AE	291	Total	C	N	O	S	0	0	0
			2336	1509	376	445	6			
1	AF	299	Total	C	N	O	S	0	0	0
			2389	1537	386	460	6			
1	AG	299	Total	C	N	O	S	0	0	0
			2386	1537	387	456	6			
1	AH	294	Total	C	N	O	S	0	0	0
			2343	1508	379	450	6			
1	AI	299	Total	C	N	O	S	0	0	0
			2389	1537	386	460	6			
1	AJ	299	Total	C	N	O	S	0	0	0
			2393	1540	387	460	6			
1	AK	293	Total	C	N	O	S	0	0	0
			2320	1495	373	446	6			
1	AL	298	Total	C	N	O	S	0	0	0
			2382	1535	385	456	6			
1	AM	299	Total	C	N	O	S	0	0	0
			2389	1537	386	460	6			
1	AN	294	Total	C	N	O	S	0	0	0
			2328	1498	377	447	6			
1	AO	299	Total	C	N	O	S	0	0	0
			2393	1540	387	460	6			
1	AP	299	Total	C	N	O	S	0	0	0
			2382	1534	386	456	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AQ	295	Total	C	N	O	S	0	0	0
			2347	1514	377	451	5			
1	AR	299	Total	C	N	O	S	0	0	0
			2390	1537	387	460	6			

- Molecule 2 is a protein called ORF46.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AS	242	Total	C	N	O	S	0	0	0
			1932	1237	313	378	4			
2	AT	242	Total	C	N	O	S	0	0	0
			1931	1238	315	374	4			
2	AU	242	Total	C	N	O	S	0	0	0
			1924	1236	315	369	4			
2	AV	241	Total	C	N	O	S	0	0	0
			1899	1215	311	369	4			
2	AW	241	Total	C	N	O	S	0	0	0
			1917	1228	312	373	4			
2	AX	241	Total	C	N	O	S	0	0	0
			1913	1224	313	372	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AS	1	GLY	-	EXPRESSION TAG	UNP Q9AZ58
AT	1	GLY	-	EXPRESSION TAG	UNP Q9AZ58
AU	1	GLY	-	EXPRESSION TAG	UNP Q9AZ58
AV	1	GLY	-	EXPRESSION TAG	UNP Q9AZ58
AW	1	GLY	-	EXPRESSION TAG	UNP Q9AZ58
AX	1	GLY	-	EXPRESSION TAG	UNP Q9AZ58

- Molecule 3 is a protein called BPP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	BA	164	Total	C	N	O	S	0	0	0
			1199	743	210	241	5			
3	BB	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			
3	BC	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			
3	BD	164	Total	C	N	O	S	0	0	0
			1199	743	210	241	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	BE	164	Total	C	N	O	S	0	0	0
			1199	743	210	241	5			
3	BF	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			
3	BG	164	Total	C	N	O	S	0	0	0
			1199	743	210	241	5			
3	BH	164	Total	C	N	O	S	0	0	0
			1205	746	213	241	5			
3	BI	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			
3	BJ	164	Total	C	N	O	S	0	0	0
			1199	743	210	241	5			
3	BK	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			
3	BL	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			
3	BM	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			
3	BN	162	Total	C	N	O	S	0	0	0
			1188	737	208	238	5			
3	BO	162	Total	C	N	O	S	0	0	0
			1188	737	208	238	5			
3	BP	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			
3	BQ	162	Total	C	N	O	S	0	0	0
			1194	740	211	238	5			
3	BR	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			
3	BS	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			
3	BT	164	Total	C	N	O	S	0	0	0
			1199	743	210	241	5			
3	BU	164	Total	C	N	O	S	0	0	0
			1199	743	210	241	5			
3	BV	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			
3	BW	164	Total	C	N	O	S	0	0	0
			1199	743	210	241	5			
3	BX	162	Total	C	N	O	S	0	0	0
			1188	737	208	238	5			
3	BY	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	BZ	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			
3	Ba	162	Total	C	N	O	S	0	0	0
			1194	740	211	238	5			
3	Bb	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			
3	Bc	164	Total	C	N	O	S	0	0	0
			1198	743	210	240	5			
3	Bd	165	Total	C	N	O	S	0	0	0
			1209	749	214	241	5			
3	Be	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			
3	Bf	164	Total	C	N	O	S	0	0	0
			1199	743	210	241	5			
3	Bg	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			
3	Bh	161	Total	C	N	O	S	0	0	0
			1186	736	210	235	5			
3	Bi	162	Total	C	N	O	S	0	0	0
			1188	737	208	238	5			
3	Bj	162	Total	C	N	O	S	0	0	0
			1194	740	211	238	5			
3	Bk	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			
3	Bl	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			
3	Bm	162	Total	C	N	O	S	0	0	0
			1188	737	208	238	5			
3	Bn	162	Total	C	N	O	S	0	0	0
			1194	740	211	238	5			
3	Bo	162	Total	C	N	O	S	0	0	0
			1194	740	211	238	5			
3	Bp	164	Total	C	N	O	S	0	0	0
			1205	746	213	241	5			
3	Bq	163	Total	C	N	O	S	0	0	0
			1200	743	212	240	5			
3	Br	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			
3	Bs	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			
3	Bt	162	Total	C	N	O	S	0	0	0
			1188	737	208	238	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Bu	162	Total	C	N	O	S	0	0	0
			1194	740	211	238	5			
3	Bv	164	Total	C	N	O	S	0	0	0
			1199	743	210	241	5			
3	Bw	163	Total	C	N	O	S	0	0	0
			1194	740	209	240	5			
3	Bx	162	Total	C	N	O	S	0	0	0
			1194	740	211	238	5			
3	By	162	Total	C	N	O	S	0	0	0
			1194	740	211	238	5			
3	Bz	163	Total	C	N	O	S	0	0	0
			1200	743	212	240	5			
3	B1	163	Total	C	N	O	S	0	0	0
			1200	743	212	240	5			
3	B2	162	Total	C	N	O	S	0	0	0
			1194	740	211	238	5			

There are 540 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	164	SER	-	EXPRESSION TAG	UNP Q9G096
BA	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BA	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BA	167	SER	-	EXPRESSION TAG	UNP Q9G096
BA	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BA	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BA	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BA	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BA	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BA	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BB	164	SER	-	EXPRESSION TAG	UNP Q9G096
BB	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BB	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BB	167	SER	-	EXPRESSION TAG	UNP Q9G096
BB	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BB	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BB	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BB	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BB	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BB	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BC	164	SER	-	EXPRESSION TAG	UNP Q9G096
BC	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BC	166	TRP	-	EXPRESSION TAG	UNP Q9G096

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
BC	167	SER	-	EXPRESSION TAG	UNP Q9G096
BC	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BC	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BC	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BC	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BC	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BC	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BD	164	SER	-	EXPRESSION TAG	UNP Q9G096
BD	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BD	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BD	167	SER	-	EXPRESSION TAG	UNP Q9G096
BD	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BD	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BD	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BD	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BD	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BD	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BE	164	SER	-	EXPRESSION TAG	UNP Q9G096
BE	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BE	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BE	167	SER	-	EXPRESSION TAG	UNP Q9G096
BE	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BE	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BE	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BE	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BE	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BE	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BF	164	SER	-	EXPRESSION TAG	UNP Q9G096
BF	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BF	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BF	167	SER	-	EXPRESSION TAG	UNP Q9G096
BF	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BF	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BF	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BF	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BF	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BF	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BG	164	SER	-	EXPRESSION TAG	UNP Q9G096
BG	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BG	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BG	167	SER	-	EXPRESSION TAG	UNP Q9G096
BG	168	HIS	-	EXPRESSION TAG	UNP Q9G096

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
BG	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BG	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BG	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BG	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BG	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BH	164	SER	-	EXPRESSION TAG	UNP Q9G096
BH	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BH	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BH	167	SER	-	EXPRESSION TAG	UNP Q9G096
BH	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BH	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BH	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BH	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BH	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BH	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BI	164	SER	-	EXPRESSION TAG	UNP Q9G096
BI	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BI	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BI	167	SER	-	EXPRESSION TAG	UNP Q9G096
BI	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BI	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BI	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BI	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BI	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BI	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BJ	164	SER	-	EXPRESSION TAG	UNP Q9G096
BJ	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BJ	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BJ	167	SER	-	EXPRESSION TAG	UNP Q9G096
BJ	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BJ	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BJ	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BJ	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BJ	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BJ	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BK	164	SER	-	EXPRESSION TAG	UNP Q9G096
BK	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BK	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BK	167	SER	-	EXPRESSION TAG	UNP Q9G096
BK	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BK	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BK	170	GLN	-	EXPRESSION TAG	UNP Q9G096

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
BK	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BK	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BK	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BL	164	SER	-	EXPRESSION TAG	UNP Q9G096
BL	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BL	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BL	167	SER	-	EXPRESSION TAG	UNP Q9G096
BL	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BL	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BL	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BL	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BL	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BL	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BM	164	SER	-	EXPRESSION TAG	UNP Q9G096
BM	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BM	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BM	167	SER	-	EXPRESSION TAG	UNP Q9G096
BM	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BM	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BM	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BM	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BM	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BM	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BN	164	SER	-	EXPRESSION TAG	UNP Q9G096
BN	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BN	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BN	167	SER	-	EXPRESSION TAG	UNP Q9G096
BN	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BN	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BN	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BN	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BN	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BN	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BO	164	SER	-	EXPRESSION TAG	UNP Q9G096
BO	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BO	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BO	167	SER	-	EXPRESSION TAG	UNP Q9G096
BO	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BO	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BO	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BO	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BO	172	GLU	-	EXPRESSION TAG	UNP Q9G096

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
BO	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BP	164	SER	-	EXPRESSION TAG	UNP Q9G096
BP	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BP	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BP	167	SER	-	EXPRESSION TAG	UNP Q9G096
BP	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BP	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BP	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BP	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BP	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BP	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BQ	164	SER	-	EXPRESSION TAG	UNP Q9G096
BQ	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BQ	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BQ	167	SER	-	EXPRESSION TAG	UNP Q9G096
BQ	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BQ	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BQ	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BQ	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BQ	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BQ	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BR	164	SER	-	EXPRESSION TAG	UNP Q9G096
BR	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BR	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BR	167	SER	-	EXPRESSION TAG	UNP Q9G096
BR	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BR	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BR	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BR	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BR	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BR	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BS	164	SER	-	EXPRESSION TAG	UNP Q9G096
BS	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BS	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BS	167	SER	-	EXPRESSION TAG	UNP Q9G096
BS	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BS	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BS	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BS	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BS	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BS	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BT	164	SER	-	EXPRESSION TAG	UNP Q9G096

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
BT	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BT	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BT	167	SER	-	EXPRESSION TAG	UNP Q9G096
BT	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BT	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BT	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BT	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BT	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BT	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BU	164	SER	-	EXPRESSION TAG	UNP Q9G096
BU	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BU	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BU	167	SER	-	EXPRESSION TAG	UNP Q9G096
BU	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BU	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BU	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BU	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BU	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BU	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BV	164	SER	-	EXPRESSION TAG	UNP Q9G096
BV	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BV	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BV	167	SER	-	EXPRESSION TAG	UNP Q9G096
BV	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BV	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BV	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BV	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BV	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BV	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BW	164	SER	-	EXPRESSION TAG	UNP Q9G096
BW	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BW	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BW	167	SER	-	EXPRESSION TAG	UNP Q9G096
BW	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BW	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BW	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BW	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BW	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BW	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BX	164	SER	-	EXPRESSION TAG	UNP Q9G096
BX	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BX	166	TRP	-	EXPRESSION TAG	UNP Q9G096

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
BX	167	SER	-	EXPRESSION TAG	UNP Q9G096
BX	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BX	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BX	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BX	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BX	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BX	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BY	164	SER	-	EXPRESSION TAG	UNP Q9G096
BY	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BY	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BY	167	SER	-	EXPRESSION TAG	UNP Q9G096
BY	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BY	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BY	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BY	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BY	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BY	173	LYS	-	EXPRESSION TAG	UNP Q9G096
BZ	164	SER	-	EXPRESSION TAG	UNP Q9G096
BZ	165	ALA	-	EXPRESSION TAG	UNP Q9G096
BZ	166	TRP	-	EXPRESSION TAG	UNP Q9G096
BZ	167	SER	-	EXPRESSION TAG	UNP Q9G096
BZ	168	HIS	-	EXPRESSION TAG	UNP Q9G096
BZ	169	PRO	-	EXPRESSION TAG	UNP Q9G096
BZ	170	GLN	-	EXPRESSION TAG	UNP Q9G096
BZ	171	PHE	-	EXPRESSION TAG	UNP Q9G096
BZ	172	GLU	-	EXPRESSION TAG	UNP Q9G096
BZ	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Ba	164	SER	-	EXPRESSION TAG	UNP Q9G096
Ba	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Ba	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Ba	167	SER	-	EXPRESSION TAG	UNP Q9G096
Ba	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Ba	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Ba	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Ba	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Ba	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Ba	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bb	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bb	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bb	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bb	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bb	168	HIS	-	EXPRESSION TAG	UNP Q9G096

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Bb	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bb	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bb	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bb	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bb	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bc	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bc	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bc	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bc	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bc	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Bc	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bc	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bc	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bc	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bc	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bd	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bd	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bd	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bd	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bd	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Bd	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bd	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bd	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bd	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bd	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Be	164	SER	-	EXPRESSION TAG	UNP Q9G096
Be	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Be	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Be	167	SER	-	EXPRESSION TAG	UNP Q9G096
Be	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Be	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Be	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Be	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Be	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Be	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bf	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bf	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bf	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bf	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bf	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Bf	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bf	170	GLN	-	EXPRESSION TAG	UNP Q9G096

