



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:48 PM UTC

PDB ID : 4V96 / pdb_00004v96
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

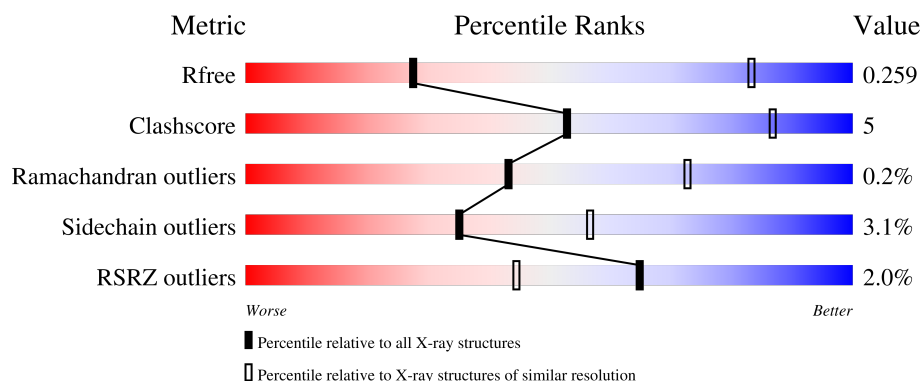
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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.



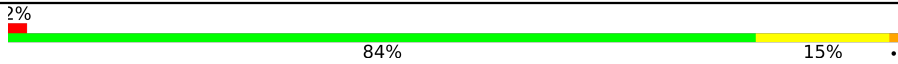
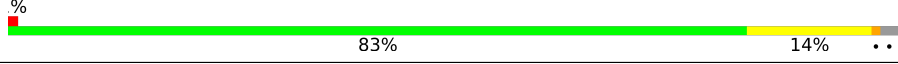
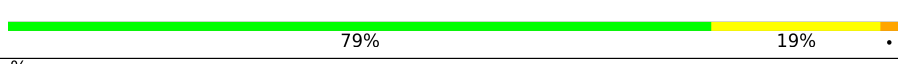
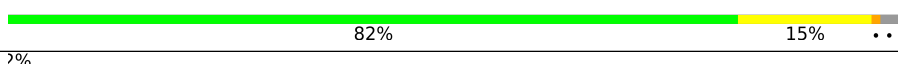
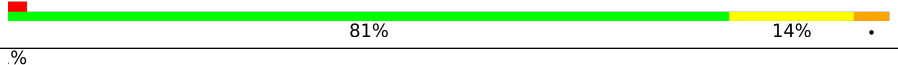
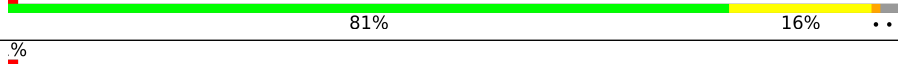
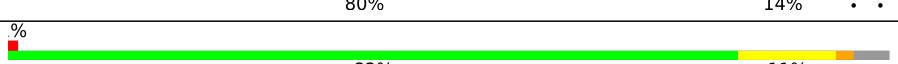
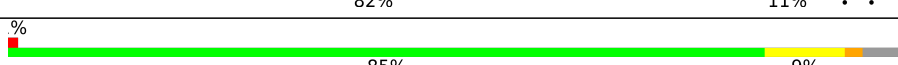
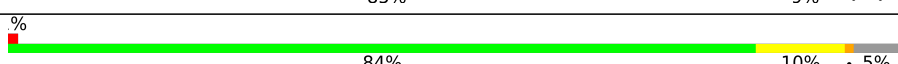
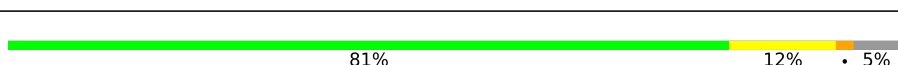
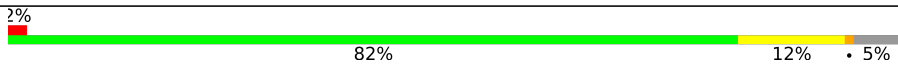
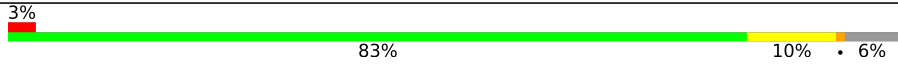
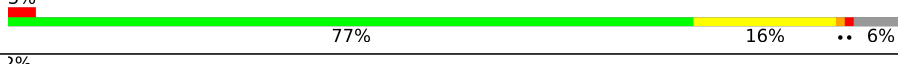
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	% 74% 22% .
1	AB	299	2% 78% 18% ..
1	AC	299	3% 77% 20% .
1	AD	299	% 83% 15% .
1	AE	299	% 83% 13% ..

