



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 22, 2024 – 08:18 AM EST

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 Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

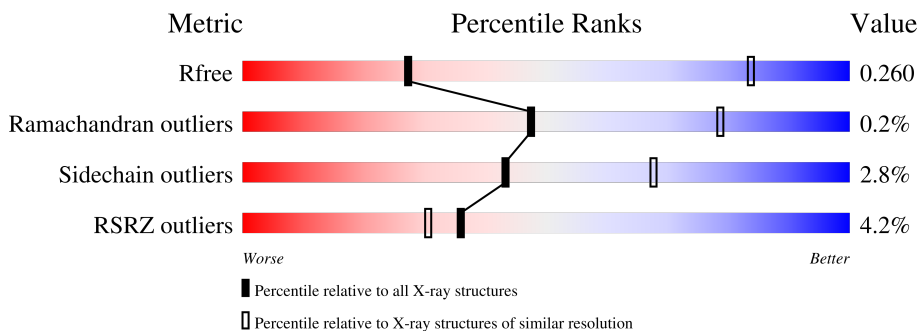
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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}	130704	1212 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	299	93% 7%
1	AB	299	3% 94% . .
1	AC	299	95% 5%
1	AD	299	94% 6%
1	AE	299	3% 95% . .
1	AF	299	% 97% .

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Mol	Chain	Length	Quality of chain
1	AG	299	94% 6%
1	AH	299	94% ..
1	AI	299	94% 6%
1	AJ	299	94% 6%
1	AK	299	94% ..
1	AL	299	95% 5%
1	AM	299	96% .
1	AN	299	94% ..
1	AO	299	96% .
1	AP	299	94% 6%
1	AQ	299	95% ..
1	AR	299	96% .
2	AS	253	92% ..
2	AT	253	91% 5% .
2	AU	253	93% ..
2	AV	253	92% . 5%
2	AW	253	93% . 5%
2	AX	253	91% 5% 5%
3	B1	173	94% . 6%
3	B2	173	93% . 6%
3	BA	173	92% . 5%
3	BB	173	91% . 6%
3	BC	173	90% 5% 6%
3	BD	173	93% . 5%
3	BE	173	94% . 5%

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Mol	Chain	Length	Quality of chain
3	BF	173	 2% 94% 6%
3	BG	173	 3% 93% 5%
3	BH	173	 2% 94% 5%
3	BI	173	 3% 94% 6%
3	BJ	173	 % 94% 5%
3	BK	173	 2% 94% 6%
3	BL	173	 3% 94% 6%
3	BM	173	 21% 93% 6%
3	BN	173	 20% 92% 6%
3	BO	173	 19% 92% 6%
3	BP	173	 18% 93% 6%
3	BQ	173	 14% 93% 6%
3	BR	173	 17% 94% 6%
3	BS	173	 % 93% 6%
3	BT	173	 % 94% 5%
3	BU	173	 5% 94% 5%
3	BV	173	 % 92% 6%
3	BW	173	 % 94% 5%
3	BX	173	 % 92% 6%
3	BY	173	 % 92% 6%
3	BZ	173	 % 93% 6%
3	Ba	173	 % 93% 6%
3	Bb	173	 2% 93% 6%
3	Bc	173	 % 94% 5%
3	Bd	173	 % 94% 5%

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Mol	Chain	Length	Quality of chain
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	18% 92% • 6%
3	Bk	173	2% 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	6% 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	15% 93% • 6%
3	Bv	173	10% 94% • 5%
3	Bw	173	6% 93% • 6%
3	Bx	173	12% 93% • 6%
3	By	173	16% 92% • 6%
3	Bz	173	3% 92% • 6%

2 Entry composition

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

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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			

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

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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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

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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, 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 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.

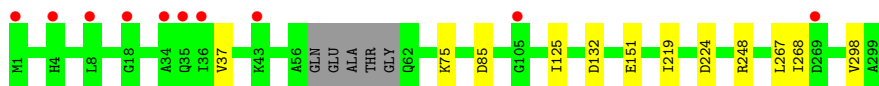
- Molecule 1: ORF48

Chain AA:  93% 7%



- Molecule 1: ORF48

Chain AB:  94% 3% 3%



- Molecule 1: ORF48

Chain AC:  95% 5%



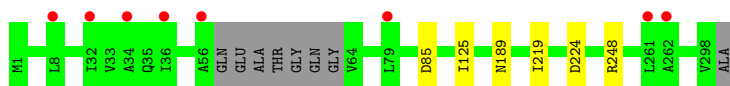
- Molecule 1: ORF48

Chain AD:  94% 6%



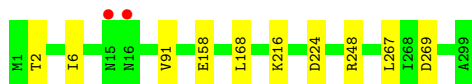
- Molecule 1: ORF48

Chain AE:  95% 3% 2%



- Molecule 1: ORF48

Chain AF:  97% 3%



• Molecule 1: ORF48



• Molecule 1: ORF48



• Molecule 1: ORF48



• Molecule 1: ORF48



• Molecule 1: ORF48



• Molecule 1: ORF48

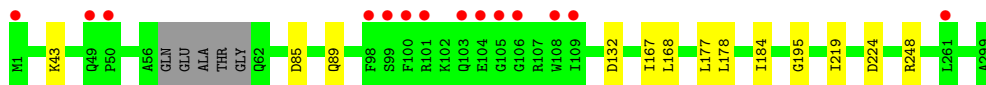


• Molecule 1: ORF48





- Molecule 1: ORF48



- Molecule 1: ORF48



- Molecule 1: ORF48



- Molecule 1: ORF48



- Molecule 1: ORF48



- Molecule 2: ORF46

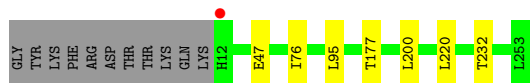


- Molecule 2: ORF46





● Molecule 2: ORF46



● Molecule 2: ORF46



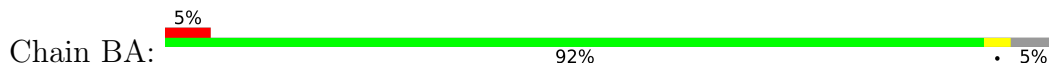
● Molecule 2: ORF46



● Molecule 2: ORF46



● Molecule 3: BPP

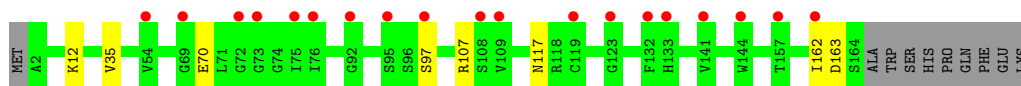


● Molecule 3: BPP



● Molecule 3: BPP





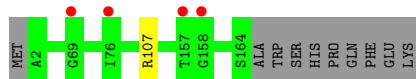
• Molecule 3: BPP



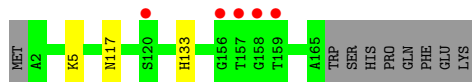
• Molecule 3: BPP



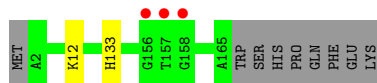
• Molecule 3: BPP



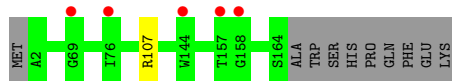
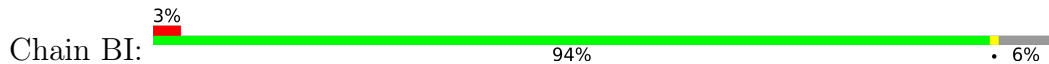
• Molecule 3: BPP



• Molecule 3: BPP

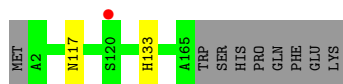


• Molecule 3: BPP

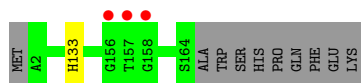


• Molecule 3: BPP

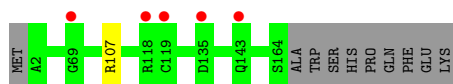




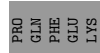
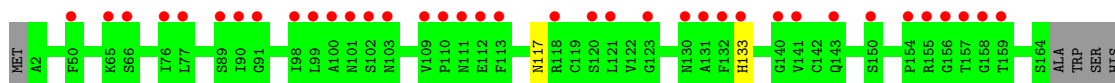
• Molecule 3: BPP



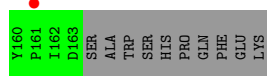
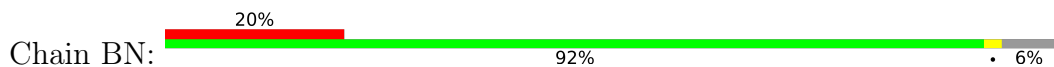
• Molecule 3: BPP



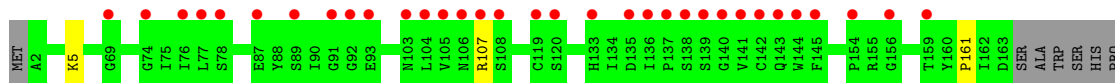
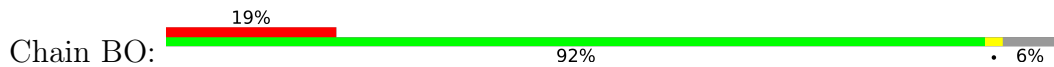
• Molecule 3: BPP