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Bf	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bf	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bf	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bg	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bg	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bg	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bg	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bg	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Bg	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bg	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bg	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bg	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bg	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bh	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bh	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bh	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bh	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bh	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Bh	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bh	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bh	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bh	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bh	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bi	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bi	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bi	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bi	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bi	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Bi	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bi	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bi	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bi	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bi	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bj	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bj	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bj	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bj	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bj	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Bj	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bj	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bj	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bj	172	GLU	-	EXPRESSION TAG	UNP Q9G096

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Bj	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bk	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bk	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bk	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bk	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bk	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Bk	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bk	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bk	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bk	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bk	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bl	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bl	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bl	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bl	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bl	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Bl	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bl	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bl	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bl	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bl	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bm	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bm	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bm	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bm	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bm	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Bm	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bm	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bm	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bm	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bm	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bn	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bn	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bn	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bn	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bn	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Bn	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bn	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bn	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bn	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bn	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bo	164	SER	-	EXPRESSION TAG	UNP Q9G096

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Bo	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bo	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bo	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bo	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Bo	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bo	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bo	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bo	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bo	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bp	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bp	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bp	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bp	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bp	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Bp	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bp	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bp	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bp	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bp	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bq	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bq	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bq	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bq	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bq	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Bq	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bq	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bq	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bq	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bq	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Br	164	SER	-	EXPRESSION TAG	UNP Q9G096
Br	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Br	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Br	167	SER	-	EXPRESSION TAG	UNP Q9G096
Br	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Br	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Br	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Br	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Br	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Br	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bs	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bs	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bs	166	TRP	-	EXPRESSION TAG	UNP Q9G096

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Bs	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bs	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Bs	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bs	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bs	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bs	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bs	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bt	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bt	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bt	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bt	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bt	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Bt	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bt	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bt	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bt	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bt	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bu	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bu	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bu	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bu	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bu	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Bu	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bu	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bu	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bu	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bu	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bv	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bv	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bv	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bv	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bv	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Bv	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bv	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bv	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bv	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bv	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bw	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bw	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bw	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bw	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bw	168	HIS	-	EXPRESSION TAG	UNP Q9G096

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Bw	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bw	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bw	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bw	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bw	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bx	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bx	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bx	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bx	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bx	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Bx	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bx	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bx	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bx	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bx	173	LYS	-	EXPRESSION TAG	UNP Q9G096
By	164	SER	-	EXPRESSION TAG	UNP Q9G096
By	165	ALA	-	EXPRESSION TAG	UNP Q9G096
By	166	TRP	-	EXPRESSION TAG	UNP Q9G096
By	167	SER	-	EXPRESSION TAG	UNP Q9G096
By	168	HIS	-	EXPRESSION TAG	UNP Q9G096
By	169	PRO	-	EXPRESSION TAG	UNP Q9G096
By	170	GLN	-	EXPRESSION TAG	UNP Q9G096
By	171	PHE	-	EXPRESSION TAG	UNP Q9G096
By	172	GLU	-	EXPRESSION TAG	UNP Q9G096
By	173	LYS	-	EXPRESSION TAG	UNP Q9G096
Bz	164	SER	-	EXPRESSION TAG	UNP Q9G096
Bz	165	ALA	-	EXPRESSION TAG	UNP Q9G096
Bz	166	TRP	-	EXPRESSION TAG	UNP Q9G096
Bz	167	SER	-	EXPRESSION TAG	UNP Q9G096
Bz	168	HIS	-	EXPRESSION TAG	UNP Q9G096
Bz	169	PRO	-	EXPRESSION TAG	UNP Q9G096
Bz	170	GLN	-	EXPRESSION TAG	UNP Q9G096
Bz	171	PHE	-	EXPRESSION TAG	UNP Q9G096
Bz	172	GLU	-	EXPRESSION TAG	UNP Q9G096
Bz	173	LYS	-	EXPRESSION TAG	UNP Q9G096
B1	164	SER	-	EXPRESSION TAG	UNP Q9G096
B1	165	ALA	-	EXPRESSION TAG	UNP Q9G096
B1	166	TRP	-	EXPRESSION TAG	UNP Q9G096
B1	167	SER	-	EXPRESSION TAG	UNP Q9G096
B1	168	HIS	-	EXPRESSION TAG	UNP Q9G096
B1	169	PRO	-	EXPRESSION TAG	UNP Q9G096
B1	170	GLN	-	EXPRESSION TAG	UNP Q9G096

Continued on next page...

Continued from previous page...

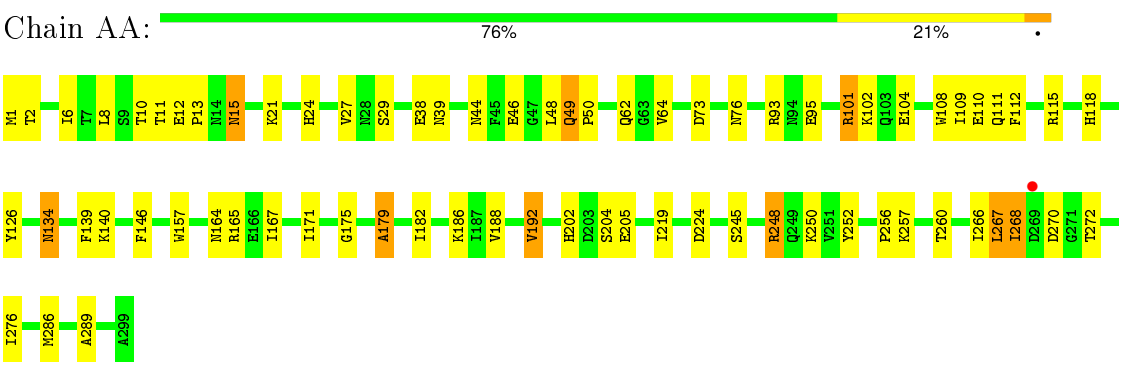
Chain	Residue	Modelled	Actual	Comment	Reference
B1	171	PHE	-	EXPRESSION TAG	UNP Q9G096
B1	172	GLU	-	EXPRESSION TAG	UNP Q9G096
B1	173	LYS	-	EXPRESSION TAG	UNP Q9G096
B2	164	SER	-	EXPRESSION TAG	UNP Q9G096
B2	165	ALA	-	EXPRESSION TAG	UNP Q9G096
B2	166	TRP	-	EXPRESSION TAG	UNP Q9G096
B2	167	SER	-	EXPRESSION TAG	UNP Q9G096
B2	168	HIS	-	EXPRESSION TAG	UNP Q9G096
B2	169	PRO	-	EXPRESSION TAG	UNP Q9G096
B2	170	GLN	-	EXPRESSION TAG	UNP Q9G096
B2	171	PHE	-	EXPRESSION TAG	UNP Q9G096
B2	172	GLU	-	EXPRESSION TAG	UNP Q9G096
B2	173	LYS	-	EXPRESSION TAG	UNP Q9G096

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

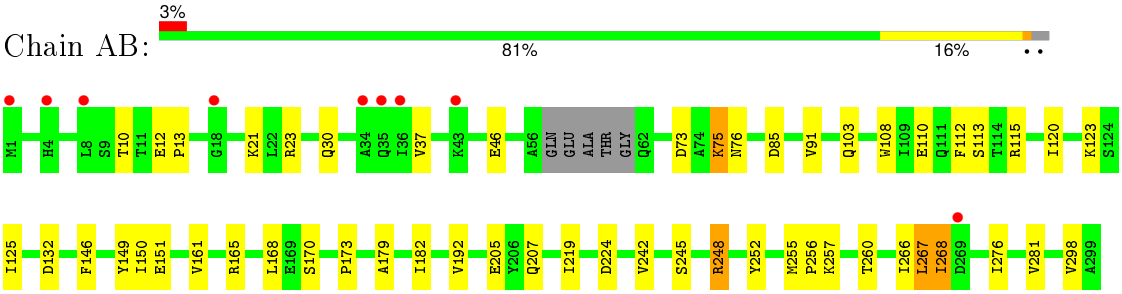
- Molecule 1: ORF48

Chain AA:



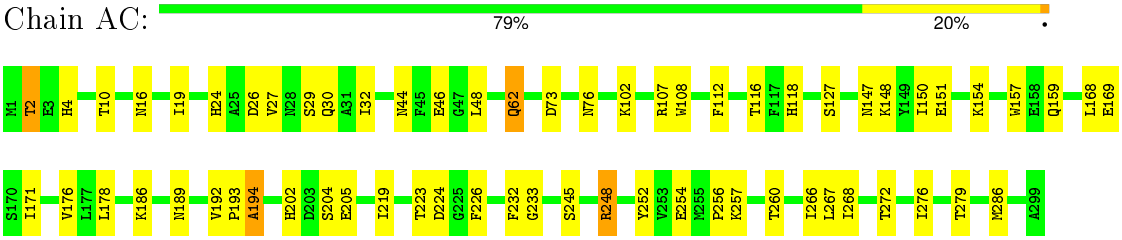
- Molecule 1: ORF48

Chain AB:



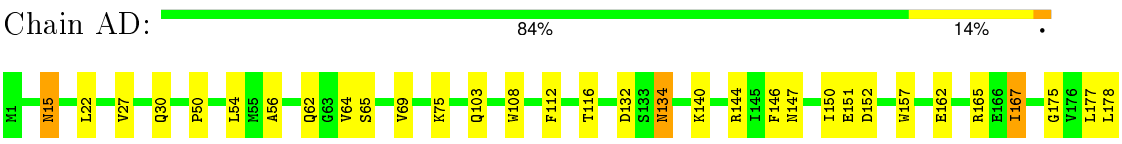
- Molecule 1: ORF48

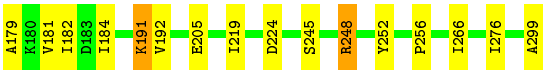
Chain AC:



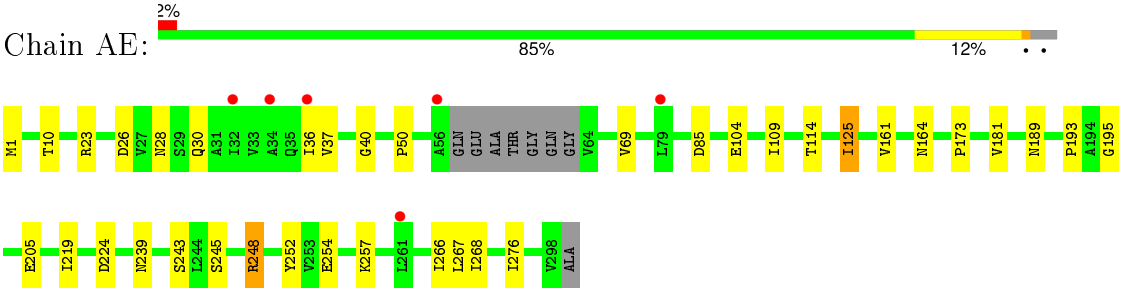
- Molecule 1: ORF48

Chain AD:

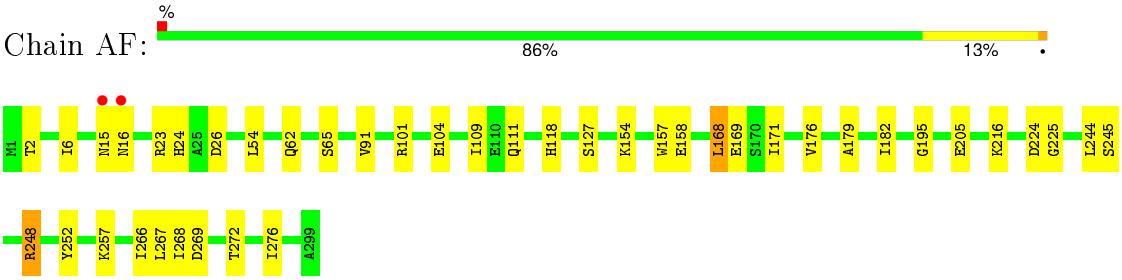




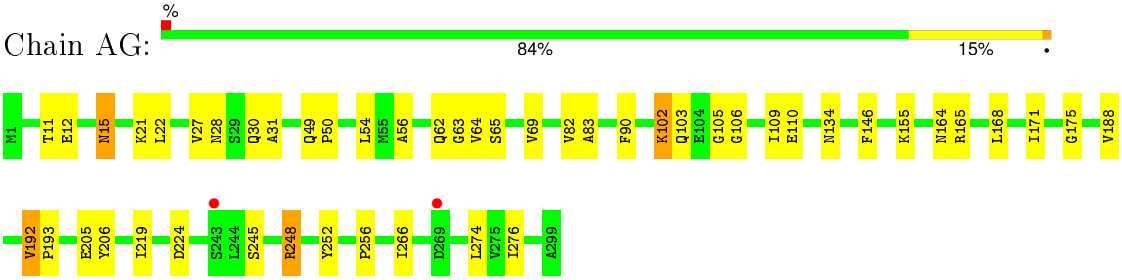
• Molecule 1: ORF48



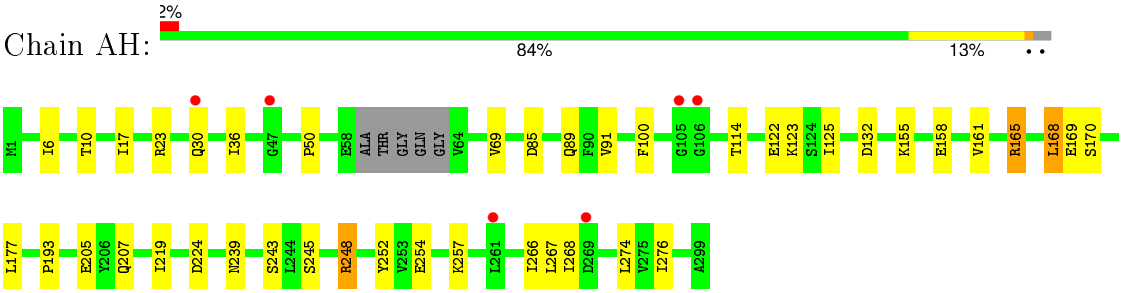
• Molecule 1: ORF48



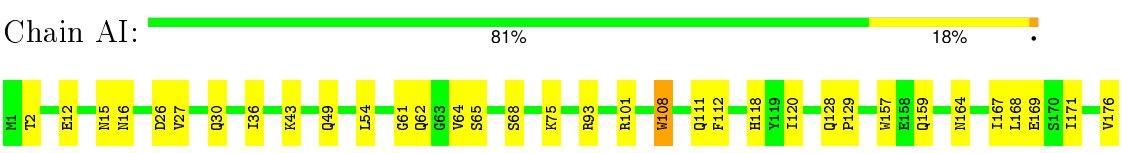
• Molecule 1: ORF48



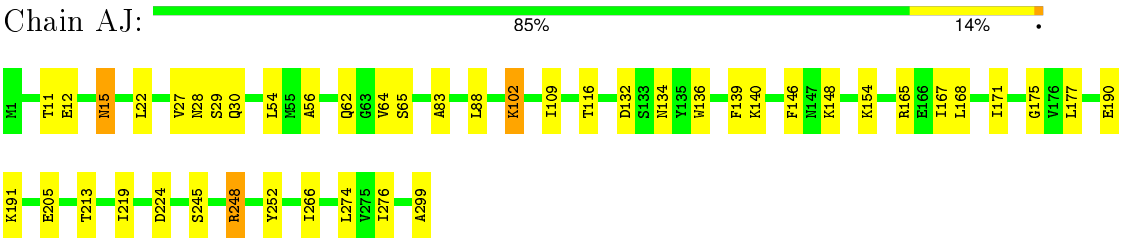
• Molecule 1: ORF48



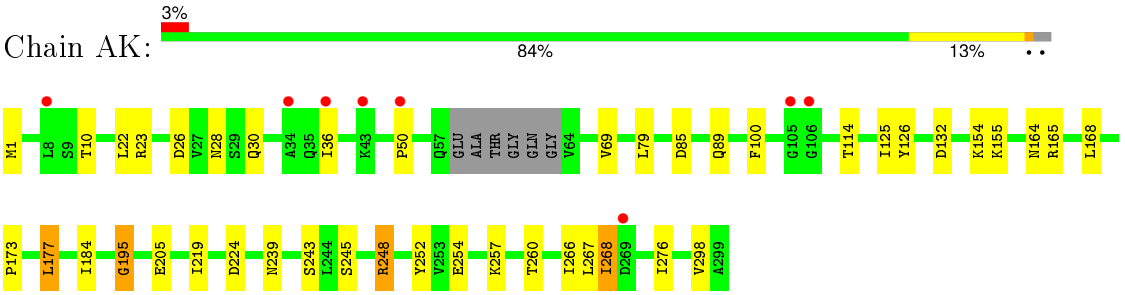
• Molecule 1: ORF48



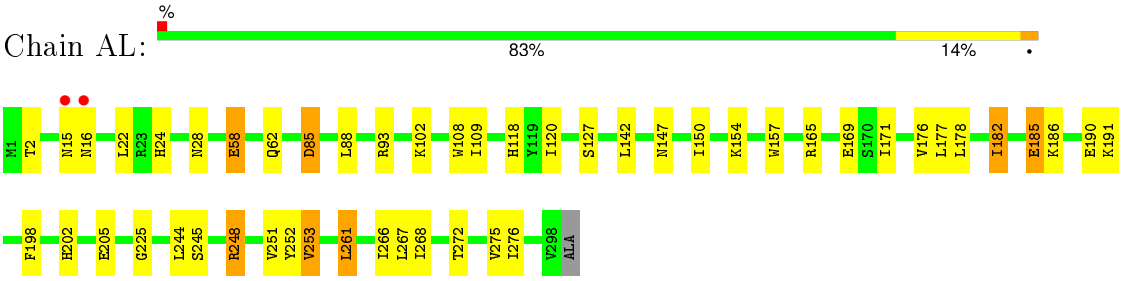
• Molecule 1: ORF48



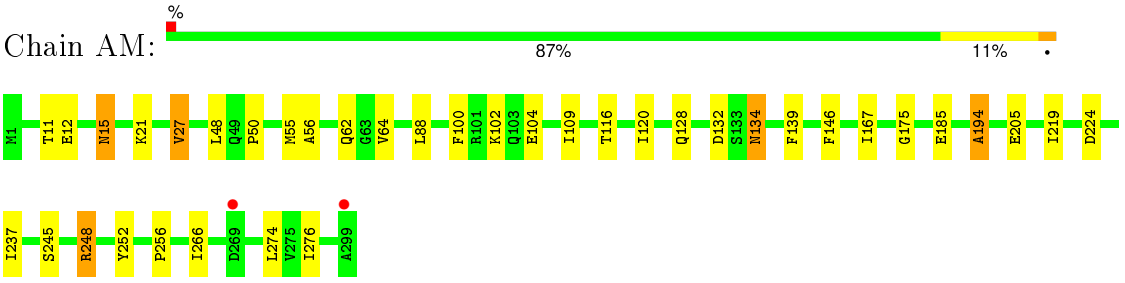
• Molecule 1: ORF48



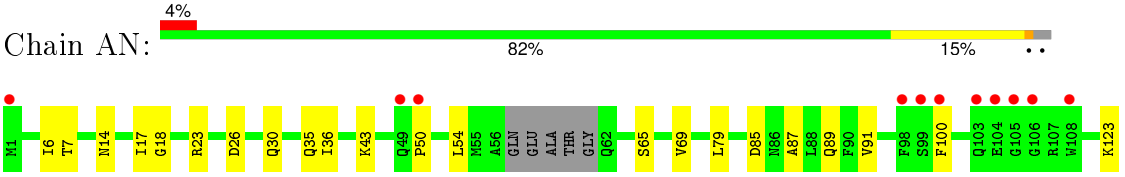
• Molecule 1: ORF48

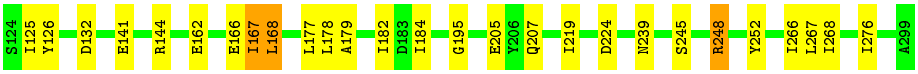


• Molecule 1: ORF48



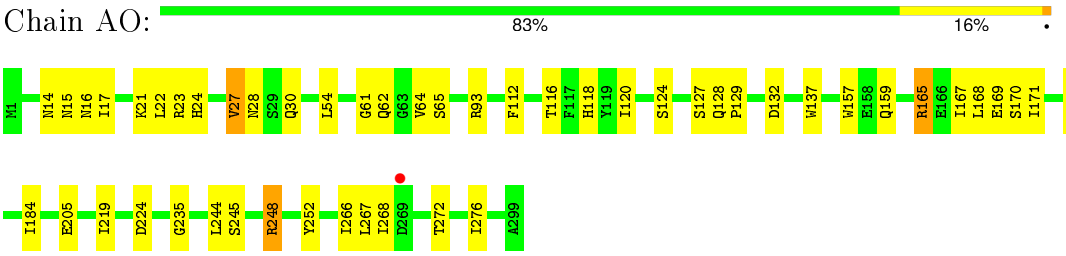
• Molecule 1: ORF48





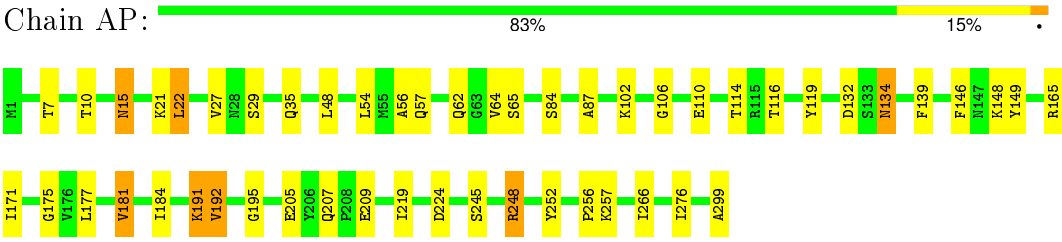
• Molecule 1: ORF48

Chain AO:



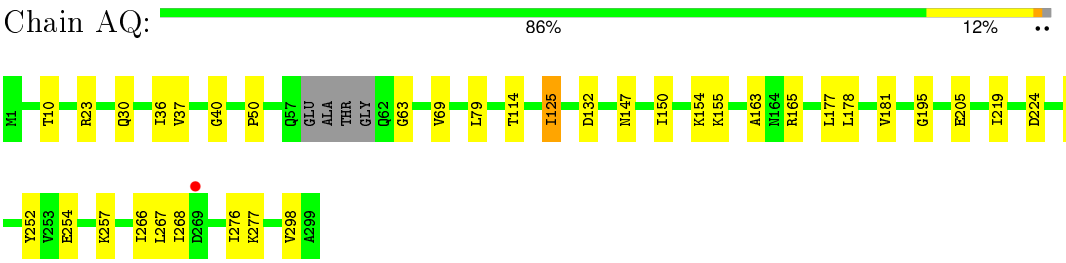
• Molecule 1: ORF48

Chain AP:



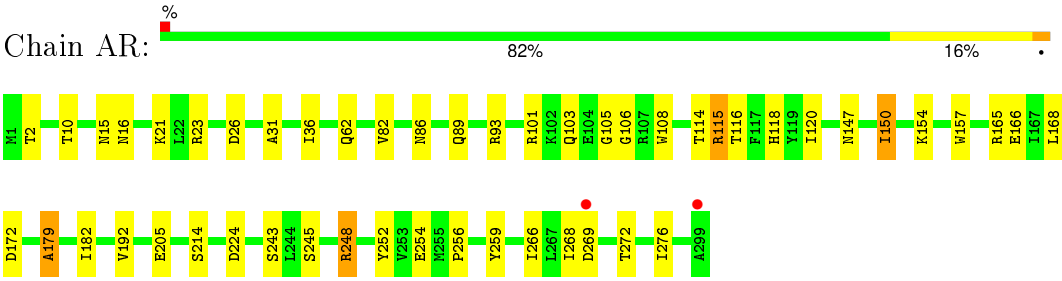
• Molecule 1: ORF48

Chain AQ:



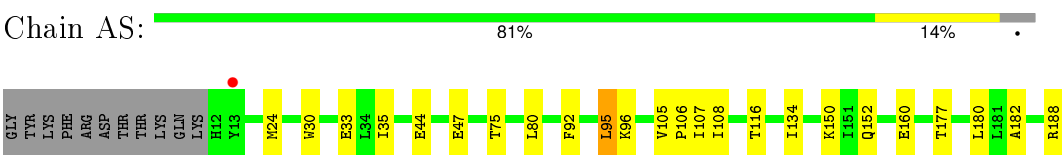
• Molecule 1: ORF48

Chain AR:



• Molecule 2: ORF46

Chain AS:



• Molecule 2: ORF46

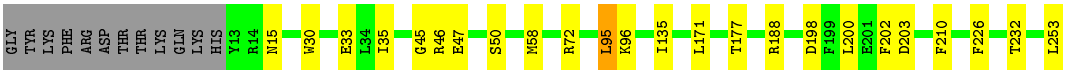
Chain AT:

• Molecule 2: ORF46

Chain AU:

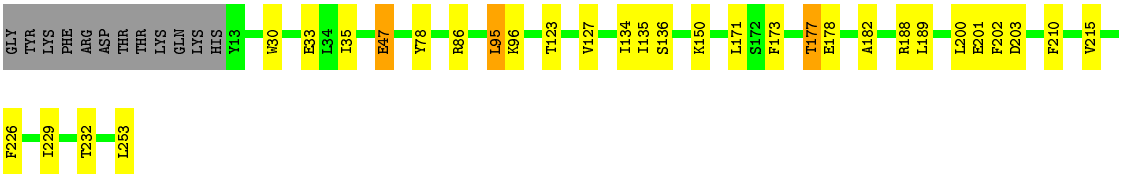
• Molecule 2: ORF46

Chain AV:



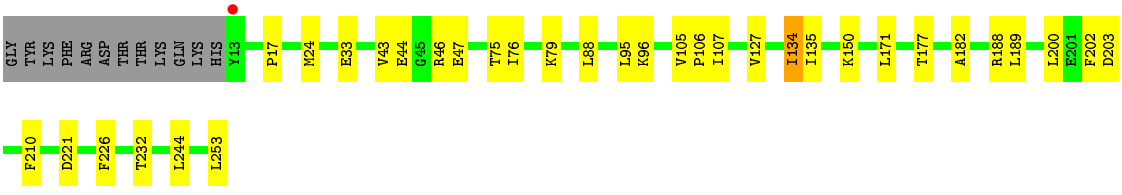
• Molecule 2: ORF46

Chain AW:



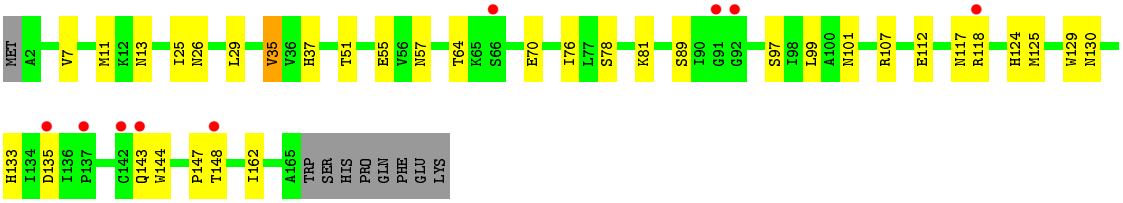
• Molecule 2: ORF46

Chain AX:

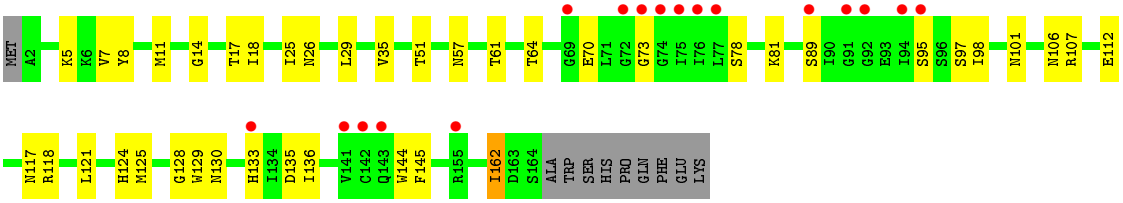


• Molecule 3: BPP

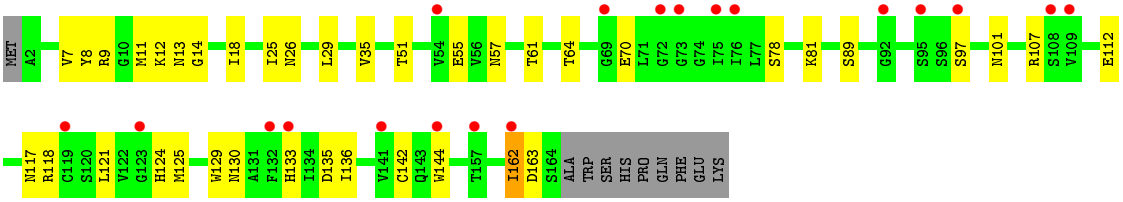
Chain BA:



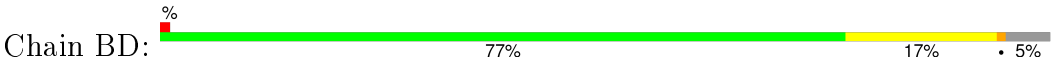
• Molecule 3: BPP

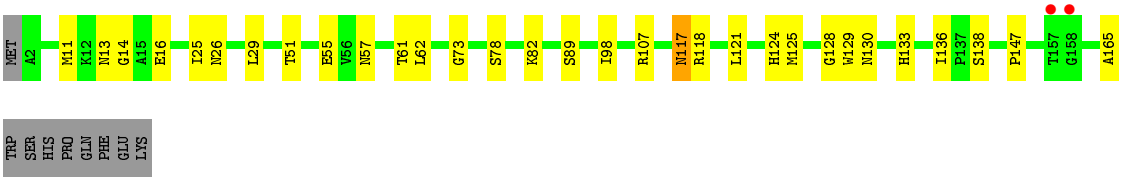


• Molecule 3: BPP

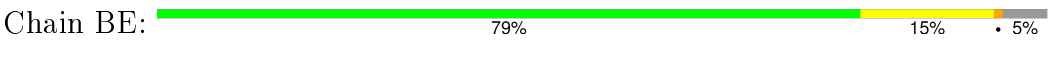


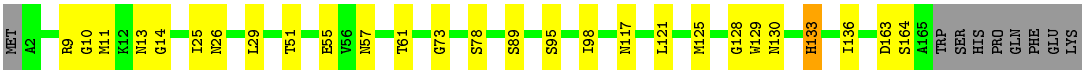
• Molecule 3: BPP



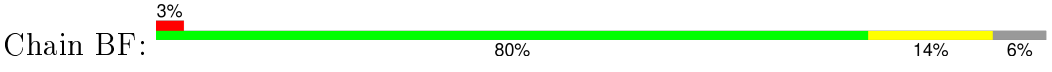


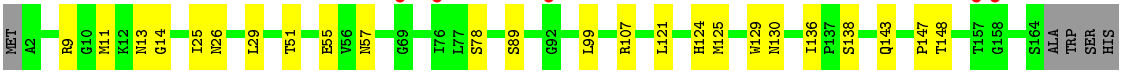
• Molecule 3: BPP





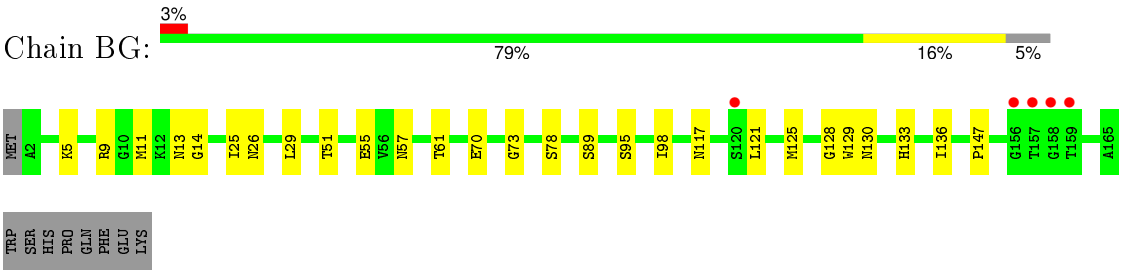
• Molecule 3: BPP





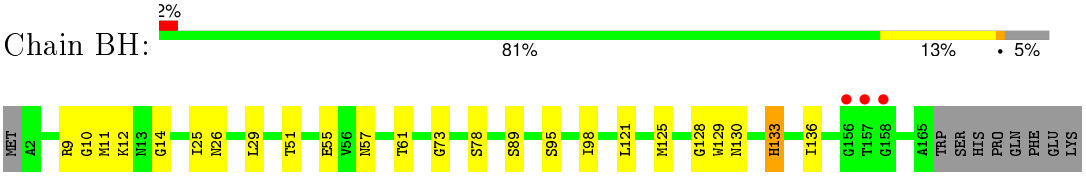
• Molecule 3: BPP

Chain BG:



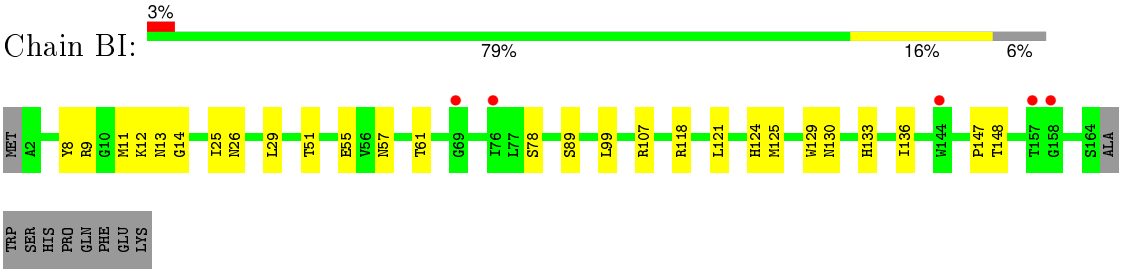
• Molecule 3: BPP

Chain BH:



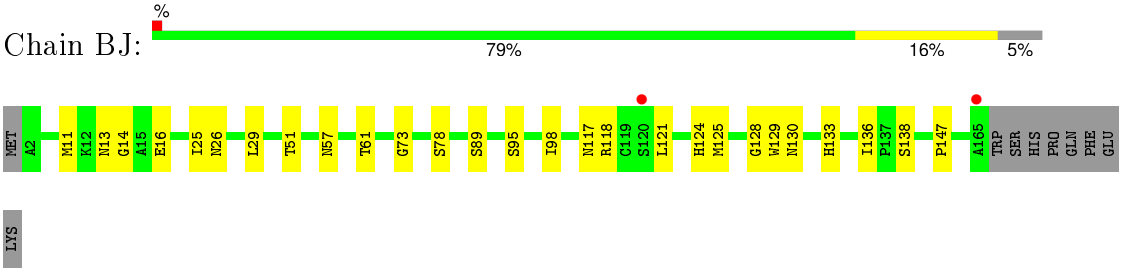
• Molecule 3: BPP

Chain BI:



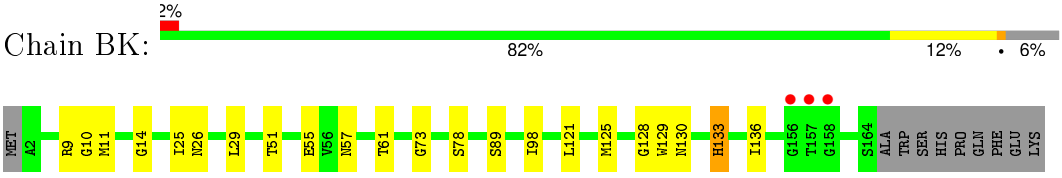
• Molecule 3: BPP

Chain BJ:



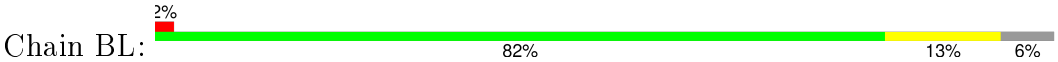
• Molecule 3: BPP

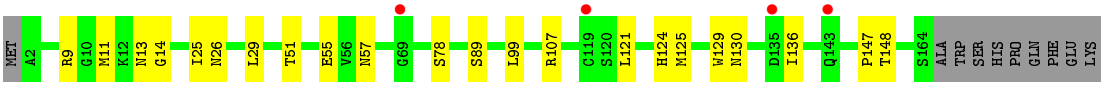
Chain BK:



• Molecule 3: BPP

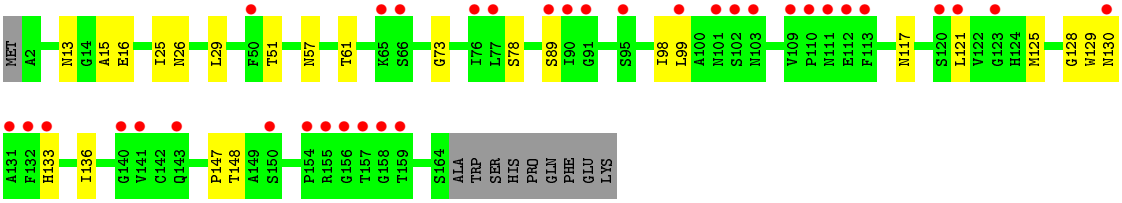
Chain BL:





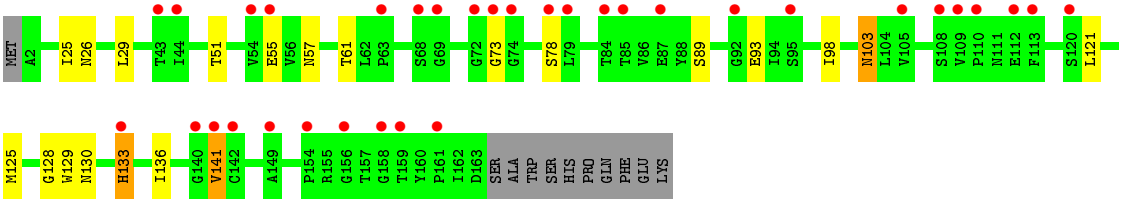
• Molecule 3: BPP

Chain BM:



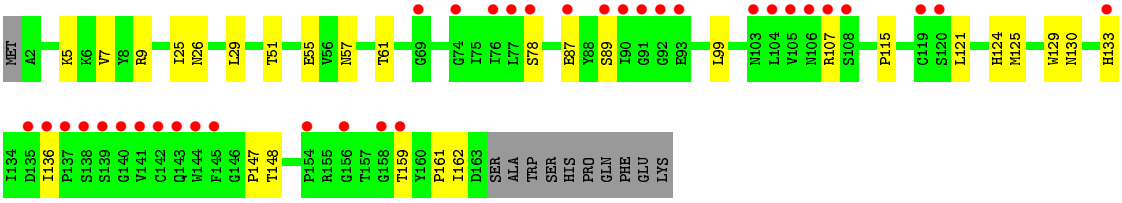
• Molecule 3: BPP

Chain BN:



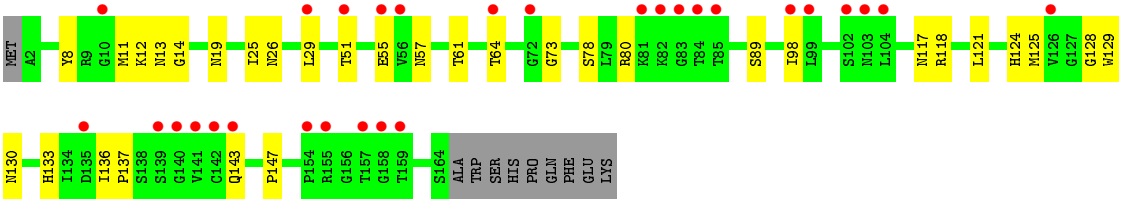
• Molecule 3: BPP

Chain BO:



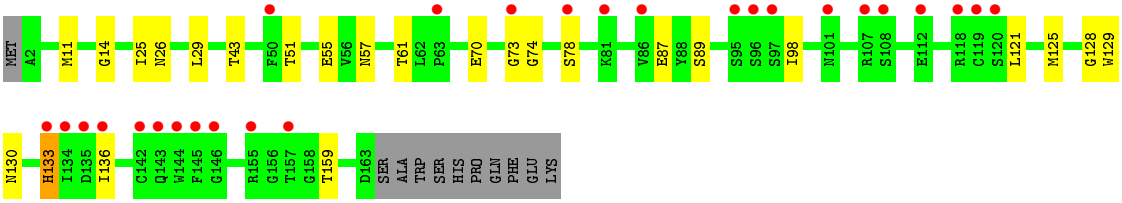
• Molecule 3: BPP

Chain BP:



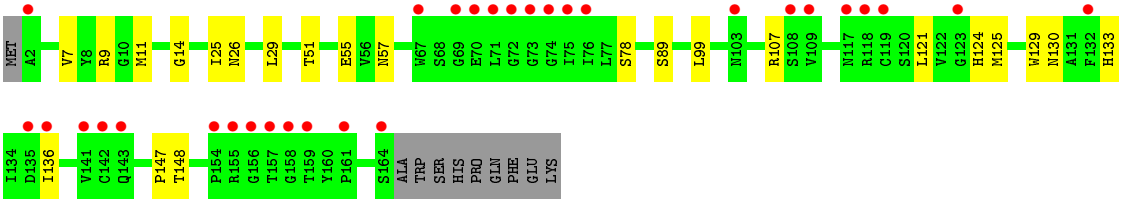
• Molecule 3: BPP

Chain BQ:



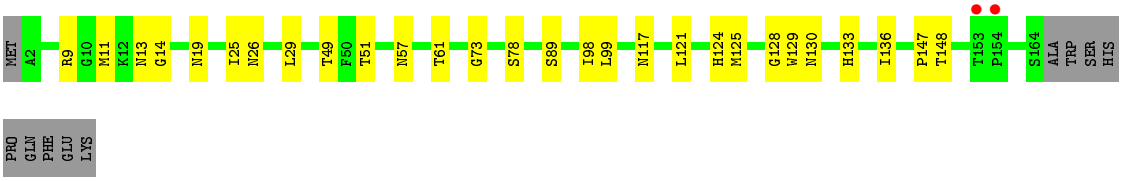
• Molecule 3: BPP

Chain BR:



• Molecule 3: BPP

Chain BS:

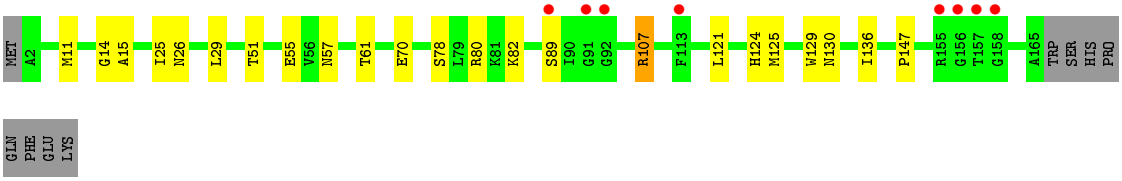


• Molecule 3: BPP

Chain BT:

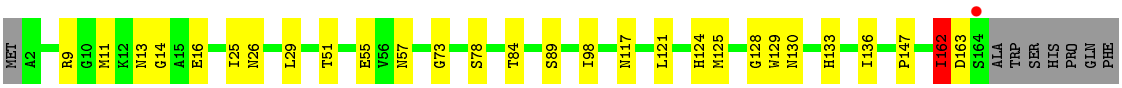
• Molecule 3: BPP

Chain BU:



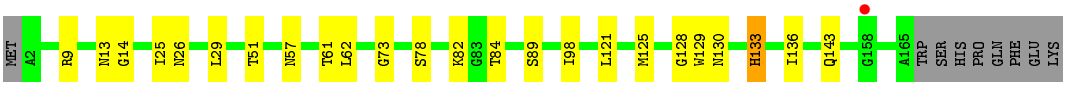
• Molecule 3: BPP

Chain BV:



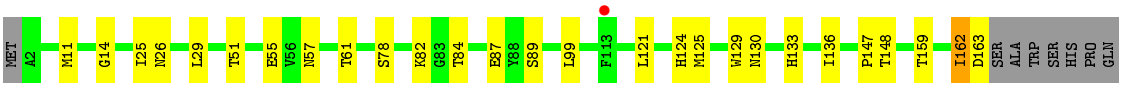
• Molecule 3: BPP

Chain BW:



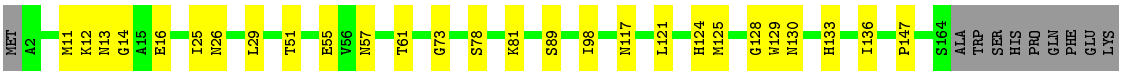
• Molecule 3: BPP

Chain BX:



• Molecule 3: BPP

Chain BY:



• Molecule 3: BPP

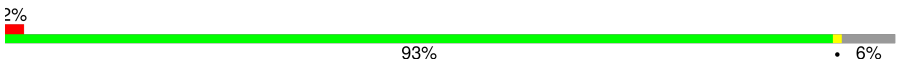
Chain BZ:

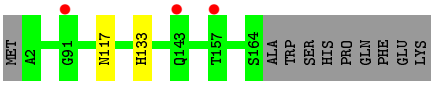
• Molecule 3: BPP

Chain Ba:

• Molecule 3: BPP

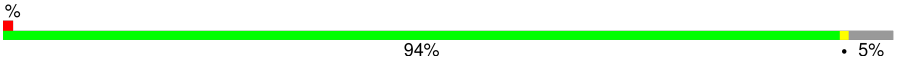
Chain Bb:

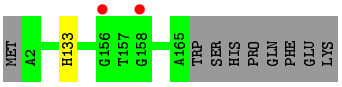




• Molecule 3: BPP

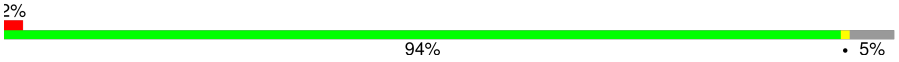
Chain Bc:

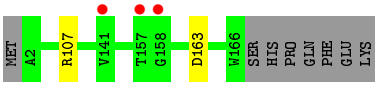




- Molecule 3: BPP

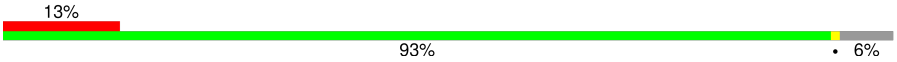
Chain Bd:

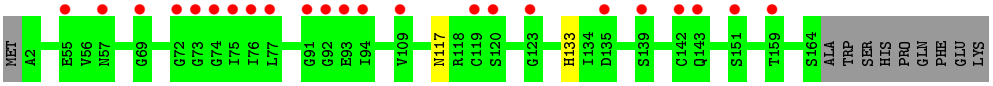




- Molecule 3: BPP

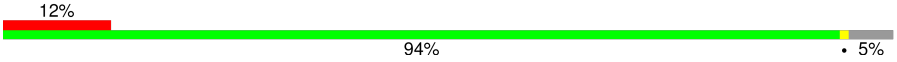
Chain Be:

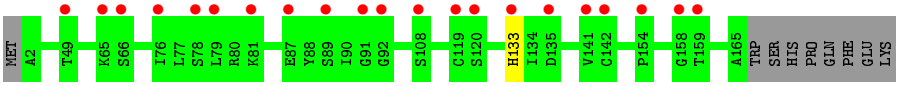




- Molecule 3: BPP

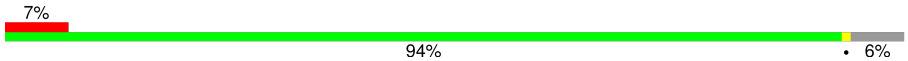
Chain Bf:

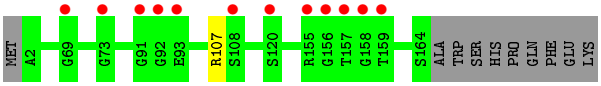




- Molecule 3: BPP

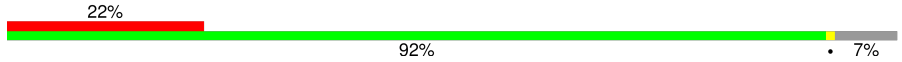
Chain Bg:

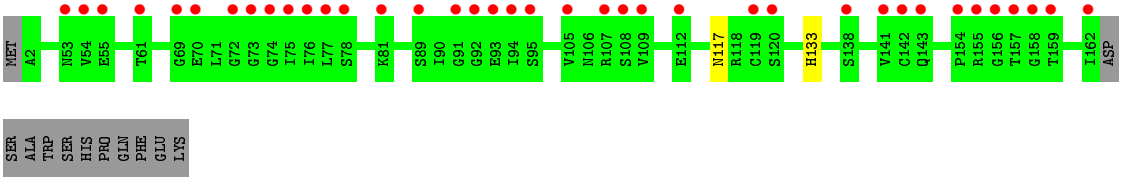




- Molecule 3: BPP

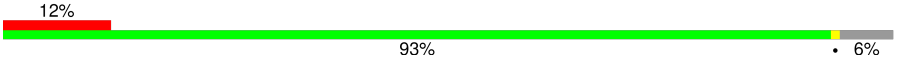
Chain Bh:

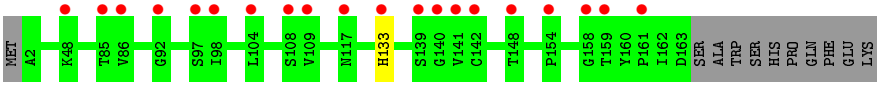




- Molecule 3: BPP

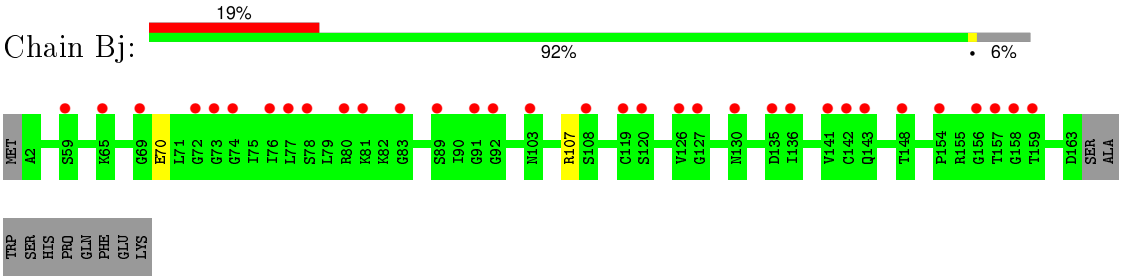
Chain Bi:





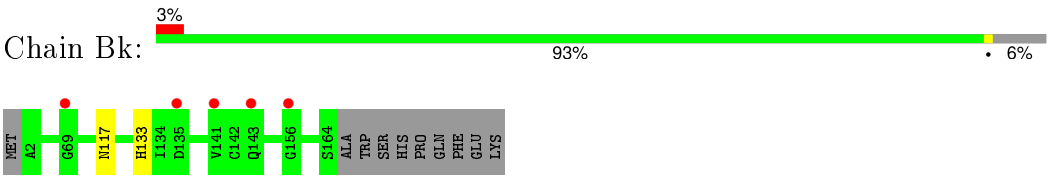
- Molecule 3: BPP

Chain Bj:



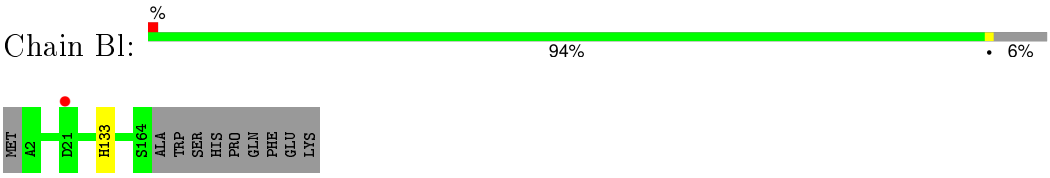
- Molecule 3: BPP

Chain Bk:



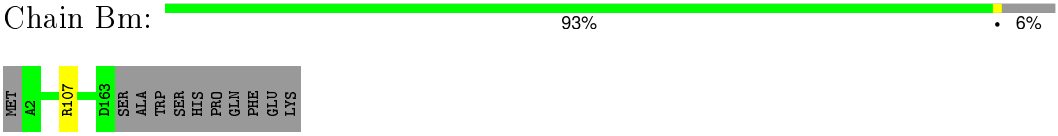
- Molecule 3: BPP

Chain Bl:



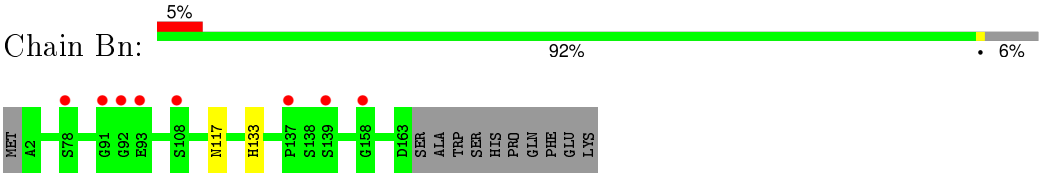
- Molecule 3: BPP

Chain Bm:



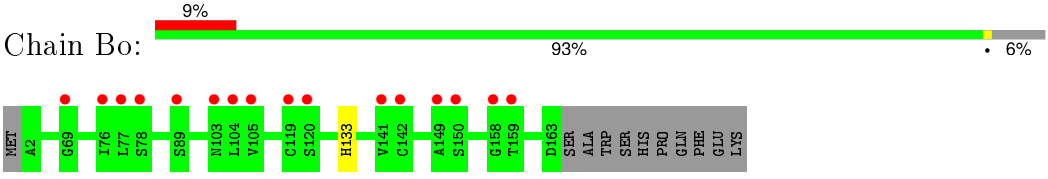
- Molecule 3: BPP

Chain Bn:



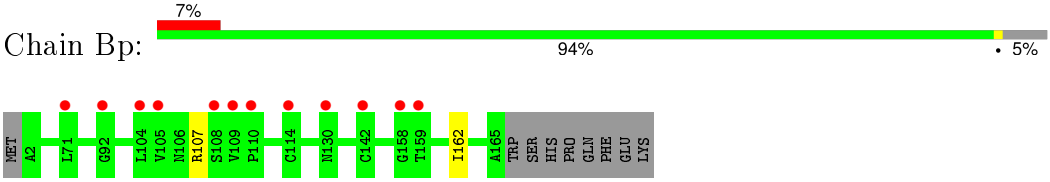
- Molecule 3: BPP

Chain Bo:



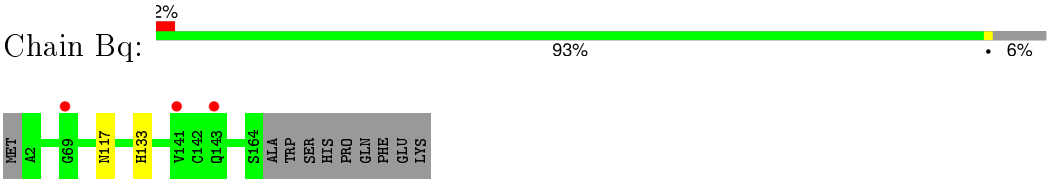
- Molecule 3: BPP

Chain Bp:



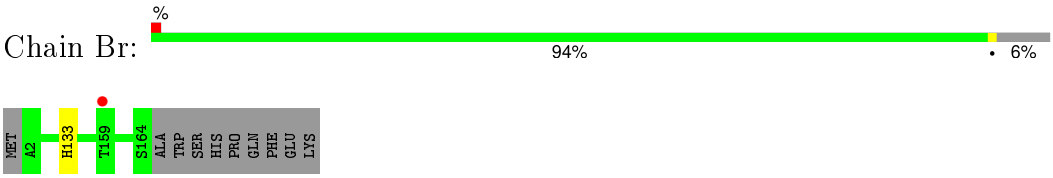
- Molecule 3: BPP

Chain Bq:



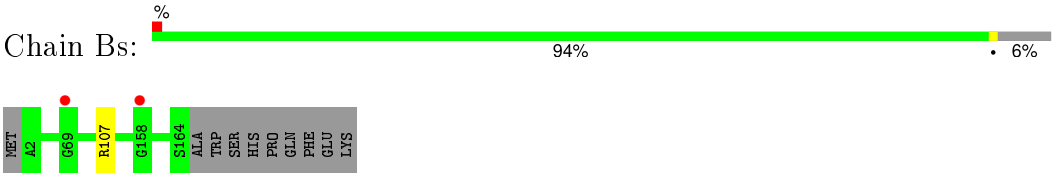
- Molecule 3: BPP

Chain Br:



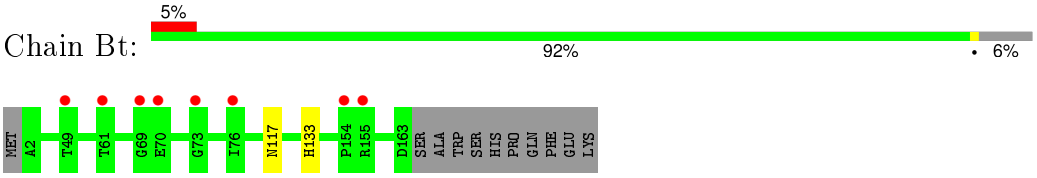
- Molecule 3: BPP

Chain Bs:



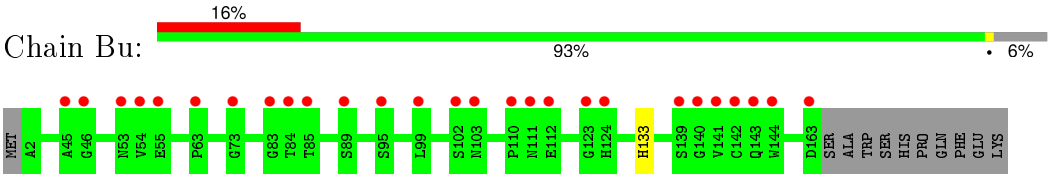
- Molecule 3: BPP

Chain Bt:



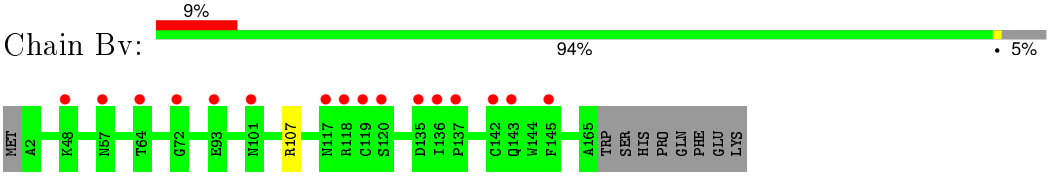
- Molecule 3: BPP

Chain Bu:



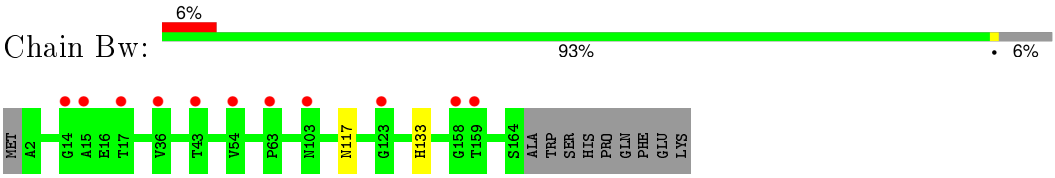
- Molecule 3: BPP

Chain Bv:



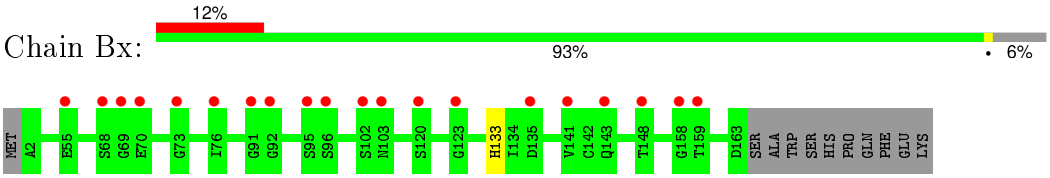
- Molecule 3: BPP

Chain Bw:



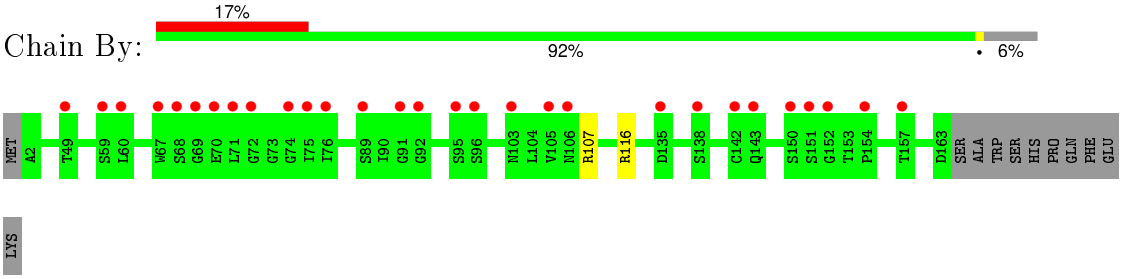
- Molecule 3: BPP

Chain Bx:



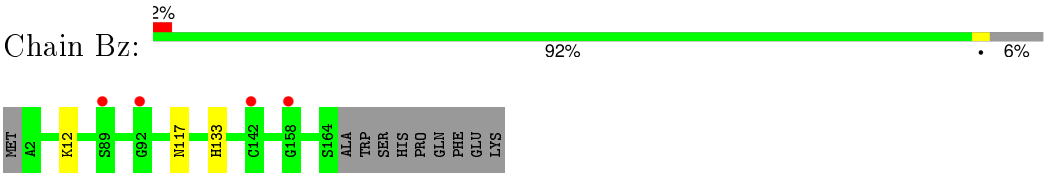
• Molecule 3: BPP

Chain By:



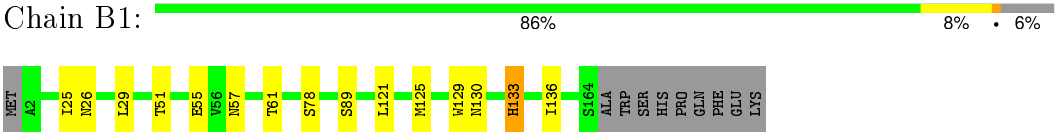
• Molecule 3: BPP

Chain Bz:



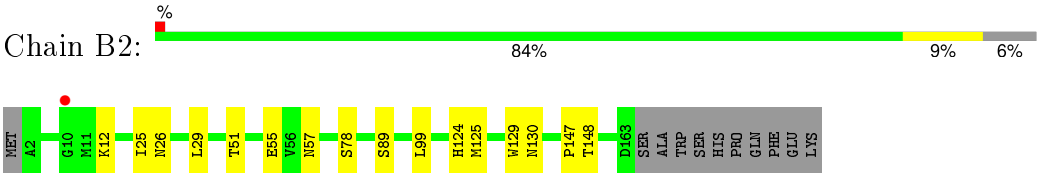
• Molecule 3: BPP

Chain B1:



• Molecule 3: BPP

Chain B2:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	163.53Å 287.36Å 323.14Å 90.00° 101.73° 90.00°	Depositor
Resolution (Å)	35.97 – 3.80 35.97 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (35.97-3.80) 99.5 (35.97-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 3.76Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.237 , 0.264 0.252 , 0.259	Depositor DCC
R_{free} test set	1422 reflections (0.50%)	DCC
Wilson B-factor (Å^2)	123.5	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 102.1	EDS
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 284701 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	118740	wwPDB-VP
Average B, all atoms (Å^2)	171.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	AA	0.49	0/2444	0.74	3/3307 (0.1%)
1	AB	0.46	0/2398	0.69	1/3243 (0.0%)
1	AC	0.49	0/2444	0.72	1/3306 (0.0%)
1	AD	0.40	0/2448	0.63	1/3311 (0.0%)
1	AE	0.41	0/2390	0.60	0/3233
1	AF	0.41	0/2444	0.62	0/3307
1	AG	0.41	0/2441	0.61	2/3302 (0.1%)
1	AH	0.41	0/2396	0.59	0/3242
1	AI	0.42	0/2444	0.62	0/3307
1	AJ	0.41	0/2448	0.62	1/3311 (0.0%)
1	AK	0.42	0/2373	0.61	2/3214 (0.1%)
1	AL	0.45	0/2437	0.66	0/3298
1	AM	0.42	0/2444	0.62	1/3307 (0.0%)
1	AN	0.42	0/2381	0.62	1/3223 (0.0%)
1	AO	0.44	0/2448	0.65	0/3311
1	AP	0.41	0/2437	0.60	0/3298
1	AQ	0.40	0/2401	0.59	0/3250
1	AR	0.43	0/2445	0.65	1/3307 (0.0%)
2	AS	0.46	0/1972	0.65	0/2669
2	AT	0.46	0/1972	0.66	1/2670 (0.0%)
2	AU	0.46	0/1965	0.66	0/2661
2	AV	0.44	0/1938	0.64	0/2625
2	AW	0.43	0/1957	0.64	0/2649
2	AX	0.45	0/1952	0.64	0/2643
3	B1	0.32	0/1222	0.49	0/1655
3	B2	0.36	0/1216	0.50	0/1647
3	BA	0.40	0/1221	0.61	0/1655
3	BB	0.42	0/1216	0.63	0/1648
3	BC	0.42	0/1216	0.63	0/1648
3	BD	0.36	0/1221	0.50	0/1655
3	BE	0.34	0/1221	0.49	0/1655
3	BF	0.34	0/1216	0.49	0/1648
3	BG	0.36	0/1221	0.51	0/1655
3	BH	0.36	0/1227	0.50	0/1662

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
3	BI	0.34	0/1216	0.49	0/1648
3	BJ	0.36	0/1221	0.51	0/1655
3	BK	0.34	0/1216	0.48	0/1648
3	BL	0.36	0/1216	0.50	0/1648
3	BM	0.35	0/1216	0.50	0/1648
3	BN	0.36	0/1210	0.50	0/1640
3	BO	0.36	0/1210	0.53	1/1640 (0.1%)
3	BP	0.36	0/1216	0.49	0/1648
3	BQ	0.35	0/1216	0.48	0/1647
3	BR	0.35	0/1216	0.48	0/1648
3	BS	0.34	0/1216	0.48	0/1648
3	BT	0.35	0/1221	0.49	0/1655
3	BU	0.35	0/1221	0.48	0/1655
3	BV	0.38	0/1216	0.55	1/1648 (0.1%)
3	BW	0.36	0/1221	0.50	0/1655
3	BX	0.35	0/1210	0.58	2/1640 (0.1%)
3	BY	0.35	0/1216	0.49	0/1648
3	BZ	0.34	0/1216	0.49	0/1648
3	Ba	0.34	0/1216	0.49	0/1647
3	Bb	0.35	0/1216	0.48	0/1648
3	Bc	0.34	0/1220	0.48	0/1654
3	Bd	0.35	0/1231	0.50	0/1668
3	Be	0.35	0/1216	0.48	0/1648
3	Bf	0.35	0/1221	0.48	0/1655
3	Bg	0.34	0/1216	0.49	0/1648
3	Bh	0.35	0/1208	0.49	0/1636
3	Bi	0.34	0/1210	0.49	0/1640
3	Bj	0.35	0/1216	0.49	0/1647
3	Bk	0.34	0/1216	0.48	0/1648
3	Bl	0.34	0/1216	0.48	0/1648
3	Bm	0.36	0/1210	0.49	0/1640
3	Bn	0.35	0/1216	0.48	0/1647
3	Bo	0.34	0/1216	0.48	0/1647
3	Bp	0.35	0/1227	0.49	0/1662
3	Bq	0.35	0/1222	0.49	0/1655
3	Br	0.35	0/1216	0.50	0/1648
3	Bs	0.36	0/1216	0.50	0/1648
3	Bt	0.36	0/1210	0.49	0/1640
3	Bu	0.36	0/1216	0.49	0/1647
3	Bv	0.35	0/1221	0.49	0/1655
3	Bw	0.35	0/1216	0.48	0/1648
3	Bx	0.34	0/1216	0.48	0/1647
3	By	0.34	0/1216	0.48	0/1647