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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	

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Mol	Chain	Length	Quality of chain
3	BE	173	
3	BF	173	
3	BG	173	
3	BH	173	
3	BI	173	
3	BJ	173	
3	BK	173	
3	BL	173	
3	BM	173	
3	BN	173	
3	BO	173	
3	BP	173	
3	BQ	173	
3	BR	173	
3	BS	173	
3	BT	173	
3	BU	173	
3	BV	173	
3	BW	173	
3	BX	173	
3	BY	173	
3	BZ	173	
3	Ba	173	
3	Bb	173	
3	Bc	173	

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Mol	Chain	Length	Quality of chain
3	Bd	173	 83% 12% 5%
3	Be	173	 80% 14% 6%
3	Bf	173	 83% 12% 5%
3	Bg	173	 84% 10% 6%
3	Bh	173	 83% 10% 7%
3	Bi	173	 82% 11% 6%
3	Bj	173	 85% 9% 6%
3	Bk	173	 83% 11% 6%
3	Bl	173	 83% 12% 6%
3	Bm	173	 85% 9% 6%
3	Bn	173	 83% 10% 6%
3	Bo	173	 82% 12% 6%
3	Bp	173	 84% 10% 5%
3	Bq	173	 84% 10% 6%
3	Br	173	 83% 11% 6%
3	Bs	173	 84% 10% 6%
3	Bt	173	 82% 12% 6%
3	Bu	173	 84% 10% 6%
3	Bv	173	 86% 9% 5%
3	Bw	173	 84% 10% 6%
3	Bx	173	 82% 11% 6%
3	By	173	 83% 10% 6%
3	Bz	173	 82% 12% 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
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			

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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
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			

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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			

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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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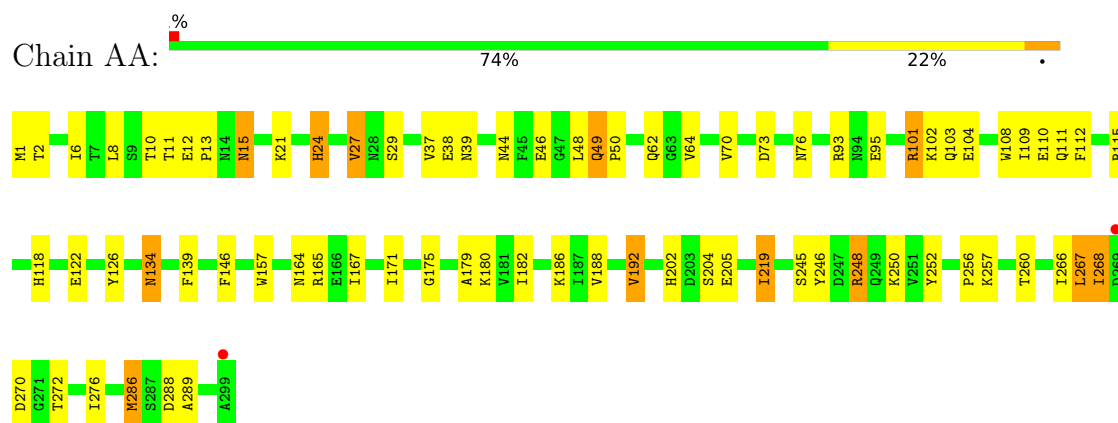
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Chain	Residue	Modelled	Actual	Comment	Reference
B1	171	PHE	-	expression tag	UNP Q9G096
B1	172	GLU	-	expression tag	UNP Q9G096
B1	173	LYS	-	expression tag	UNP Q9G096
B2	164	SER	-	expression tag	UNP Q9G096
B2	165	ALA	-	expression tag	UNP Q9G096
B2	166	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