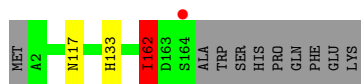
• Molecule 3: BPP



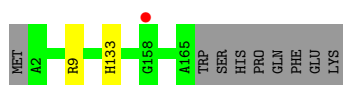
• Molecule 3: BPP



• Molecule 3: BPP



• Molecule 3: BPP



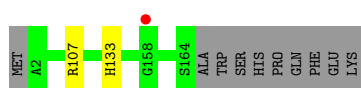
• Molecule 3: BPP



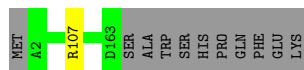
• Molecule 3: BPP



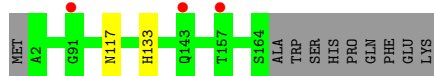
• Molecule 3: BPP



• Molecule 3: BPP



• Molecule 3: BPP

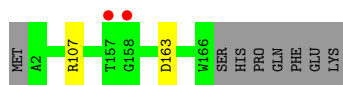


• Molecule 3: BPP

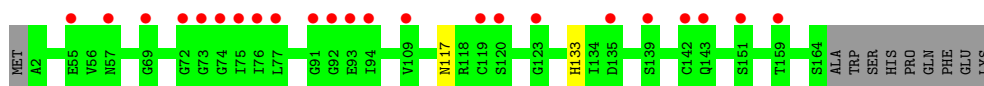
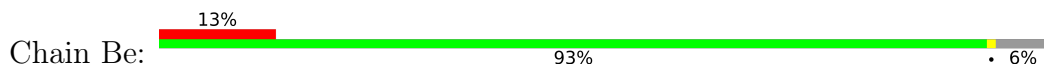




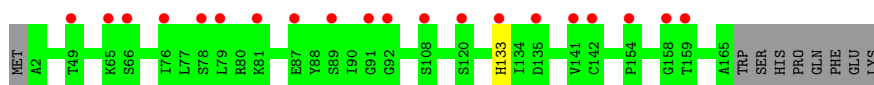
• Molecule 3: BPP



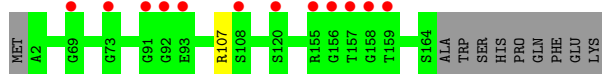
• Molecule 3: BPP



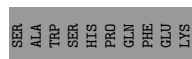
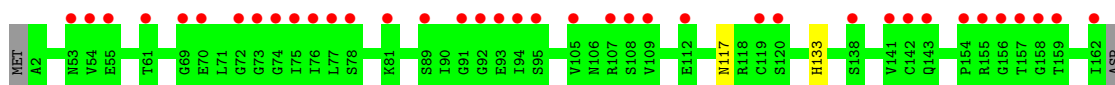
• Molecule 3: BPP



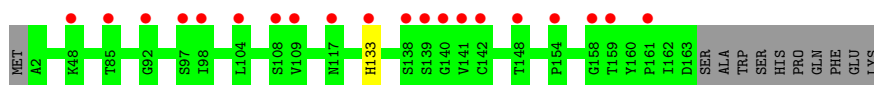
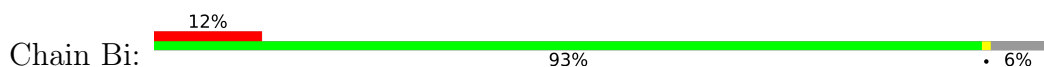
• Molecule 3: BPP



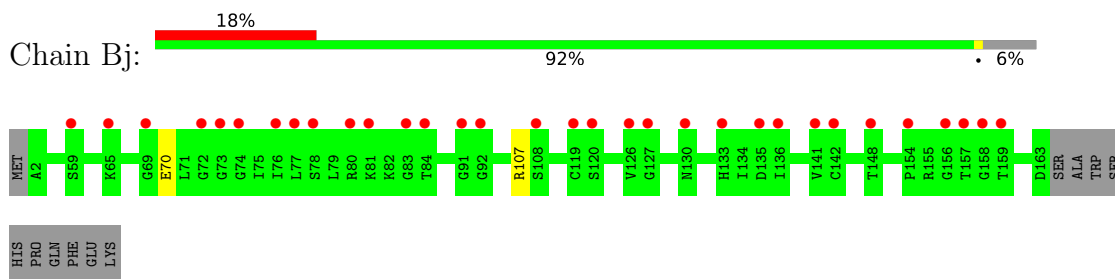
• Molecule 3: BPP



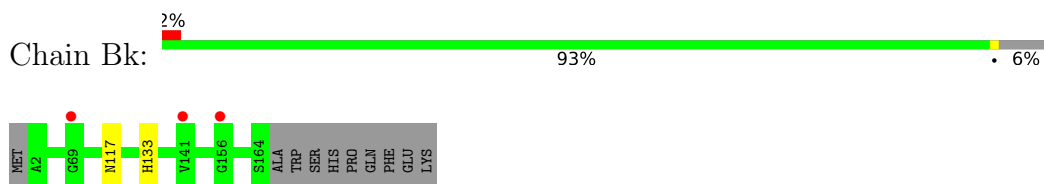
• Molecule 3: BPP



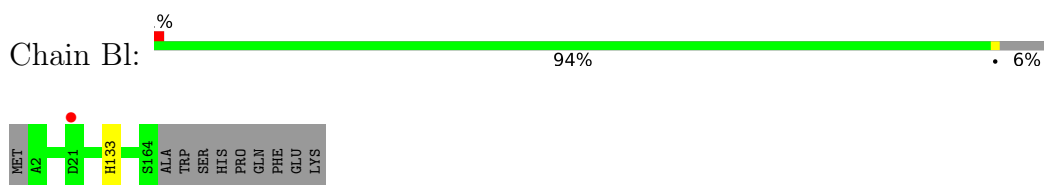
- Molecule 3: BPP



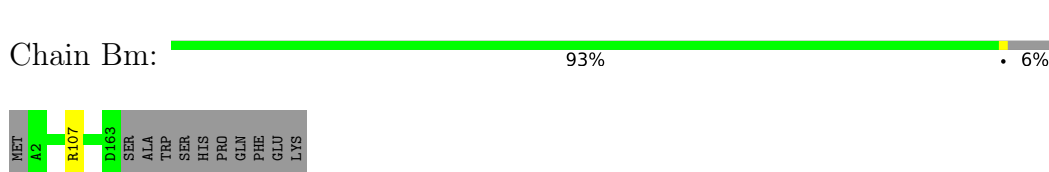
- Molecule 3: BPP



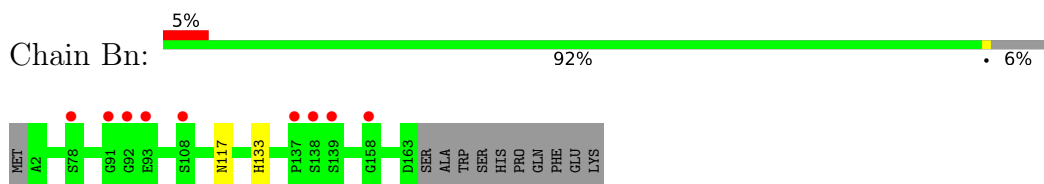
- Molecule 3: BPP



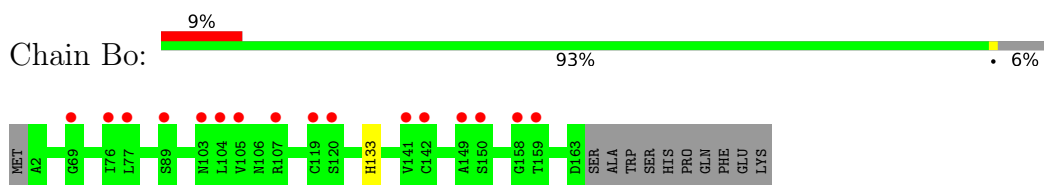
- Molecule 3: BPP



- Molecule 3: BPP

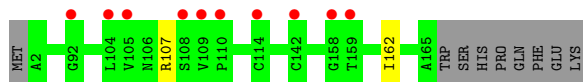


- Molecule 3: BPP

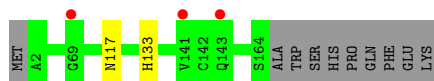


- Molecule 3: BPP

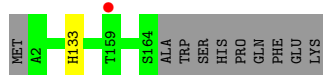




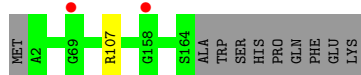
- Molecule 3: BPP



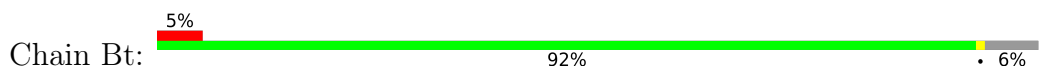
- Molecule 3: BPP



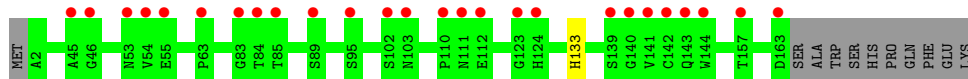
- Molecule 3: BPP



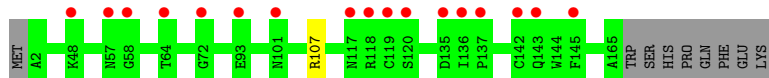
- Molecule 3: BPP



- Molecule 3: BPP

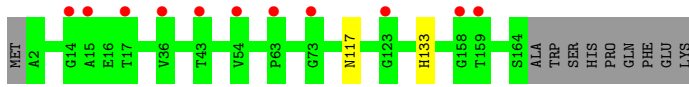


- Molecule 3: BPP

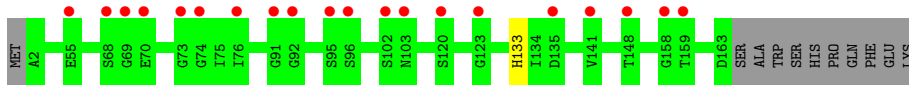


- Molecule 3: BPP

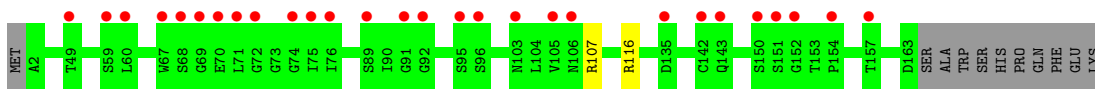
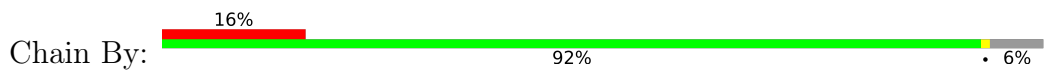