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
3	Bz	0.33	0/1222	0.49	0/1655
All	All	0.39	0/121148	0.57	19/164062 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	BV	0	1

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	BX	163	ASP	N-CA-CB	-8.21	95.81	110.60
1	AR	179	ALA	CB-CA-C	7.90	121.95	110.10
3	BV	162	ILE	CB-CA-C	7.86	127.31	111.60
3	BX	162	ILE	CB-CA-C	7.70	126.99	111.60
1	AJ	83	ALA	CB-CA-C	7.48	121.31	110.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	BV	162	ILE	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	2389	0	2333	57	0
1	AB	2345	0	2295	35	0
1	AC	2389	0	2340	46	0
1	AD	2393	0	2344	30	0
1	AE	2336	0	2292	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AF	2389	0	2333	26	0
1	AG	2386	0	2338	31	0
1	AH	2343	0	2280	24	0
1	AI	2389	0	2333	34	0
1	AJ	2393	0	2344	29	0
1	AK	2320	0	2246	36	0
1	AL	2382	0	2330	38	0
1	AM	2389	0	2333	23	0
1	AN	2328	0	2253	28	0
1	AO	2393	0	2344	29	0
1	AP	2382	0	2327	31	0
1	AQ	2347	0	2281	20	0
1	AR	2390	0	2335	38	0
2	AS	1932	0	1882	30	0
2	AT	1931	0	1886	17	0
2	AU	1924	0	1879	19	0
2	AV	1899	0	1836	17	0
2	AW	1917	0	1865	31	0
2	AX	1913	0	1867	22	0
3	B1	1200	0	1182	14	0
3	B2	1194	0	1177	15	0
3	BA	1199	0	1176	36	0
3	BB	1194	0	1171	32	0
3	BC	1194	0	1171	37	0
3	BD	1199	0	1176	30	0
3	BE	1199	0	1176	25	0
3	BF	1194	0	1171	25	0
3	BG	1199	0	1176	29	0
3	BH	1205	0	1187	23	0
3	BI	1194	0	1171	31	0
3	BJ	1199	0	1176	28	0
3	BK	1194	0	1171	20	0
3	BL	1194	0	1171	20	0
3	BM	1194	0	1171	23	0
3	BN	1188	0	1166	22	0
3	BO	1188	0	1166	25	0
3	BP	1194	0	1171	35	0
3	BQ	1194	0	1177	22	0
3	BR	1194	0	1171	24	0
3	BS	1194	0	1171	28	0
3	BT	1199	0	1176	24	0
3	BU	1199	0	1176	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	BV	1194	0	1170	25	0
3	BW	1199	0	1176	22	0
3	BX	1188	0	1166	23	0
3	BY	1194	0	1171	24	0
3	BZ	1194	0	1171	29	0
3	Ba	1194	0	1177	0	0
3	Bb	1194	0	1171	0	0
3	Bc	1198	0	1173	0	0
3	Bd	1209	0	1186	0	0
3	Be	1194	0	1171	0	0
3	Bf	1199	0	1176	0	0
3	Bg	1194	0	1171	0	0
3	Bh	1186	0	1173	0	0
3	Bi	1188	0	1166	0	0
3	Bj	1194	0	1177	0	0
3	Bk	1194	0	1171	0	0
3	Bl	1194	0	1171	0	0
3	Bm	1188	0	1166	0	0
3	Bn	1194	0	1177	0	0
3	Bo	1194	0	1177	0	0
3	Bp	1205	0	1187	0	0
3	Bq	1200	0	1182	0	0
3	Br	1194	0	1171	0	0
3	Bs	1194	0	1171	0	0
3	Bt	1188	0	1166	0	0
3	Bu	1194	0	1177	0	0
3	Bv	1199	0	1176	0	0
3	Bw	1194	0	1171	0	0
3	Bx	1194	0	1177	0	0
3	By	1194	0	1177	0	0
3	Bz	1200	0	1182	0	0
All	All	118740	0	116287	1033	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 4.

The worst 5 of 1033 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:AI:108:TRP:CZ2	1:AK:125:ILE:HD11	1.37	1.59
2:AW:127:VAL:HG23	2:AW:134:ILE:CD1	1.44	1.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AI:108:TRP:CH2	1:AK:125:ILE:HD11	1.73	1.22
1:AI:108:TRP:CZ2	1:AK:125:ILE:CD1	2.29	1.15
2:AW:127:VAL:CG2	2:AW:134:ILE:CD1	2.27	1.11

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 X-ray entries followed by that with respect to entries of similar resolution.

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	AA	297/299 (99%)	284 (96%)	11 (4%)	2 (1%)	26 72
1	AB	290/299 (97%)	273 (94%)	17 (6%)	0	100 100
1	AC	297/299 (99%)	274 (92%)	23 (8%)	0	100 100
1	AD	297/299 (99%)	276 (93%)	19 (6%)	2 (1%)	26 72
1	AE	287/299 (96%)	268 (93%)	19 (7%)	0	100 100
1	AF	297/299 (99%)	277 (93%)	19 (6%)	1 (0%)	46 83
1	AG	297/299 (99%)	278 (94%)	14 (5%)	5 (2%)	11 56
1	AH	290/299 (97%)	271 (93%)	18 (6%)	1 (0%)	46 83
1	AI	297/299 (99%)	275 (93%)	20 (7%)	2 (1%)	26 72
1	AJ	297/299 (99%)	275 (93%)	20 (7%)	2 (1%)	26 72
1	AK	289/299 (97%)	270 (93%)	19 (7%)	0	100 100
1	AL	296/299 (99%)	276 (93%)	19 (6%)	1 (0%)	46 83
1	AM	297/299 (99%)	276 (93%)	19 (6%)	2 (1%)	26 72
1	AN	290/299 (97%)	270 (93%)	20 (7%)	0	100 100
1	AO	297/299 (99%)	276 (93%)	20 (7%)	1 (0%)	46 83
1	AP	297/299 (99%)	281 (95%)	13 (4%)	3 (1%)	19 66
1	AQ	291/299 (97%)	269 (92%)	21 (7%)	1 (0%)	46 83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AR	297/299 (99%)	277 (93%)	17 (6%)	3 (1%)	19	66
2	AS	240/253 (95%)	215 (90%)	24 (10%)	1 (0%)	39	80
2	AT	240/253 (95%)	218 (91%)	22 (9%)	0	100	100
2	AU	240/253 (95%)	215 (90%)	25 (10%)	0	100	100
2	AV	239/253 (94%)	217 (91%)	22 (9%)	0	100	100
2	AW	239/253 (94%)	217 (91%)	22 (9%)	0	100	100
2	AX	239/253 (94%)	217 (91%)	22 (9%)	0	100	100
3	B1	161/173 (93%)	157 (98%)	4 (2%)	0	100	100
3	B2	160/173 (92%)	154 (96%)	6 (4%)	0	100	100
3	BA	162/173 (94%)	159 (98%)	3 (2%)	0	100	100
3	BB	161/173 (93%)	158 (98%)	3 (2%)	0	100	100
3	BC	161/173 (93%)	158 (98%)	3 (2%)	0	100	100
3	BD	162/173 (94%)	154 (95%)	8 (5%)	0	100	100
3	BE	162/173 (94%)	157 (97%)	5 (3%)	0	100	100
3	BF	161/173 (93%)	155 (96%)	6 (4%)	0	100	100
3	BG	162/173 (94%)	155 (96%)	7 (4%)	0	100	100
3	BH	162/173 (94%)	157 (97%)	5 (3%)	0	100	100
3	BI	161/173 (93%)	154 (96%)	7 (4%)	0	100	100
3	BJ	162/173 (94%)	156 (96%)	6 (4%)	0	100	100
3	BK	161/173 (93%)	157 (98%)	4 (2%)	0	100	100
3	BL	161/173 (93%)	154 (96%)	7 (4%)	0	100	100
3	BM	161/173 (93%)	155 (96%)	6 (4%)	0	100	100
3	BN	160/173 (92%)	156 (98%)	4 (2%)	0	100	100
3	BO	160/173 (92%)	153 (96%)	7 (4%)	0	100	100
3	BP	161/173 (93%)	154 (96%)	7 (4%)	0	100	100
3	BQ	160/173 (92%)	156 (98%)	4 (2%)	0	100	100
3	BR	161/173 (93%)	154 (96%)	7 (4%)	0	100	100
3	BS	161/173 (93%)	156 (97%)	5 (3%)	0	100	100
3	BT	162/173 (94%)	157 (97%)	5 (3%)	0	100	100
3	BU	162/173 (94%)	154 (95%)	8 (5%)	0	100	100
3	BV	161/173 (93%)	155 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	BW	162/173 (94%)	157 (97%)	5 (3%)	0	100	100
3	BX	160/173 (92%)	153 (96%)	7 (4%)	0	100	100
3	BY	161/173 (93%)	155 (96%)	6 (4%)	0	100	100
3	BZ	161/173 (93%)	157 (98%)	4 (2%)	0	100	100
3	Ba	160/173 (92%)	151 (94%)	9 (6%)	0	100	100
3	Bb	161/173 (93%)	155 (96%)	6 (4%)	0	100	100
3	Bc	162/173 (94%)	158 (98%)	4 (2%)	0	100	100
3	Bd	163/173 (94%)	155 (95%)	8 (5%)	0	100	100
3	Be	161/173 (93%)	155 (96%)	6 (4%)	0	100	100
3	Bf	162/173 (94%)	157 (97%)	5 (3%)	0	100	100
3	Bg	161/173 (93%)	154 (96%)	7 (4%)	0	100	100
3	Bh	159/173 (92%)	154 (97%)	5 (3%)	0	100	100
3	Bi	160/173 (92%)	156 (98%)	4 (2%)	0	100	100
3	Bj	160/173 (92%)	155 (97%)	5 (3%)	0	100	100
3	Bk	161/173 (93%)	155 (96%)	6 (4%)	0	100	100
3	Bl	161/173 (93%)	157 (98%)	4 (2%)	0	100	100
3	Bm	160/173 (92%)	154 (96%)	6 (4%)	0	100	100
3	Bn	160/173 (92%)	154 (96%)	6 (4%)	0	100	100
3	Bo	160/173 (92%)	156 (98%)	4 (2%)	0	100	100
3	Bp	162/173 (94%)	154 (95%)	8 (5%)	0	100	100
3	Bq	161/173 (93%)	155 (96%)	6 (4%)	0	100	100
3	Br	161/173 (93%)	157 (98%)	4 (2%)	0	100	100
3	Bs	161/173 (93%)	154 (96%)	7 (4%)	0	100	100
3	Bt	160/173 (92%)	154 (96%)	6 (4%)	0	100	100
3	Bu	160/173 (92%)	156 (98%)	4 (2%)	0	100	100
3	Bv	162/173 (94%)	154 (95%)	8 (5%)	0	100	100
3	Bw	161/173 (93%)	155 (96%)	6 (4%)	0	100	100
3	Bx	160/173 (92%)	156 (98%)	4 (2%)	0	100	100
3	By	160/173 (92%)	153 (96%)	7 (4%)	0	100	100
3	Bz	161/173 (93%)	155 (96%)	6 (4%)	0	100	100
All	All	15429/16242 (95%)	14631 (95%)	771 (5%)	27 (0%)	52	86

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AF	269	ASP
1	AA	175	GLY
1	AM	175	GLY
1	AD	27	VAL
1	AG	27	VAL

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 X-ray entries followed by that with respect to entries of similar resolution.