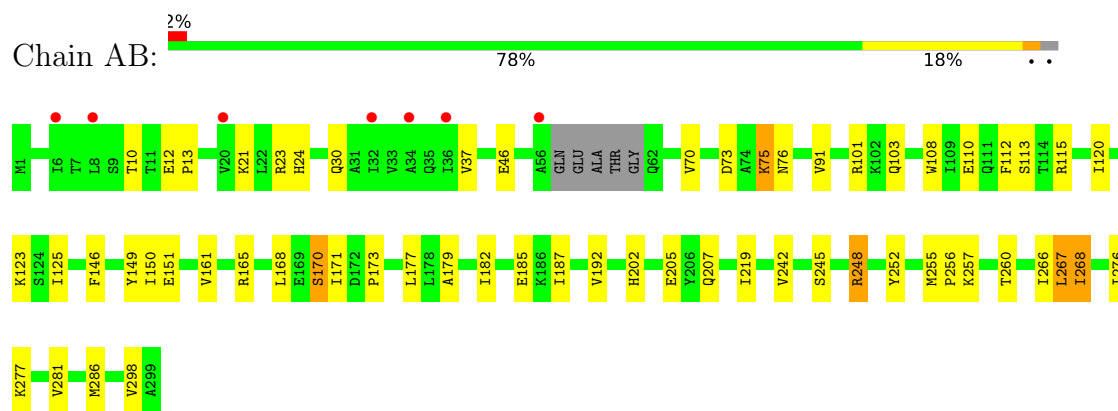
3 Residue-property plots [i](#)

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.

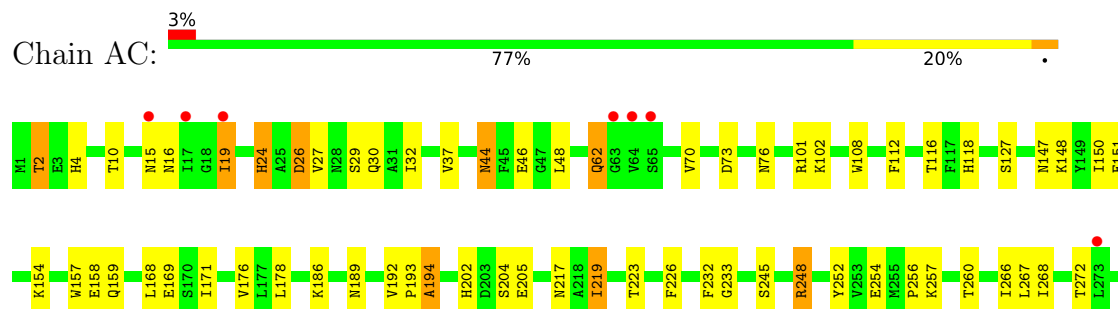
• Molecule 1: ORF48

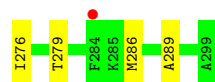


• Molecule 1: ORF48

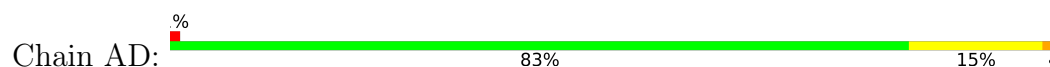


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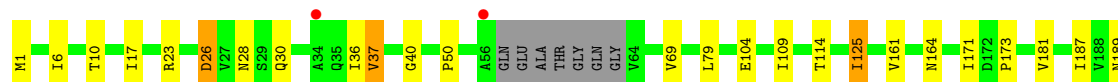
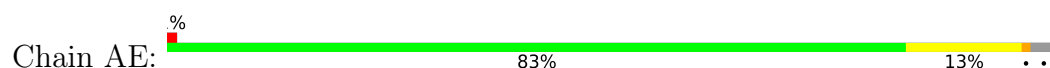