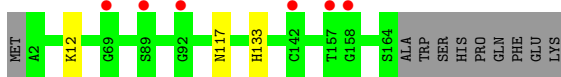
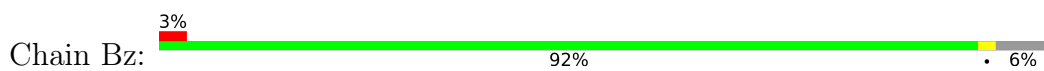
- Molecule 3: BPP



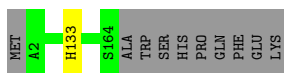
- Molecule 3: BPP



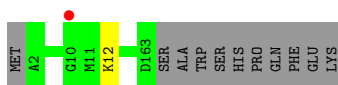
- Molecule 3: BPP



- Molecule 3: BPP



- Molecule 3: BPP



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
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.76Å)	Xtrriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.237 , 0.264 0.254 , 0.260	Depositor DCC
R_{free} test set	1424 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å ²)	123.5	Xtrriage
Anisotropy	0.206	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 102.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtrriage
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

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	AA	192	VAL	CB-CA-C	6.46	123.67	111.40
1	AG	192	VAL	CB-CA-C	6.20	123.17	111.40
1	AM	194	ALA	N-CA-C	6.19	127.70	111.00
3	BO	161	PRO	O-C-N	-6.14	112.88	122.70
1	AN	195	GLY	N-CA-C	6.04	128.20	113.10
2	AT	115	TYR	CB-CA-C	6.00	122.40	110.40
1	AA	268	ILE	CB-CA-C	5.70	123.00	111.60
1	AC	194	ALA	N-CA-C	5.59	126.11	111.00
1	AB	268	ILE	CB-CA-C	5.54	122.67	111.60
1	AK	268	ILE	CB-CA-C	5.33	122.27	111.60
1	AG	83	ALA	CB-CA-C	5.28	118.02	110.10
1	AK	195	GLY	N-CA-C	5.11	125.86	113.10
1	AD	162	GLU	CB-CG-CD	5.09	127.95	114.20
1	AA	179	ALA	CB-CA-C	5.01	117.61	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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	22	60
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%)	22	60
1	AE	287/299 (96%)	268 (93%)	19 (7%)	0	100	100
1	AF	297/299 (99%)	277 (93%)	19 (6%)	1 (0%)	41	74
1	AG	297/299 (99%)	278 (94%)	14 (5%)	5 (2%)	9	43
1	AH	290/299 (97%)	271 (93%)	18 (6%)	1 (0%)	41	74
1	AI	297/299 (99%)	275 (93%)	20 (7%)	2 (1%)	22	60
1	AJ	297/299 (99%)	275 (93%)	20 (7%)	2 (1%)	22	60
1	AK	289/299 (97%)	270 (93%)	19 (7%)	0	100	100
1	AL	296/299 (99%)	276 (93%)	19 (6%)	1 (0%)	41	74
1	AM	297/299 (99%)	276 (93%)	19 (6%)	2 (1%)	22	60
1	AN	290/299 (97%)	270 (93%)	20 (7%)	0	100	100
1	AO	297/299 (99%)	276 (93%)	20 (7%)	1 (0%)	41	74
1	AP	297/299 (99%)	281 (95%)	13 (4%)	3 (1%)	15	52
1	AQ	291/299 (97%)	269 (92%)	21 (7%)	1 (0%)	41	74
1	AR	297/299 (99%)	277 (93%)	17 (6%)	3 (1%)	15	52
2	AS	240/253 (95%)	215 (90%)	24 (10%)	1 (0%)	34	70
2	AT	240/253 (95%)	218 (91%)	22 (9%)	0	100	100
2	AU	240/253 (95%)	215 (90%)	25 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	47	79

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AF	269	ASP
1	AA	175	GLY

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Mol	Chain	Res	Type
1	AM	175	GLY
1	AD	27	VAL
1	AG	27	VAL
1	AG	175	GLY
1	AJ	27	VAL
1	AJ	175	GLY
1	AP	27	VAL
1	AP	175	GLY
1	AA	27	VAL
1	AG	193	PRO
1	AL	28	ASN
1	AM	27	VAL
1	AD	175	GLY
1	AI	269	ASP
1	AP	106	GLY
1	AR	269	ASP
1	AQ	63	GLY
1	AR	105	GLY
1	AR	171	ILE
1	AH	193	PRO
1	AG	105	GLY
1	AO	235	GLY
1	AG	106	GLY
2	AS	197	GLY
1	AI	235	GLY

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%)	20	51
1	AB	255/261 (98%)	244 (96%)	11 (4%)	29	58
1	AC	260/261 (100%)	247 (95%)	13 (5%)	24	55
1	AD	261/261 (100%)	247 (95%)	14 (5%)	22	53
1	AE	256/261 (98%)	250 (98%)	6 (2%)	50	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AF	260/261 (100%)	251 (96%)	9 (4%)	36	64
1	AG	259/261 (99%)	249 (96%)	10 (4%)	32	60
1	AH	254/261 (97%)	242 (95%)	12 (5%)	26	56
1	AI	260/261 (100%)	245 (94%)	15 (6%)	20	51
1	AJ	261/261 (100%)	247 (95%)	14 (5%)	22	53
1	AK	250/261 (96%)	239 (96%)	11 (4%)	28	57
1	AL	259/261 (99%)	246 (95%)	13 (5%)	24	55
1	AM	260/261 (100%)	249 (96%)	11 (4%)	30	58
1	AN	250/261 (96%)	238 (95%)	12 (5%)	25	56
1	AO	261/261 (100%)	250 (96%)	11 (4%)	30	58
1	AP	258/261 (99%)	242 (94%)	16 (6%)	18	49
1	AQ	254/261 (97%)	244 (96%)	10 (4%)	32	60
1	AR	260/261 (100%)	253 (97%)	7 (3%)	44	69
2	AS	212/229 (93%)	205 (97%)	7 (3%)	38	65
2	AT	212/229 (93%)	200 (94%)	12 (6%)	20	52
2	AU	209/229 (91%)	202 (97%)	7 (3%)	38	65
2	AV	204/229 (89%)	196 (96%)	8 (4%)	32	60
2	AW	209/229 (91%)	203 (97%)	6 (3%)	42	67
2	AX	209/229 (91%)	197 (94%)	12 (6%)	20	52
3	B1	133/142 (94%)	132 (99%)	1 (1%)	81	89
3	B2	132/142 (93%)	131 (99%)	1 (1%)	81	89
3	BA	132/142 (93%)	127 (96%)	5 (4%)	33	61
3	BB	132/142 (93%)	126 (96%)	6 (4%)	27	57
3	BC	132/142 (93%)	124 (94%)	8 (6%)	18	50
3	BD	132/142 (93%)	129 (98%)	3 (2%)	50	72
3	BE	132/142 (93%)	131 (99%)	1 (1%)	81	89
3	BF	132/142 (93%)	131 (99%)	1 (1%)	81	89
3	BG	132/142 (93%)	129 (98%)	3 (2%)	50	72
3	BH	133/142 (94%)	131 (98%)	2 (2%)	65	81
3	BI	132/142 (93%)	131 (99%)	1 (1%)	81	89
3	BJ	132/142 (93%)	130 (98%)	2 (2%)	65	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	BK	132/142 (93%)	131 (99%)	1 (1%)	81	89
3	BL	132/142 (93%)	131 (99%)	1 (1%)	81	89
3	BM	132/142 (93%)	130 (98%)	2 (2%)	65	81
3	BN	131/142 (92%)	128 (98%)	3 (2%)	50	72
3	BO	131/142 (92%)	129 (98%)	2 (2%)	65	81
3	BP	132/142 (93%)	130 (98%)	2 (2%)	65	81
3	BQ	132/142 (93%)	131 (99%)	1 (1%)	81	89
3	BR	132/142 (93%)	131 (99%)	1 (1%)	81	89
3	BS	132/142 (93%)	130 (98%)	2 (2%)	65	81
3	BT	132/142 (93%)	131 (99%)	1 (1%)	81	89
3	BU	132/142 (93%)	131 (99%)	1 (1%)	81	89
3	BV	132/142 (93%)	129 (98%)	3 (2%)	50	72
3	BW	132/142 (93%)	130 (98%)	2 (2%)	65	81
3	BX	131/142 (92%)	131 (100%)	0	100	100
3	BY	132/142 (93%)	128 (97%)	4 (3%)	41	66
3	BZ	132/142 (93%)	130 (98%)	2 (2%)	65	81
3	Ba	132/142 (93%)	131 (99%)	1 (1%)	81	89
3	Bb	132/142 (93%)	130 (98%)	2 (2%)	65	81
3	Bc	131/142 (92%)	130 (99%)	1 (1%)	81	89
3	Bd	132/142 (93%)	130 (98%)	2 (2%)	65	81
3	Be	132/142 (93%)	130 (98%)	2 (2%)	65	81
3	Bf	132/142 (93%)	131 (99%)	1 (1%)	81	89
3	Bg	132/142 (93%)	131 (99%)	1 (1%)	81	89
3	Bh	131/142 (92%)	129 (98%)	2 (2%)	65	81
3	Bi	131/142 (92%)	130 (99%)	1 (1%)	81	89
3	Bj	132/142 (93%)	130 (98%)	2 (2%)	65	81
3	Bk	132/142 (93%)	130 (98%)	2 (2%)	65	81
3	Bl	132/142 (93%)	131 (99%)	1 (1%)	81	89
3	Bm	131/142 (92%)	130 (99%)	1 (1%)	81	89
3	Bn	132/142 (93%)	130 (98%)	2 (2%)	65	81
3	Bo	132/142 (93%)	131 (99%)	1 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Bp	133/142 (94%)	131 (98%)	2 (2%)	65	81
3	Bq	133/142 (94%)	131 (98%)	2 (2%)	65	81
3	Br	132/142 (93%)	131 (99%)	1 (1%)	81	89
3	Bs	132/142 (93%)	131 (99%)	1 (1%)	81	89
3	Bt	131/142 (92%)	129 (98%)	2 (2%)	65	81
3	Bu	132/142 (93%)	131 (99%)	1 (1%)	81	89
3	Bv	132/142 (93%)	131 (99%)	1 (1%)	81	89
3	Bw	132/142 (93%)	130 (98%)	2 (2%)	65	81
3	Bx	132/142 (93%)	131 (99%)	1 (1%)	81	89
3	By	132/142 (93%)	130 (98%)	2 (2%)	65	81
3	Bz	133/142 (94%)	130 (98%)	3 (2%)	50	72
All	All	13018/13740 (95%)	12654 (97%)	364 (3%)	43	68