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	AA	260/261 (100%)	245 (94%)	15 (6%)	25 66
1	AB	255/261 (98%)	244 (96%)	11 (4%)	35 74
1	AC	260/261 (100%)	247 (95%)	13 (5%)	30 70
1	AD	261/261 (100%)	247 (95%)	14 (5%)	27 68
1	AE	256/261 (98%)	250 (98%)	6 (2%)	58 84
1	AF	260/261 (100%)	251 (96%)	9 (4%)	43 78
1	AG	259/261 (99%)	249 (96%)	10 (4%)	39 75
1	AH	254/261 (97%)	242 (95%)	12 (5%)	32 72
1	AI	260/261 (100%)	245 (94%)	15 (6%)	25 66
1	AJ	261/261 (100%)	247 (95%)	14 (5%)	27 68
1	AK	250/261 (96%)	239 (96%)	11 (4%)	35 73
1	AL	259/261 (99%)	246 (95%)	13 (5%)	30 70
1	AM	260/261 (100%)	249 (96%)	11 (4%)	36 74
1	AN	250/261 (96%)	238 (95%)	12 (5%)	31 71
1	AO	261/261 (100%)	250 (96%)	11 (4%)	36 74
1	AP	258/261 (99%)	242 (94%)	16 (6%)	23 64
1	AQ	254/261 (97%)	244 (96%)	10 (4%)	39 75
1	AR	260/261 (100%)	253 (97%)	7 (3%)	52 82
2	AS	212/229 (93%)	205 (97%)	7 (3%)	45 79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AT	212/229 (93%)	200 (94%)	12 (6%)	25	67
2	AU	209/229 (91%)	202 (97%)	7 (3%)	45	79
2	AV	204/229 (89%)	196 (96%)	8 (4%)	39	75
2	AW	209/229 (91%)	203 (97%)	6 (3%)	50	81
2	AX	209/229 (91%)	197 (94%)	12 (6%)	25	67
3	B1	133/142 (94%)	132 (99%)	1 (1%)	86	94
3	B2	132/142 (93%)	131 (99%)	1 (1%)	86	94
3	BA	132/142 (93%)	127 (96%)	5 (4%)	40	76
3	BB	132/142 (93%)	126 (96%)	6 (4%)	34	73
3	BC	132/142 (93%)	124 (94%)	8 (6%)	23	65
3	BD	132/142 (93%)	129 (98%)	3 (2%)	58	84
3	BE	132/142 (93%)	131 (99%)	1 (1%)	86	94
3	BF	132/142 (93%)	131 (99%)	1 (1%)	86	94
3	BG	132/142 (93%)	129 (98%)	3 (2%)	58	84
3	BH	133/142 (94%)	131 (98%)	2 (2%)	72	90
3	BI	132/142 (93%)	131 (99%)	1 (1%)	86	94
3	BJ	132/142 (93%)	130 (98%)	2 (2%)	72	90
3	BK	132/142 (93%)	131 (99%)	1 (1%)	86	94
3	BL	132/142 (93%)	131 (99%)	1 (1%)	86	94
3	BM	132/142 (93%)	130 (98%)	2 (2%)	72	90
3	BN	131/142 (92%)	128 (98%)	3 (2%)	58	84
3	BO	131/142 (92%)	129 (98%)	2 (2%)	72	90
3	BP	132/142 (93%)	130 (98%)	2 (2%)	72	90
3	BQ	132/142 (93%)	131 (99%)	1 (1%)	86	94
3	BR	132/142 (93%)	131 (99%)	1 (1%)	86	94
3	BS	132/142 (93%)	130 (98%)	2 (2%)	72	90
3	BT	132/142 (93%)	131 (99%)	1 (1%)	86	94
3	BU	132/142 (93%)	131 (99%)	1 (1%)	86	94
3	BV	132/142 (93%)	129 (98%)	3 (2%)	58	84
3	BW	132/142 (93%)	130 (98%)	2 (2%)	72	90
3	BX	131/142 (92%)	131 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	BY	132/142 (93%)	128 (97%)	4 (3%)	48	80
3	BZ	132/142 (93%)	130 (98%)	2 (2%)	72	90
3	Ba	132/142 (93%)	131 (99%)	1 (1%)	86	94
3	Bb	132/142 (93%)	130 (98%)	2 (2%)	72	90
3	Bc	131/142 (92%)	130 (99%)	1 (1%)	86	94
3	Bd	132/142 (93%)	130 (98%)	2 (2%)	72	90
3	Be	132/142 (93%)	130 (98%)	2 (2%)	72	90
3	Bf	132/142 (93%)	131 (99%)	1 (1%)	86	94
3	Bg	132/142 (93%)	131 (99%)	1 (1%)	86	94
3	Bh	131/142 (92%)	129 (98%)	2 (2%)	72	90
3	Bi	131/142 (92%)	130 (99%)	1 (1%)	86	94
3	Bj	132/142 (93%)	130 (98%)	2 (2%)	72	90
3	Bk	132/142 (93%)	130 (98%)	2 (2%)	72	90
3	Bl	132/142 (93%)	131 (99%)	1 (1%)	86	94
3	Bm	131/142 (92%)	130 (99%)	1 (1%)	86	94
3	Bn	132/142 (93%)	130 (98%)	2 (2%)	72	90
3	Bo	132/142 (93%)	131 (99%)	1 (1%)	86	94
3	Bp	133/142 (94%)	131 (98%)	2 (2%)	72	90
3	Bq	133/142 (94%)	131 (98%)	2 (2%)	72	90
3	Br	132/142 (93%)	131 (99%)	1 (1%)	86	94
3	Bs	132/142 (93%)	131 (99%)	1 (1%)	86	94
3	Bt	131/142 (92%)	129 (98%)	2 (2%)	72	90
3	Bu	132/142 (93%)	131 (99%)	1 (1%)	86	94
3	Bv	132/142 (93%)	131 (99%)	1 (1%)	86	94
3	Bw	132/142 (93%)	130 (98%)	2 (2%)	72	90
3	Bx	132/142 (93%)	131 (99%)	1 (1%)	86	94
3	By	132/142 (93%)	130 (98%)	2 (2%)	72	90
3	Bz	133/142 (94%)	130 (98%)	3 (2%)	58	84
All	All	13018/13740 (95%)	12654 (97%)	364 (3%)	51	81

5 of 364 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AN	224	ASP
1	AR	2	THR
3	Bj	107	ARG
1	AO	116	THR
1	AP	134	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 243 such sidechains are listed below:

Mol	Chain	Res	Type
3	BK	19	ASN
3	BT	19	ASN
3	Bw	19	ASN
3	BL	103	ASN
3	BO	133	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	AA	299/299 (100%)	-0.36	1 (0%) 94 89	84, 119, 162, 188	0
1	AB	294/299 (98%)	-0.10	9 (3%) 52 36	94, 149, 206, 237	0
1	AC	299/299 (100%)	-0.29	0 100 100	95, 124, 160, 180	0
1	AD	299/299 (100%)	-0.36	0 100 100	86, 128, 175, 206	0
1	AE	291/299 (97%)	-0.07	6 (2%) 67 51	89, 159, 213, 249	0
1	AF	299/299 (100%)	-0.28	2 (0%) 89 80	90, 132, 167, 183	0
1	AG	299/299 (100%)	-0.35	2 (0%) 89 80	95, 133, 180, 203	0
1	AH	294/299 (98%)	-0.11	6 (2%) 68 53	103, 176, 237, 261	0
1	AI	299/299 (100%)	-0.30	0 100 100	94, 135, 163, 180	0
1	AJ	299/299 (100%)	-0.38	0 100 100	88, 121, 160, 183	0
1	AK	293/299 (97%)	-0.13	8 (2%) 58 42	94, 140, 229, 255	0
1	AL	298/299 (99%)	-0.33	2 (0%) 89 80	92, 122, 157, 172	0
1	AM	299/299 (100%)	-0.28	2 (0%) 89 80	85, 124, 188, 230	0
1	AN	294/299 (98%)	0.04	11 (3%) 45 30	92, 156, 235, 269	0
1	AO	299/299 (100%)	-0.30	1 (0%) 94 89	91, 129, 164, 182	0
1	AP	299/299 (100%)	-0.36	0 100 100	92, 129, 171, 193	0
1	AQ	295/299 (98%)	-0.17	1 (0%) 94 89	111, 172, 217, 240	0
1	AR	299/299 (100%)	-0.18	2 (0%) 89 80	95, 138, 197, 218	0
2	AS	242/253 (95%)	-0.40	1 (0%) 93 87	84, 124, 195, 234	0
2	AT	242/253 (95%)	-0.37	2 (0%) 87 77	88, 122, 191, 233	0
2	AU	242/253 (95%)	-0.41	1 (0%) 93 87	83, 121, 188, 235	0
2	AV	241/253 (95%)	-0.40	0 100 100	82, 125, 205, 257	0
2	AW	241/253 (95%)	-0.32	0 100 100	83, 125, 200, 246	0
2	AX	241/253 (95%)	-0.40	1 (0%) 93 87	86, 119, 192, 232	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
3	B1	163/173 (94%)	-0.17	0 100 100	134, 174, 213, 233	0
3	B2	162/173 (93%)	-0.27	1 (0%) 90 82	106, 137, 159, 179	0
3	BA	164/173 (94%)	0.26	9 (5%) 29 19	103, 260, 278, 283	0
3	BB	163/173 (94%)	0.45	17 (10%) 8 6	112, 254, 272, 279	0
3	BC	163/173 (94%)	0.43	19 (11%) 6 5	113, 261, 278, 280	0
3	BD	164/173 (94%)	-0.25	2 (1%) 81 67	112, 160, 181, 206	0
3	BE	164/173 (94%)	-0.27	0 100 100	112, 157, 189, 219	0
3	BF	163/173 (94%)	-0.10	5 (3%) 52 36	118, 183, 239, 258	0
3	BG	164/173 (94%)	-0.19	5 (3%) 54 37	97, 159, 203, 216	0
3	BH	164/173 (94%)	-0.11	3 (1%) 71 56	102, 148, 177, 214	0
3	BI	163/173 (94%)	-0.07	5 (3%) 52 36	99, 177, 221, 229	0
3	BJ	164/173 (94%)	-0.03	2 (1%) 81 67	106, 179, 218, 232	0
3	BK	163/173 (94%)	-0.11	3 (1%) 71 56	107, 171, 210, 235	0
3	BL	163/173 (94%)	-0.06	4 (2%) 61 44	116, 190, 228, 239	0
3	BM	163/173 (94%)	1.10	35 (21%) 1 1	133, 280, 292, 295	0
3	BN	162/173 (93%)	0.88	34 (20%) 1 1	149, 265, 278, 282	0
3	BO	162/173 (93%)	1.15	35 (21%) 1 1	147, 276, 292, 295	0
3	BP	163/173 (94%)	0.84	29 (17%) 2 2	162, 274, 286, 288	0
3	BQ	162/173 (93%)	0.93	27 (16%) 2 2	176, 241, 272, 278	0
3	BR	163/173 (94%)	0.91	31 (19%) 2 1	179, 271, 290, 294	0
3	BS	163/173 (94%)	-0.00	2 (1%) 81 67	163, 198, 224, 233	0
3	BT	164/173 (94%)	-0.03	2 (1%) 81 67	149, 196, 218, 227	0
3	BU	164/173 (94%)	0.15	8 (4%) 33 22	148, 204, 241, 256	0
3	BV	163/173 (94%)	-0.36	1 (0%) 90 82	125, 150, 191, 214	0
3	BW	164/173 (94%)	-0.24	1 (0%) 90 82	121, 146, 163, 187	0
3	BX	162/173 (93%)	-0.25	1 (0%) 90 82	118, 143, 179, 200	0
3	BY	163/173 (94%)	-0.25	0 100 100	127, 154, 182, 202	0
3	BZ	163/173 (94%)	-0.23	1 (0%) 90 82	116, 151, 180, 209	0
3	Ba	162/173 (93%)	-0.24	0 100 100	124, 148, 179, 196	0
3	Bb	163/173 (94%)	-0.10	3 (1%) 71 56	144, 200, 239, 255	0
3	Bc	164/173 (94%)	-0.20	2 (1%) 81 67	119, 196, 228, 240	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
3	Bd	165/173 (95%)	-0.03	3 (1%) 71 56	120, 187, 209, 215	0
3	Be	163/173 (94%)	0.57	23 (14%) 4 3	128, 282, 288, 291	0
3	Bf	164/173 (94%)	0.55	21 (12%) 5 4	107, 277, 289, 291	0
3	Bg	163/173 (94%)	0.38	12 (7%) 17 11	109, 273, 286, 288	0
3	Bh	161/173 (93%)	1.11	38 (23%) 1 1	194, 259, 275, 278	0
3	Bi	162/173 (93%)	0.61	20 (12%) 5 5	164, 256, 274, 276	0
3	Bj	162/173 (93%)	1.03	33 (20%) 1 1	181, 259, 276, 278	0
3	Bk	163/173 (94%)	0.04	5 (3%) 52 36	160, 187, 214, 231	0
3	Bl	163/173 (94%)	-0.09	1 (0%) 90 82	161, 184, 203, 232	0
3	Bm	162/173 (93%)	-0.07	0 100 100	156, 181, 202, 213	0
3	Bn	162/173 (93%)	0.28	8 (4%) 33 22	146, 208, 256, 274	0
3	Bo	162/173 (93%)	0.32	16 (9%) 9 6	142, 203, 230, 238	0
3	Bp	164/173 (94%)	0.31	12 (7%) 18 11	133, 210, 240, 252	0
3	Bq	163/173 (94%)	-0.02	3 (1%) 71 56	108, 192, 220, 232	0
3	Br	163/173 (94%)	-0.07	1 (0%) 90 82	100, 172, 207, 237	0
3	Bs	163/173 (94%)	-0.08	2 (1%) 81 67	99, 168, 208, 227	0
3	Bt	162/173 (93%)	0.41	8 (4%) 33 22	146, 213, 232, 257	0
3	Bu	162/173 (93%)	0.63	27 (16%) 2 2	138, 239, 271, 275	0
3	Bv	164/173 (94%)	0.61	16 (9%) 10 6	128, 225, 251, 257	0
3	Bw	163/173 (94%)	0.53	11 (6%) 21 12	182, 216, 245, 253	0
3	Bx	162/173 (93%)	0.59	20 (12%) 5 5	203, 239, 274, 280	0
3	By	162/173 (93%)	0.81	29 (17%) 2 2	195, 252, 267, 272	0
3	Bz	163/173 (94%)	-0.12	4 (2%) 61 44	130, 170, 232, 238	0
All	All	15597/16242 (96%)	0.01	658 (4%) 40 26	82, 163, 274, 295	0

The worst 5 of 658 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	BQ	135	ASP	13.7
3	BO	91	GLY	13.5
3	BR	69	GLY	12.6
3	BO	92	GLY	11.4
3	BQ	120	SER	9.8

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.