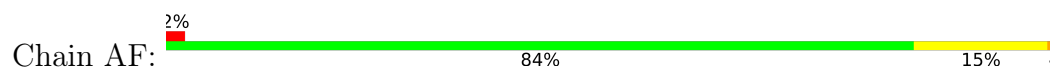
• Molecule 1: ORF48



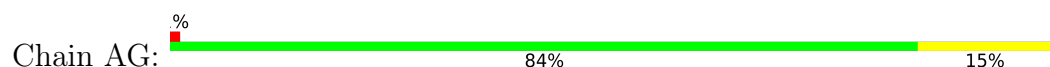
• Molecule 1: ORF48



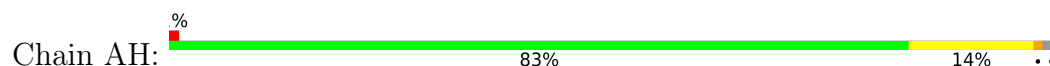
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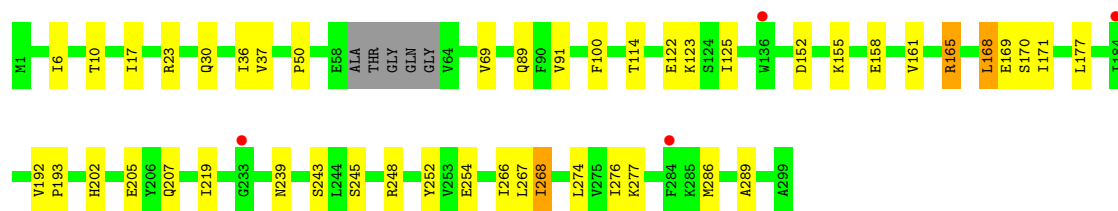


• Molecule 1: ORF48



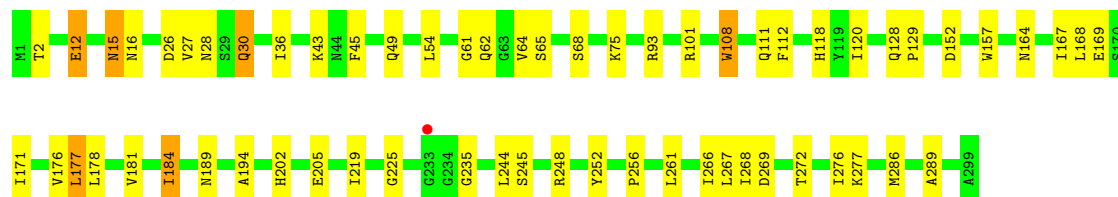
• Molecule 1: ORF48





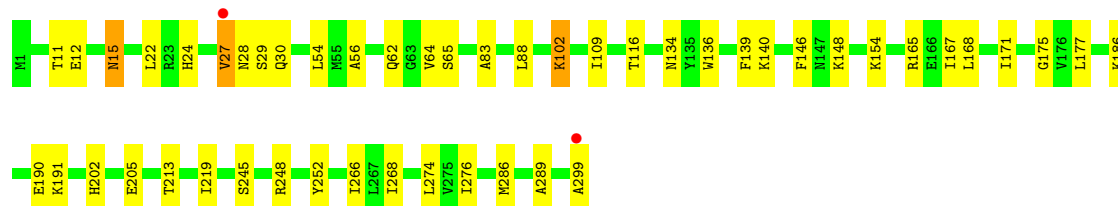
• Molecule 1: ORF48

Chain AI: 79% 19% .



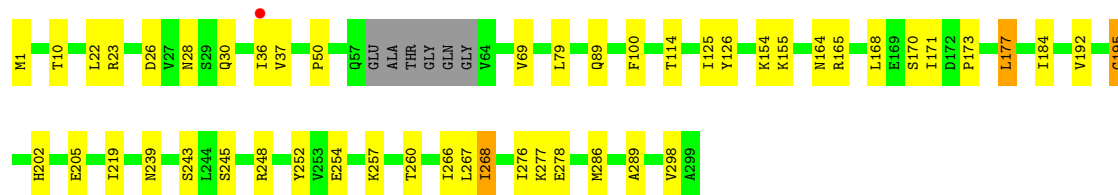
• Molecule 1: ORF48

Chain AJ: 84% 15% .