All (364) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	15	ASN
1	AA	49	GLN
1	AA	62	GLN
1	AA	64	VAL
1	AA	101	ARG
1	AA	134	ASN
1	AA	139	PHE
1	AA	140	LYS
1	AA	171	ILE
1	AA	186	LYS
1	AA	224	ASP
1	AA	248	ARG
1	AA	250	LYS
1	AA	267	LEU
1	AA	272	THR
1	AB	37	VAL
1	AB	75	LYS
1	AB	85	ASP
1	AB	125	ILE
1	AB	132	ASP
1	AB	151	GLU
1	AB	219	ILE

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Mol	Chain	Res	Type
1	AB	224	ASP
1	AB	248	ARG
1	AB	267	LEU
1	AB	298	VAL
1	AC	2	THR
1	AC	27	VAL
1	AC	62	GLN
1	AC	107	ARG
1	AC	116	THR
1	AC	159	GLN
1	AC	168	LEU
1	AC	178	LEU
1	AC	186	LYS
1	AC	189	ASN
1	AC	224	ASP
1	AC	248	ARG
1	AC	267	LEU
1	AD	15	ASN
1	AD	62	GLN
1	AD	75	LYS
1	AD	116	THR
1	AD	132	ASP
1	AD	134	ASN
1	AD	140	LYS
1	AD	144	ARG
1	AD	147	ASN
1	AD	167	ILE
1	AD	178	LEU
1	AD	191	LYS
1	AD	224	ASP
1	AD	248	ARG
1	AE	85	ASP
1	AE	125	ILE
1	AE	189	ASN
1	AE	219	ILE
1	AE	224	ASP
1	AE	248	ARG
1	AF	2	THR
1	AF	6	ILE
1	AF	91	VAL
1	AF	158	GLU
1	AF	168	LEU

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Mol	Chain	Res	Type
1	AF	216	LYS
1	AF	224	ASP
1	AF	248	ARG
1	AF	267	LEU
1	AG	15	ASN
1	AG	28	ASN
1	AG	49	GLN
1	AG	62	GLN
1	AG	102	LYS
1	AG	103	GLN
1	AG	134	ASN
1	AG	155	LYS
1	AG	224	ASP
1	AG	248	ARG
1	AH	85	ASP
1	AH	89	GLN
1	AH	125	ILE
1	AH	132	ASP
1	AH	155	LYS
1	AH	165	ARG
1	AH	168	LEU
1	AH	169	GLU
1	AH	219	ILE
1	AH	224	ASP
1	AH	248	ARG
1	AH	257	LYS
1	AI	2	THR
1	AI	12	GLU
1	AI	27	VAL
1	AI	62	GLN
1	AI	75	LYS
1	AI	108	TRP
1	AI	159	GLN
1	AI	168	LEU
1	AI	177	LEU
1	AI	178	LEU
1	AI	184	ILE
1	AI	189	ASN
1	AI	224	ASP
1	AI	248	ARG
1	AI	267	LEU
1	AJ	15	ASN

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Mol	Chain	Res	Type
1	AJ	28	ASN
1	AJ	62	GLN
1	AJ	88	LEU
1	AJ	102	LYS
1	AJ	116	THR
1	AJ	132	ASP
1	AJ	134	ASN
1	AJ	139	PHE
1	AJ	140	LYS
1	AJ	148	LYS
1	AJ	154	LYS
1	AJ	224	ASP
1	AJ	248	ARG
1	AK	85	ASP
1	AK	89	GLN
1	AK	132	ASP
1	AK	154	LYS
1	AK	155	LYS
1	AK	165	ARG
1	AK	177	LEU
1	AK	219	ILE
1	AK	224	ASP
1	AK	248	ARG
1	AK	298	VAL
1	AL	2	THR
1	AL	22	LEU
1	AL	58	GLU
1	AL	62	GLN
1	AL	85	ASP
1	AL	108	TRP
1	AL	165	ARG
1	AL	182	ILE
1	AL	185	GLU
1	AL	248	ARG
1	AL	253	VAL
1	AL	261	LEU
1	AL	267	LEU
1	AM	15	ASN
1	AM	27	VAL
1	AM	55	MET
1	AM	62	GLN
1	AM	88	LEU

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Mol	Chain	Res	Type
1	AM	116	THR
1	AM	132	ASP
1	AM	134	ASN
1	AM	139	PHE
1	AM	224	ASP
1	AM	248	ARG
1	AN	43	LYS
1	AN	85	ASP
1	AN	89	GLN
1	AN	132	ASP
1	AN	167	ILE
1	AN	168	LEU
1	AN	177	LEU
1	AN	178	LEU
1	AN	184	ILE
1	AN	219	ILE
1	AN	224	ASP
1	AN	248	ARG
1	AO	23	ARG
1	AO	27	VAL
1	AO	62	GLN
1	AO	116	THR
1	AO	159	GLN
1	AO	165	ARG
1	AO	170	SER
1	AO	219	ILE
1	AO	224	ASP
1	AO	248	ARG
1	AO	267	LEU
1	AP	15	ASN
1	AP	22	LEU
1	AP	57	GLN
1	AP	62	GLN
1	AP	102	LYS
1	AP	116	THR
1	AP	132	ASP
1	AP	134	ASN
1	AP	139	PHE
1	AP	148	LYS
1	AP	181	VAL
1	AP	191	LYS
1	AP	192	VAL

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Mol	Chain	Res	Type
1	AP	209	GLU
1	AP	224	ASP
1	AP	248	ARG
1	AQ	125	ILE
1	AQ	132	ASP
1	AQ	155	LYS
1	AQ	165	ARG
1	AQ	178	LEU
1	AQ	219	ILE
1	AQ	224	ASP
1	AQ	248	ARG
1	AQ	277	LYS
1	AQ	298	VAL
1	AR	2	THR
1	AR	62	GLN
1	AR	115	ARG
1	AR	116	THR
1	AR	150	ILE
1	AR	224	ASP
1	AR	248	ARG
2	AS	47	GLU
2	AS	95	LEU
2	AS	177	THR
2	AS	200	LEU
2	AS	221	ASP
2	AS	232	THR
2	AS	243	GLU
2	AT	47	GLU
2	AT	76	ILE
2	AT	86	ARG
2	AT	95	LEU
2	AT	134	ILE
2	AT	135	ILE
2	AT	177	THR
2	AT	200	LEU
2	AT	221	ASP
2	AT	232	THR
2	AT	244	LEU
2	AT	246	ILE
2	AU	47	GLU
2	AU	76	ILE
2	AU	95	LEU

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Mol	Chain	Res	Type
2	AU	177	THR
2	AU	200	LEU
2	AU	220	LEU
2	AU	232	THR
2	AV	47	GLU
2	AV	58	MET
2	AV	95	LEU
2	AV	135	ILE
2	AV	177	THR
2	AV	198	ASP
2	AV	200	LEU
2	AV	232	THR
2	AW	47	GLU
2	AW	86	ARG
2	AW	95	LEU
2	AW	177	THR
2	AW	200	LEU
2	AW	232	THR
2	AX	46	ARG
2	AX	47	GLU
2	AX	79	LYS
2	AX	88	LEU
2	AX	95	LEU
2	AX	134	ILE
2	AX	135	ILE
2	AX	177	THR
2	AX	200	LEU
2	AX	221	ASP
2	AX	232	THR
2	AX	244	LEU
3	BA	35	VAL
3	BA	70	GLU
3	BA	97	SER
3	BA	107	ARG
3	BA	117	ASN
3	BB	35	VAL
3	BB	70	GLU
3	BB	97	SER
3	BB	107	ARG
3	BB	117	ASN
3	BB	162	ILE
3	BC	12	LYS

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Mol	Chain	Res	Type
3	BC	35	VAL
3	BC	70	GLU
3	BC	97	SER
3	BC	107	ARG
3	BC	117	ASN
3	BC	162	ILE
3	BC	163	ASP
3	BD	117	ASN
3	BD	118	ARG
3	BD	133	HIS
3	BE	133	HIS
3	BF	107	ARG
3	BG	5	LYS
3	BG	117	ASN
3	BG	133	HIS
3	BH	12	LYS
3	BH	133	HIS
3	BI	107	ARG
3	BJ	117	ASN
3	BJ	133	HIS
3	BK	133	HIS
3	BL	107	ARG
3	BM	117	ASN
3	BM	133	HIS
3	BN	103	ASN
3	BN	133	HIS
3	BN	141	VAL
3	BO	5	LYS
3	BO	107	ARG
3	BP	117	ASN
3	BP	133	HIS
3	BQ	133	HIS
3	BR	107	ARG
3	BS	117	ASN
3	BS	133	HIS
3	BT	133	HIS
3	BU	107	ARG
3	BV	117	ASN
3	BV	133	HIS
3	BV	162	ILE
3	BW	9	ARG
3	BW	133	HIS

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Mol	Chain	Res	Type
3	BY	12	LYS
3	BY	81	LYS
3	BY	117	ASN
3	BY	133	HIS
3	BZ	107	ARG
3	BZ	133	HIS
3	Ba	107	ARG
3	Bb	117	ASN
3	Bb	133	HIS
3	Bc	133	HIS
3	Bd	107	ARG
3	Bd	163	ASP
3	Be	117	ASN
3	Be	133	HIS
3	Bf	133	HIS
3	Bg	107	ARG
3	Bh	117	ASN
3	Bh	133	HIS
3	Bi	133	HIS
3	Bj	70	GLU
3	Bj	107	ARG
3	Bk	117	ASN
3	Bk	133	HIS
3	Bl	133	HIS
3	Bm	107	ARG
3	Bn	117	ASN
3	Bn	133	HIS
3	Bo	133	HIS
3	Bp	107	ARG
3	Bp	162	ILE
3	Bq	117	ASN
3	Bq	133	HIS
3	Br	133	HIS
3	Bs	107	ARG
3	Bt	117	ASN
3	Bt	133	HIS
3	Bu	133	HIS
3	Bv	107	ARG
3	Bw	117	ASN
3	Bw	133	HIS
3	Bx	133	HIS
3	By	107	ARG

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Mol	Chain	Res	Type
3	B _y	116	ARG
3	B _z	12	LYS
3	B _z	117	ASN
3	B _z	133	HIS
3	B1	133	HIS
3	B2	12	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (243) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	15	ASN
1	AA	44	ASN
1	AA	49	GLN
1	AA	62	GLN
1	AA	89	GLN
1	AA	134	ASN
1	AA	164	ASN
1	AA	202	HIS
1	AA	280	GLN
1	AB	30	GLN
1	AC	24	HIS
1	AC	30	GLN
1	AC	44	ASN
1	AC	111	GLN
1	AC	159	GLN
1	AC	189	ASN
1	AC	202	HIS
1	AD	15	ASN
1	AD	134	ASN
1	AE	239	ASN
1	AF	111	GLN
1	AG	15	ASN
1	AG	62	GLN
1	AG	164	ASN
1	AH	103	GLN
1	AH	164	ASN
1	AH	239	ASN
1	AI	24	HIS
1	AI	30	GLN
1	AI	49	GLN
1	AI	62	GLN
1	AI	89	GLN

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Mol	Chain	Res	Type
1	AI	111	GLN
1	AJ	15	ASN
1	AJ	62	GLN
1	AK	147	ASN
1	AK	164	ASN
1	AK	239	ASN
1	AL	24	HIS
1	AL	118	HIS
1	AL	202	HIS
1	AM	15	ASN
1	AM	62	GLN
1	AM	89	GLN
1	AM	111	GLN
1	AM	134	ASN
1	AN	147	ASN
1	AN	239	ASN
1	AO	24	HIS
1	AO	28	ASN
1	AO	49	GLN
1	AO	62	GLN
1	AO	89	GLN
1	AO	111	GLN
1	AO	147	ASN
1	AP	15	ASN
1	AP	62	GLN
1	AQ	30	GLN
1	AQ	239	ASN
1	AR	24	HIS
1	AR	62	GLN
1	AR	111	GLN
2	AS	59	GLN
2	AS	66	ASN
2	AS	102	GLN
2	AS	205	GLN
2	AT	59	GLN
2	AT	66	ASN
2	AT	102	GLN
2	AT	205	GLN
2	AU	15	ASN
2	AU	59	GLN
2	AU	66	ASN
2	AU	89	GLN

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Mol	Chain	Res	Type
2	AU	102	GLN
2	AU	217	ASN
2	AV	15	ASN
2	AV	66	ASN
2	AV	102	GLN
2	AW	102	GLN
2	AW	217	ASN
2	AX	15	ASN
2	AX	59	GLN
2	AX	102	GLN
3	BA	133	HIS
3	BA	143	GLN
3	BB	133	HIS
3	BC	133	HIS
3	BD	19	ASN
3	BD	26	ASN
3	BD	133	HIS
3	BE	19	ASN
3	BE	133	HIS
3	BF	19	ASN
3	BF	57	ASN
3	BF	103	ASN
3	BF	133	HIS
3	BG	19	ASN
3	BG	26	ASN
3	BG	133	HIS
3	BH	19	ASN
3	BH	133	HIS
3	BI	19	ASN
3	BI	57	ASN
3	BI	103	ASN
3	BI	133	HIS
3	BJ	19	ASN
3	BJ	26	ASN
3	BJ	133	HIS
3	BK	19	ASN
3	BK	133	HIS
3	BL	19	ASN
3	BL	57	ASN
3	BL	103	ASN
3	BL	133	HIS
3	BM	19	ASN

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Mol	Chain	Res	Type
3	BM	26	ASN
3	BM	133	HIS
3	BN	19	ASN
3	BN	103	ASN
3	BN	133	HIS
3	BO	19	ASN
3	BO	57	ASN
3	BO	133	HIS
3	BP	19	ASN
3	BP	133	HIS
3	BP	143	GLN
3	BQ	19	ASN
3	BQ	133	HIS
3	BR	19	ASN
3	BR	57	ASN
3	BR	103	ASN
3	BR	133	HIS
3	BS	19	ASN
3	BS	26	ASN
3	BS	133	HIS
3	BT	19	ASN
3	BT	133	HIS
3	BU	19	ASN
3	BU	57	ASN
3	BU	103	ASN
3	BU	133	HIS
3	BV	19	ASN
3	BV	26	ASN
3	BV	133	HIS
3	BW	19	ASN
3	BW	133	HIS
3	BW	143	GLN
3	BX	19	ASN
3	BX	57	ASN
3	BX	103	ASN
3	BX	133	HIS
3	BY	19	ASN
3	BY	133	HIS
3	BZ	19	ASN
3	BZ	133	HIS
3	Ba	19	ASN
3	Ba	57	ASN

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Mol	Chain	Res	Type
3	Ba	103	ASN
3	Ba	133	HIS
3	Bb	19	ASN
3	Bb	133	HIS
3	Bc	19	ASN
3	Bc	133	HIS
3	Bd	19	ASN
3	Bd	57	ASN
3	Bd	103	ASN
3	Bd	133	HIS
3	Be	19	ASN
3	Be	26	ASN
3	Be	133	HIS
3	Bf	19	ASN
3	Bf	133	HIS
3	Bf	143	GLN
3	Bg	19	ASN
3	Bg	57	ASN
3	Bg	103	ASN
3	Bg	133	HIS
3	Bh	19	ASN
3	Bh	26	ASN
3	Bh	133	HIS
3	Bi	19	ASN
3	Bi	133	HIS
3	Bj	19	ASN
3	Bj	57	ASN
3	Bj	103	ASN
3	Bj	133	HIS
3	Bk	19	ASN
3	Bk	26	ASN
3	Bk	133	HIS
3	Bl	19	ASN
3	Bl	133	HIS
3	Bm	19	ASN
3	Bm	57	ASN
3	Bm	103	ASN
3	Bm	133	HIS
3	Bn	19	ASN
3	Bn	26	ASN
3	Bn	133	HIS
3	Bo	19	ASN

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Mol	Chain	Res	Type
3	Bo	133	HIS
3	Bp	19	ASN
3	Bp	57	ASN
3	Bp	103	ASN
3	Bp	133	HIS
3	Bq	19	ASN
3	Bq	26	ASN
3	Bq	133	HIS
3	Br	19	ASN
3	Br	133	HIS
3	Bs	13	ASN
3	Bs	19	ASN
3	Bs	57	ASN
3	Bs	103	ASN
3	Bs	133	HIS
3	Bt	19	ASN
3	Bt	133	HIS
3	Bu	19	ASN
3	Bu	133	HIS
3	Bv	13	ASN
3	Bv	19	ASN
3	Bv	57	ASN
3	Bv	103	ASN
3	Bv	133	HIS
3	Bw	19	ASN
3	Bw	26	ASN
3	Bw	133	HIS
3	Bx	19	ASN
3	Bx	133	HIS
3	By	13	ASN
3	By	19	ASN
3	By	57	ASN
3	By	103	ASN
3	By	133	HIS
3	Bz	19	ASN
3	Bz	26	ASN
3	Bz	133	HIS
3	B1	19	ASN
3	B1	133	HIS
3	B2	19	ASN
3	B2	57	ASN
3	B2	103	ASN

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Mol	Chain	Res	Type
3	B2	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 monosaccharides 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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%)	-0.40	1 (0%) 94 91	84, 119, 162, 188	0
1	AB	294/299 (98%)	-0.14	10 (3%) 45 37	94, 149, 206, 237	0
1	AC	299/299 (100%)	-0.32	0 100 100	95, 124, 160, 180	0
1	AD	299/299 (100%)	-0.39	0 100 100	86, 128, 175, 206	0
1	AE	291/299 (97%)	-0.11	8 (2%) 54 45	89, 159, 213, 249	0
1	AF	299/299 (100%)	-0.32	2 (0%) 87 83	90, 132, 167, 183	0
1	AG	299/299 (100%)	-0.38	2 (0%) 87 83	95, 133, 180, 203	0
1	AH	294/299 (98%)	-0.14	6 (2%) 65 58	103, 176, 237, 261	0
1	AI	299/299 (100%)	-0.34	0 100 100	94, 135, 163, 180	0
1	AJ	299/299 (100%)	-0.42	0 100 100	88, 121, 160, 183	0
1	AK	293/299 (97%)	-0.17	5 (1%) 70 62	94, 140, 229, 255	0
1	AL	298/299 (99%)	-0.36	2 (0%) 87 83	92, 122, 157, 172	0
1	AM	299/299 (100%)	-0.31	2 (0%) 87 83	85, 124, 188, 230	0
1	AN	294/299 (98%)	0.02	14 (4%) 30 26	92, 156, 235, 269	0
1	AO	299/299 (100%)	-0.34	0 100 100	91, 129, 164, 182	0
1	AP	299/299 (100%)	-0.40	0 100 100	92, 129, 171, 193	0
1	AQ	295/299 (98%)	-0.20	3 (1%) 82 76	111, 172, 217, 240	0
1	AR	299/299 (100%)	-0.21	2 (0%) 87 83	95, 138, 197, 218	0
2	AS	242/253 (95%)	-0.43	1 (0%) 92 89	84, 124, 195, 234	0
2	AT	242/253 (95%)	-0.40	2 (0%) 86 81	88, 122, 191, 233	0
2	AU	242/253 (95%)	-0.44	1 (0%) 92 89	83, 121, 188, 235	0
2	AV	241/253 (95%)	-0.43	0 100 100	82, 125, 205, 257	0
2	AW	241/253 (95%)	-0.35	0 100 100	83, 125, 200, 246	0
2	AX	241/253 (95%)	-0.43	1 (0%) 92 89	86, 119, 192, 232	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	B1	163/173 (94%)	-0.19	0 100 100	134, 174, 213, 233	0
3	B2	162/173 (93%)	-0.30	1 (0%) 89 85	106, 137, 159, 179	0
3	BA	164/173 (94%)	0.21	9 (5%) 25 21	103, 260, 278, 283	0
3	BB	163/173 (94%)	0.42	17 (10%) 6 5	112, 254, 272, 279	0
3	BC	163/173 (94%)	0.41	19 (11%) 4 5	113, 261, 278, 280	0
3	BD	164/173 (94%)	-0.27	2 (1%) 79 72	112, 160, 181, 206	0
3	BE	164/173 (94%)	-0.28	0 100 100	112, 157, 189, 219	0
3	BF	163/173 (94%)	-0.12	4 (2%) 57 49	118, 183, 239, 258	0
3	BG	164/173 (94%)	-0.22	5 (3%) 50 40	97, 159, 203, 216	0
3	BH	164/173 (94%)	-0.14	3 (1%) 68 61	102, 148, 177, 214	0
3	BI	163/173 (94%)	-0.10	5 (3%) 49 40	99, 177, 221, 229	0
3	BJ	164/173 (94%)	-0.07	1 (0%) 89 85	106, 179, 218, 232	0
3	BK	163/173 (94%)	-0.12	3 (1%) 68 61	107, 171, 210, 235	0
3	BL	163/173 (94%)	-0.09	5 (3%) 49 40	116, 190, 228, 239	0
3	BM	163/173 (94%)	1.05	37 (22%) 0 0	133, 280, 292, 295	0
3	BN	162/173 (93%)	0.87	35 (21%) 0 1	149, 265, 278, 282	0
3	BO	162/173 (93%)	1.10	33 (20%) 1 1	147, 276, 292, 295	0
3	BP	163/173 (94%)	0.83	31 (19%) 1 1	162, 274, 286, 288	0
3	BQ	162/173 (93%)	0.88	24 (14%) 2 2	176, 241, 272, 278	0
3	BR	163/173 (94%)	0.87	30 (18%) 1 1	179, 271, 290, 294	0
3	BS	163/173 (94%)	-0.05	1 (0%) 89 85	163, 198, 224, 233	0
3	BT	164/173 (94%)	-0.07	2 (1%) 79 72	149, 196, 218, 227	0
3	BU	164/173 (94%)	0.15	9 (5%) 25 21	148, 204, 241, 256	0
3	BV	163/173 (94%)	-0.39	1 (0%) 89 85	125, 150, 191, 214	0
3	BW	164/173 (94%)	-0.27	1 (0%) 89 85	121, 146, 163, 187	0
3	BX	162/173 (93%)	-0.28	1 (0%) 89 85	118, 143, 179, 200	0
3	BY	163/173 (94%)	-0.27	0 100 100	127, 154, 182, 202	0
3	BZ	163/173 (94%)	-0.25	1 (0%) 89 85	116, 151, 180, 209	0
3	Ba	162/173 (93%)	-0.27	0 100 100	124, 148, 179, 196	0
3	Bb	163/173 (94%)	-0.13	3 (1%) 68 61	144, 200, 239, 255	0
3	Bc	164/173 (94%)	-0.23	1 (0%) 89 85	119, 196, 228, 240	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
3	Bd	165/173 (95%)	-0.08	2 (1%) 79 72	120, 187, 209, 215	0
3	Be	163/173 (94%)	0.54	23 (14%) 2 3	128, 282, 288, 291	0
3	Bf	164/173 (94%)	0.50	20 (12%) 4 4	107, 277, 289, 291	0
3	Bg	163/173 (94%)	0.36	12 (7%) 14 11	109, 273, 286, 288	0
3	Bh	161/173 (93%)	1.08	38 (23%) 0 0	194, 259, 275, 278	0
3	Bi	162/173 (93%)	0.60	20 (12%) 4 4	164, 256, 274, 276	0
3	Bj	162/173 (93%)	1.01	32 (19%) 1 1	181, 259, 276, 278	0
3	Bk	163/173 (94%)	-0.01	3 (1%) 68 61	160, 187, 214, 231	0
3	Bl	163/173 (94%)	-0.13	1 (0%) 89 85	161, 184, 203, 232	0
3	Bm	162/173 (93%)	-0.10	0 100 100	156, 181, 202, 213	0
3	Bn	162/173 (93%)	0.27	9 (5%) 24 20	146, 208, 256, 274	0
3	Bo	162/173 (93%)	0.29	16 (9%) 7 6	142, 203, 230, 238	0
3	Bp	164/173 (94%)	0.26	10 (6%) 21 17	133, 210, 240, 252	0
3	Bq	163/173 (94%)	-0.04	3 (1%) 68 61	108, 192, 220, 232	0
3	Br	163/173 (94%)	-0.10	1 (0%) 89 85	100, 172, 207, 237	0
3	Bs	163/173 (94%)	-0.10	2 (1%) 79 72	99, 168, 208, 227	0
3	Bt	162/173 (93%)	0.39	8 (4%) 29 25	146, 213, 232, 257	0
3	Bu	162/173 (93%)	0.61	26 (16%) 1 2	138, 239, 271, 275	0
3	Bv	164/173 (94%)	0.58	17 (10%) 6 5	128, 225, 251, 257	0
3	Bw	163/173 (94%)	0.52	11 (6%) 17 14	182, 216, 245, 253	0
3	Bx	162/173 (93%)	0.58	20 (12%) 4 4	203, 239, 274, 280	0
3	By	162/173 (93%)	0.79	28 (17%) 1 1	195, 252, 267, 272	0
3	Bz	163/173 (94%)	-0.15	6 (3%) 41 34	130, 170, 232, 238	0
All	All	15597/16242 (96%)	-0.02	654 (4%) 36 30	82, 163, 274, 295	0

All (654) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	BO	91	GLY	13.5
3	BQ	135	ASP	13.4
3	BR	69	GLY	12.6
3	BO	92	GLY	11.2
3	BQ	120	SER	9.6
3	BM	91	GLY	9.0

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Mol	Chain	Res	Type	RSRZ
3	BB	73	GLY	8.5
3	Bh	76	ILE	8.5
3	Bh	92	GLY	8.3
3	Bg	69	GLY	8.1
3	BO	78	SER	8.0
3	Bh	91	GLY	7.7
3	BN	108	SER	7.7
3	Bt	69	GLY	7.6
3	Bj	91	GLY	7.4
3	BO	89	SER	7.3
3	BM	133	HIS	7.2
3	BO	76	ILE	7.2
3	BO	135	ASP	7.1
3	Bj	69	GLY	7.1
3	BR	70	GLU	6.9
3	BQ	119	CYS	6.8
3	BQ	145	PHE	6.8
3	Bj	120	SER	6.8
3	Bf	89	SER	6.7
3	Bg	158	GLY	6.5
3	Bg	157	THR	6.4
3	BN	109	VAL	6.3
3	Bj	74	GLY	6.3
3	Bv	118	ARG	6.2
3	BM	158	GLY	6.2
3	BM	131	ALA	6.1
3	BU	92	GLY	6.1
3	Bv	135	ASP	6.0
3	BP	83	GLY	5.9
3	By	92	GLY	5.9
3	BP	158	GLY	5.8
3	BC	133	HIS	5.8
3	BU	91	GLY	5.8
3	BN	159	THR	5.7
3	Bh	74	GLY	5.7
3	Bf	159	THR	5.7
1	AE	34	ALA	5.6
3	BR	76	ILE	5.6
3	Be	73	GLY	5.6
3	Bi	159	THR	5.5
3	BO	139	SER	5.5
2	AT	12	HIS	5.5

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Mol	Chain	Res	Type	RSRZ
3	BB	74	GLY	5.5
3	Bx	158	GLY	5.4
3	BR	159	THR	5.4
3	Bv	57	ASN	5.3
3	Bp	108	SER	5.3
3	BM	76	ILE	5.2
3	BR	155	ARG	5.2
3	Be	74	GLY	5.2
3	BC	132	PHE	5.2
3	Bh	120	SER	5.2
3	Bj	119	CYS	5.1
3	BO	145	PHE	5.1
3	BQ	133	HIS	5.1
3	Bj	157	THR	5.1
3	BR	154	PRO	5.1
3	By	69	GLY	5.1
3	BO	120	SER	5.0
3	BA	91	GLY	5.0
3	Bj	73	GLY	5.0
3	BM	154	PRO	5.0
3	BQ	118	ARG	5.0
3	BN	140	GLY	5.0
3	Bf	78	SER	4.9
3	Bg	92	GLY	4.9
3	Be	76	ILE	4.8
1	AE	56	ALA	4.8
3	BM	120	SER	4.8
3	By	91	GLY	4.8
3	Bh	156	GLY	4.8
3	Be	69	GLY	4.8
3	BU	156	GLY	4.8
3	Be	92	GLY	4.7
1	AF	16	ASN	4.7
3	Be	142	CYS	4.6
3	BN	69	GLY	4.6
3	Bh	159	THR	4.6
3	BB	69	GLY	4.6
3	Bf	120	SER	4.6
3	BO	154	PRO	4.6
3	BO	141	VAL	4.6
3	Bi	158	GLY	4.6
3	BM	112	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
3	Bw	15	ALA	4.6
3	BM	103	ASN	4.5
3	Bt	70	GLU	4.5
3	Bg	73	GLY	4.5
3	BR	123	GLY	4.5
3	BN	133	HIS	4.5
3	Bu	143	GLN	4.5
3	Bh	73	GLY	4.5
3	Bx	141	VAL	4.5
3	BO	74	GLY	4.5
3	By	143	GLN	4.4
3	Bv	119	CYS	4.4
3	BM	89	SER	4.4
3	BO	142	CYS	4.4
3	BM	101	ASN	4.3
3	BP	141	VAL	4.3
3	BP	143	GLN	4.3
3	BP	139	SER	4.3
3	BR	75	ILE	4.3
3	BP	135	ASP	4.3
3	BM	90	ILE	4.3
3	BC	123	GLY	4.3
3	Bc	158	GLY	4.3
3	Bt	76	ILE	4.3
3	Bn	92	GLY	4.3
3	Bt	154	PRO	4.2
3	BP	84	THR	4.2
3	BH	156	GLY	4.2
3	BP	159	THR	4.2
3	BR	157	THR	4.2
3	BO	133	HIS	4.1
3	BP	142	CYS	4.1
3	Bp	92	GLY	4.1
3	Bg	120	SER	4.1
1	AN	49	GLN	4.1
3	Be	109	VAL	4.1
3	BQ	143	GLN	4.1
3	Bi	104	LEU	4.1
3	Bx	76	ILE	4.0
3	Be	135	ASP	4.0
3	BN	110	PRO	4.0
3	Bh	75	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
3	Bi	141	VAL	4.0
3	BN	55	GLU	4.0
3	BT	120	SER	4.0
3	Bn	91	GLY	4.0
3	Bi	161	PRO	3.9
3	Bi	117	ASN	3.9
3	Be	72	GLY	3.9
3	BM	159	THR	3.9
3	BQ	136	ILE	3.9
3	Bh	93	GLU	3.9
3	BA	142	CYS	3.8
3	BN	84	THR	3.8
1	AN	106	GLY	3.8
3	Bj	135	ASP	3.8
3	Bh	77	LEU	3.8
3	BB	75	ILE	3.8
3	Bj	81	LYS	3.8
3	Bn	93	GLU	3.8
3	BO	108	SER	3.8
3	BM	132	PHE	3.8
3	BN	92	GLY	3.8
3	BR	108	SER	3.8
3	Bv	143	GLN	3.7
3	Bu	163	ASP	3.7
3	BH	158	GLY	3.7
3	BR	117	ASN	3.7
3	Bz	158	GLY	3.7
3	BM	156	GLY	3.7
3	Bt	155	ARG	3.7
3	BR	141	VAL	3.7
3	BA	92	GLY	3.7
3	By	76	ILE	3.7
3	BC	97	SER	3.7
3	Bh	72	GLY	3.7
3	BA	148	THR	3.7
3	Bj	142	CYS	3.7
3	Bx	70	GLU	3.7
3	BP	157	THR	3.7
3	Bx	55	GLU	3.7
3	BN	44	ILE	3.6
3	Bg	93	GLU	3.6
3	Bj	92	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
3	Bf	76	ILE	3.6
3	Bj	77	LEU	3.6
3	Bp	105	VAL	3.6
3	BI	158	GLY	3.6
3	Bu	103	ASN	3.6
1	AH	105	GLY	3.6
3	BN	158	GLY	3.6
1	AH	261	LEU	3.6
3	Bh	108	SER	3.6
3	Bf	108	SER	3.6
3	BB	91	GLY	3.6
3	Bx	69	GLY	3.6
3	BO	137	PRO	3.6
1	AK	105	GLY	3.6
3	Bp	109	VAL	3.5
3	Bx	103	ASN	3.5
3	Bf	65	LYS	3.5
3	BU	113	PHE	3.5
3	Bv	101	ASN	3.5
3	BB	142	CYS	3.5
3	Bf	141	VAL	3.5
3	BQ	96	SER	3.5
3	BP	56	VAL	3.5
3	BG	120	SER	3.5
3	BN	85	THR	3.5
3	BN	74	GLY	3.4
3	BM	111	ASN	3.4
3	Bi	140	GLY	3.4
3	Bu	83	GLY	3.4
3	Bx	159	THR	3.4
3	Bv	137	PRO	3.4
3	BP	82	LYS	3.4
3	Bi	108	SER	3.4
3	BB	72	GLY	3.4
3	Bf	91	GLY	3.4
3	Bj	141	VAL	3.4
3	BU	158	GLY	3.4
3	By	72	GLY	3.4
3	BR	142	CYS	3.4
3	BN	154	PRO	3.4
3	BR	74	GLY	3.4
3	BB	94	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
3	By	71	LEU	3.3
3	Be	91	GLY	3.3
3	BR	72	GLY	3.3
3	BR	118	ARG	3.3
3	Bx	95	SER	3.3
3	BC	73	GLY	3.3
3	BQ	63	PRO	3.3
3	Bs	158	GLY	3.3
3	BM	123	GLY	3.3
3	BR	103	ASN	3.3
3	Bi	98	ILE	3.3
3	BF	69	GLY	3.3
3	BO	105	VAL	3.3
3	Bo	105	VAL	3.3
3	By	70	GLU	3.3
3	BP	85	THR	3.2
3	Bv	64	THR	3.2
3	BR	156	GLY	3.2
3	Bj	127	GLY	3.2
3	BU	157	THR	3.2
1	AN	105	GLY	3.2
3	BN	73	GLY	3.2
3	Bq	69	GLY	3.2
1	AG	269	ASP	3.2
3	Bh	78	SER	3.2
3	Bx	123	GLY	3.2
3	Bg	156	GLY	3.2
3	Bu	46	GLY	3.2
3	Bo	69	GLY	3.2
3	Bi	142	CYS	3.2
3	Bh	157	THR	3.2
3	BP	10	GLY	3.2
3	BN	149	ALA	3.2
1	AL	15	ASN	3.2
3	Bj	148	THR	3.2
3	Bw	158	GLY	3.2
3	Bf	142	CYS	3.1
3	BU	155	ARG	3.1
1	AN	108	TRP	3.1
3	Bj	78	SER	3.1
3	Bw	54	VAL	3.1
3	BB	76	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	AQ	269	ASP	3.1
3	Bh	138	SER	3.1
3	Bo	150	SER	3.1
3	Bf	79	LEU	3.1
3	BP	55	GLU	3.1
3	Bw	63	PRO	3.1
3	BO	119	CYS	3.1
1	AB	34	ALA	3.1
3	Be	75	ILE	3.1
3	BH	157	THR	3.1
3	BO	136	ILE	3.1
3	BM	77	LEU	3.1
3	BR	158	GLY	3.1
3	Bu	123	GLY	3.1
3	Bu	45	ALA	3.1
3	Bh	142	CYS	3.1
3	By	67	TRP	3.1
3	Bg	159	THR	3.1
3	Bv	120	SER	3.1
3	BR	143	GLN	3.1
3	Bk	156	GLY	3.1
3	Bo	141	VAL	3.0
3	BQ	95	SER	3.0
1	AE	261	LEU	3.0
3	Bf	158	GLY	3.0
3	BA	137	PRO	3.0
3	Bv	136	ILE	3.0
1	AH	269	ASP	3.0
3	BA	135	ASP	3.0
3	By	68	SER	3.0
3	Bv	48	LYS	3.0
1	AN	100	PHE	3.0
3	BR	73	GLY	3.0
3	Bv	145	PHE	3.0
3	Bx	92	GLY	3.0
3	Bu	102	SER	3.0
3	BG	158	GLY	3.0
3	Bn	137	PRO	3.0
1	AK	106	GLY	3.0
3	BP	102	SER	3.0
3	BP	155	ARG	2.9
3	BO	144	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
3	BP	140	GLY	2.9
3	BM	155	ARG	2.9
3	Bj	159	THR	2.9
3	BB	92	GLY	2.9
3	Bi	133	HIS	2.9
3	BQ	97	SER	2.9
3	Bf	66	SER	2.9
3	Bo	149	ALA	2.9
3	Bo	89	SER	2.9
1	AH	30	GLN	2.9
3	BK	158	GLY	2.9
3	Bu	142	CYS	2.9
1	AN	98	PHE	2.9
3	BM	143	GLN	2.9
3	By	154	PRO	2.8
3	BO	107	ARG	2.8
3	By	152	GLY	2.8
3	BM	110	PRO	2.8
3	BN	156	GLY	2.8
3	By	151	SER	2.8
3	Bp	142	CYS	2.8
3	BM	102	SER	2.8
3	Bj	156	GLY	2.8
1	AB	36	ILE	2.8
3	Bp	104	LEU	2.8
3	BQ	86	VAL	2.8
3	Be	143	GLN	2.8
3	BR	67	TRP	2.8
3	BM	113	PHE	2.8
3	Bo	76	ILE	2.8
3	By	135	ASP	2.8
3	Bh	112	GLU	2.8
3	By	75	ILE	2.8
3	By	142	CYS	2.8
3	BF	76	ILE	2.8
3	Bf	49	THR	2.8
3	BJ	120	SER	2.8
1	AN	1	MET	2.8
1	AK	43	LYS	2.8
1	AN	103	GLN	2.8
3	Bb	143	GLN	2.8
3	Bi	148	THR	2.7

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Mol	Chain	Res	Type	RSRZ
3	BQ	81	LYS	2.7
3	Bh	141	VAL	2.7
3	Bu	54	VAL	2.7
3	Bx	73	GLY	2.7
3	BP	51	THR	2.7
2	AX	13	TYR	2.7
3	BC	95	SER	2.7
3	Bo	142	CYS	2.7
3	BI	69	GLY	2.7
3	Bo	159	THR	2.7
3	BP	103	ASN	2.7
3	BM	141	VAL	2.7
3	Bt	61	THR	2.7
3	Bj	136	ILE	2.7
3	Bh	105	VAL	2.7
3	BP	72	GLY	2.7
3	Bn	139	SER	2.7
3	BC	162	ILE	2.7
3	Bk	69	GLY	2.7
3	BM	66	SER	2.7
3	BN	113	PHE	2.7
3	Be	93	GLU	2.7
3	Bh	89	SER	2.7
3	Bh	95	SER	2.7
3	Bw	36	VAL	2.7
3	BI	76	ILE	2.7
3	Bu	139	SER	2.6
3	BO	103	ASN	2.6
3	Bj	154	PRO	2.6
3	Be	119	CYS	2.6
3	BC	141	VAL	2.6
3	BN	54	VAL	2.6
1	AN	99	SER	2.6
3	Be	123	GLY	2.6
3	BO	143	GLN	2.6
3	By	60	LEU	2.6
3	Bu	89	SER	2.6
3	By	150	SER	2.6
3	BQ	142	CYS	2.6
3	BR	71	LEU	2.6
3	BM	65	LYS	2.6
3	Bo	77	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
3	BM	157	THR	2.6
1	AB	43	LYS	2.6
3	Bh	158	GLY	2.6
3	Bq	143	GLN	2.6
3	BQ	73	GLY	2.6
3	Bn	108	SER	2.6
3	Bu	95	SER	2.6
3	Bp	159	THR	2.6
3	BB	77	LEU	2.6
3	BC	54	VAL	2.6
3	BN	120	SER	2.6
3	BQ	108	SER	2.6
3	Bh	119	CYS	2.6
3	BP	126	VAL	2.6
3	BC	108	SER	2.6
3	Bt	49	THR	2.6
3	Bg	108	SER	2.6
3	Be	55	GLU	2.5
3	BB	143	GLN	2.5
3	Bh	61	THR	2.5
3	Bu	141	VAL	2.5
3	Bn	78	SER	2.5
3	BN	105	VAL	2.5
1	AA	269	ASP	2.5
3	BQ	101	ASN	2.5
3	Bj	65	LYS	2.5
3	Bu	110	PRO	2.5
3	Bj	59	SER	2.5
3	BZ	158	GLY	2.5
3	Bu	53	ASN	2.5
3	Bv	117	ASN	2.5
3	BB	89	SER	2.5
3	Bi	48	LYS	2.5
3	BL	143	GLN	2.5
3	BO	106	ASN	2.5
3	BU	89	SER	2.5
3	Bu	55	GLU	2.5
3	Bw	159	THR	2.5
1	AE	79	LEU	2.5
3	Bf	154	PRO	2.5
3	Bu	111	ASN	2.5
3	BC	92	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
3	Bs	69	GLY	2.5
1	AM	299	ALA	2.5
3	Bf	87	GLU	2.5
3	Bf	133	HIS	2.5
3	Be	77	LEU	2.5
3	BC	69	GLY	2.5
3	Bd	157	THR	2.5
3	Be	120	SER	2.5
3	BP	99	LEU	2.5
3	By	157	THR	2.5
3	Bx	102	SER	2.4
3	BC	75	ILE	2.4
3	BM	140	GLY	2.4
3	BM	99	LEU	2.4
1	AB	18	GLY	2.4
1	AB	269	ASP	2.4
3	BN	68	SER	2.4
3	Bx	68	SER	2.4
3	BP	98	ILE	2.4
3	Bf	92	GLY	2.4
3	Bu	140	GLY	2.4
1	AH	106	GLY	2.4
3	Bj	108	SER	2.4
3	Bu	84	THR	2.4
3	BR	109	VAL	2.4
3	Bj	126	VAL	2.4
3	Bo	158	GLY	2.4
3	BP	81	LYS	2.4
3	By	59	SER	2.4
3	By	95	SER	2.4
3	By	103	ASN	2.4
3	BL	69	GLY	2.4
3	BA	66	SER	2.4
3	Bf	135	ASP	2.4
3	Bh	55	GLU	2.4
3	Bw	17	THR	2.4
3	BM	130	ASN	2.4
3	Bp	158	GLY	2.4
1	AR	299	ALA	2.4
3	BG	159	THR	2.4
3	BO	159	THR	2.4
3	BC	109	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
3	BN	141	VAL	2.4
3	BP	154	PRO	2.4
3	BD	158	GLY	2.4
3	BN	78	SER	2.4
3	BN	112	GLU	2.4
3	BM	150	SER	2.4
3	Bl	21	ASP	2.4
3	BM	121	LEU	2.4
3	BO	77	LEU	2.4
1	AR	269	ASP	2.4
3	BR	164	SER	2.4
3	Bx	96	SER	2.4
3	Be	159	THR	2.4
3	BN	142	CYS	2.4
3	Bk	141	VAL	2.4
3	Bb	91	GLY	2.4
3	Bu	85	THR	2.4
3	Bh	143	GLN	2.3
3	Bv	93	GLU	2.3
3	Bg	91	GLY	2.3
3	Bi	139	SER	2.3
3	BQ	157	THR	2.3
3	Bo	104	LEU	2.3
3	Bv	142	CYS	2.3
3	BO	93	GLU	2.3
3	Bi	109	VAL	2.3
3	Bx	91	GLY	2.3
3	BC	76	ILE	2.3
3	BC	119	CYS	2.3
3	Bh	155	ARG	2.3
3	By	89	SER	2.3
3	By	105	VAL	2.3
3	Bj	83	GLY	2.3
3	Bu	144	TRP	2.3
3	Bx	120	SER	2.3
3	BR	161	PRO	2.3
3	Bx	135	ASP	2.3
3	Be	139	SER	2.3
3	BM	50	PHE	2.3
1	AN	104	GLU	2.3
1	AB	4	HIS	2.3
1	AB	8	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	BB	155	ARG	2.3
3	BF	158	GLY	2.3
3	Bb	157	THR	2.3
3	Bn	158	GLY	2.3
3	Br	159	THR	2.3
3	Bo	119	CYS	2.3
3	Bh	81	LYS	2.3
3	BP	104	LEU	2.3
3	Bh	154	PRO	2.3
3	Bj	72	GLY	2.3
3	BN	72	GLY	2.3
3	BF	157	THR	2.3
3	BO	104	LEU	2.3
1	AB	35	GLN	2.3
3	BA	118	ARG	2.2
3	Bu	124	HIS	2.3
3	BO	87	GLU	2.2
3	BX	113	PHE	2.2
3	Bw	14	GLY	2.2
3	Be	57	ASN	2.2
3	Bi	85	THR	2.2
3	Bh	94	ILE	2.2
3	By	96	SER	2.2
3	BD	157	THR	2.2
3	Bh	162	ILE	2.2
3	BQ	155	ARG	2.2
1	AB	105	GLY	2.2
3	BW	158	GLY	2.2
3	Bh	53	ASN	2.2
3	BB	141	VAL	2.2
3	BQ	134	ILE	2.2
3	BK	157	THR	2.2
3	BO	69	GLY	2.2
3	B2	10	GLY	2.2
1	AN	50	PRO	2.2
3	BB	133	HIS	2.2
3	BG	157	THR	2.2
3	Bj	76	ILE	2.2
3	Bj	84	THR	2.2
1	AN	101	ARG	2.2
3	BQ	107	ARG	2.2
3	Be	151	SER	2.2

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Mol	Chain	Res	Type	RSRZ
3	Bf	81	LYS	2.2
3	BR	132	PHE	2.2
3	Bo	107	ARG	2.2
3	BM	109	VAL	2.2
1	AN	109	ILE	2.2
3	BN	63	PRO	2.2
3	Bi	97	SER	2.2
1	AK	50	PRO	2.2
3	BG	156	GLY	2.2
3	Bi	92	GLY	2.2
3	By	74	GLY	2.2
3	Bp	114	CYS	2.2
3	BP	29	LEU	2.2
3	BN	161	PRO	2.2
3	BS	154	PRO	2.2
3	Bj	158	GLY	2.2
3	Bz	92	GLY	2.2
1	AE	36	ILE	2.2
3	Be	94	ILE	2.2
3	Bw	123	GLY	2.1
3	Bg	155	ARG	2.1
3	By	49	THR	2.1
3	Bz	157	THR	2.1
3	BC	144	TRP	2.1
3	BT	165	ALA	2.1
1	AF	15	ASN	2.1
3	BC	157	THR	2.1
3	Bv	72	GLY	2.1
1	AM	269	ASP	2.1
2	AU	12	HIS	2.1
3	BI	157	THR	2.1
3	BO	140	GLY	2.1
3	BN	81	LYS	2.1
3	Bh	70	GLU	2.1
3	BM	100	ALA	2.1
3	Bj	130	ASN	2.1
3	Bi	154	PRO	2.1
1	AN	261	LEU	2.1
3	Bq	141	VAL	2.1
3	By	106	ASN	2.1
3	Bu	112	GLU	2.1
1	AG	243	SER	2.1

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Mol	Chain	Res	Type	RSRZ
3	BB	95	SER	2.1
3	BQ	50	PHE	2.1
3	Bo	120	SER	2.1
3	Bw	43	THR	2.1
1	AQ	276	ILE	2.1
2	AT	13	TYR	2.1
1	AB	1	MET	2.1
3	BQ	78	SER	2.1
3	Bx	74	GLY	2.1
3	BN	95	SER	2.1
2	AS	221	ASP	2.1
3	BK	156	GLY	2.1
3	BN	79	LEU	2.1
3	Bt	73	GLY	2.1
3	Bv	58	GLY	2.1
3	Bh	107	ARG	2.1
3	BR	2	ALA	2.1
3	BL	118	ARG	2.1
3	Bp	110	PRO	2.1
3	Bz	89	SER	2.1
3	BL	119	CYS	2.1
3	Bo	103	ASN	2.1
3	Bh	54	VAL	2.1
3	BO	138	SER	2.0
3	BO	156	GLY	2.1
3	Bi	138	SER	2.0
3	BI	144	TRP	2.0
3	Bu	157	THR	2.0
3	Bz	142	CYS	2.0
3	BR	57	ASN	2.0
1	AH	80	LYS	2.0
3	Bz	69	GLY	2.0
3	Bh	109	VAL	2.0
3	Bd	158	GLY	2.0
3	BM	118	ARG	2.0
3	Bx	148	THR	2.0
3	BA	143	GLN	2.0
3	BP	123	GLY	2.0
3	BP	153	THR	2.0
3	Bh	69	GLY	2.0
3	Bw	73	GLY	2.0
1	AE	32	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
3	Bj	80	ARG	2.0
1	AE	8	LEU	2.0
1	AQ	275	VAL	2.0
3	Bu	63	PRO	2.0
3	Bj	133	HIS	2.0
3	BC	72	GLY	2.0
3	BL	135	ASP	2.0
3	BM	98	ILE	2.0
3	BP	100	ALA	2.0
3	BR	139	SER	2.0
3	BV	164	SER	2.0
3	Bn	138	SER	2.0
3	BN	87	GLU	2.0
1	AE	262	ALA	2.0
1	AK	269	ASP	2.0
3	BN	135	ASP	2.0
1	AL	16	ASN	2.0
3	BU	93	GLU	2.0

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 monosaccharides 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.