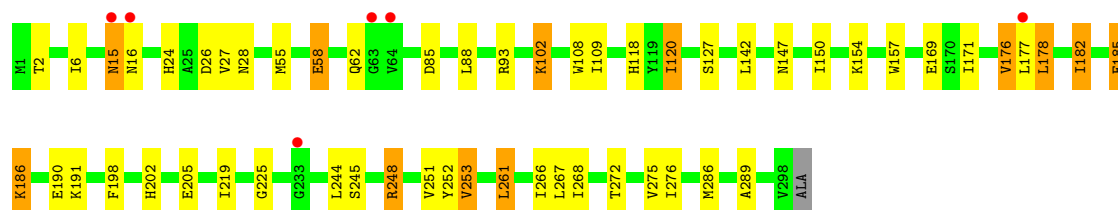
• Molecule 1: ORF48

Chain AK: 82% 15% ..

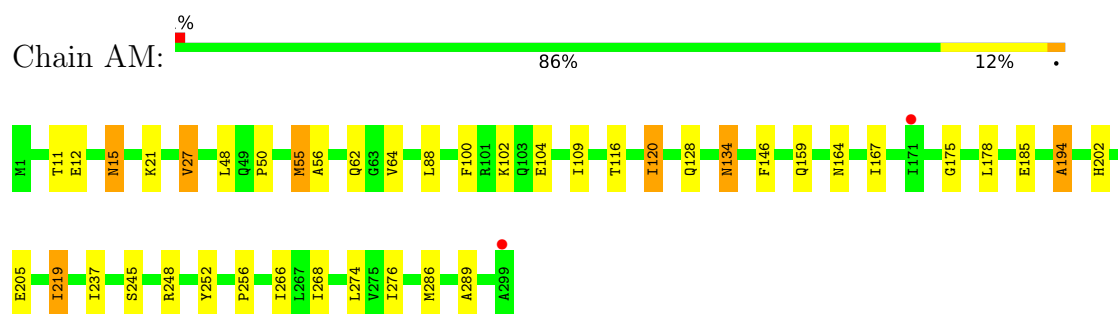


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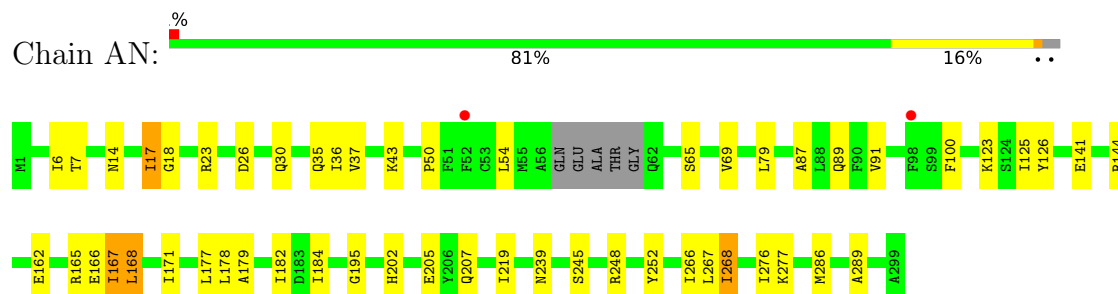
Chain AL: 81% 14% .



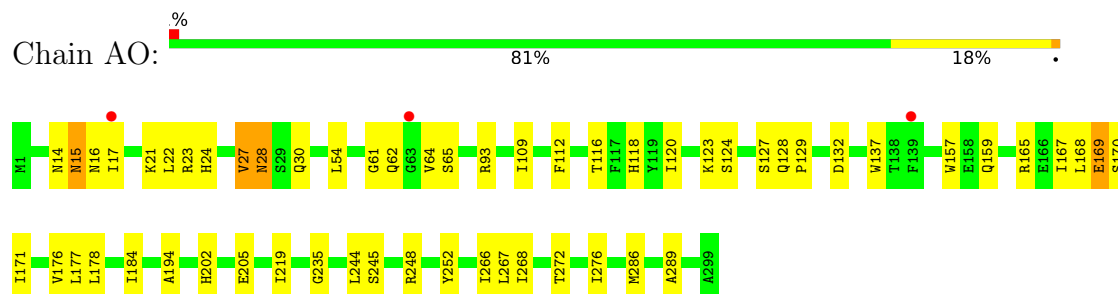
• Molecule 1: ORF48



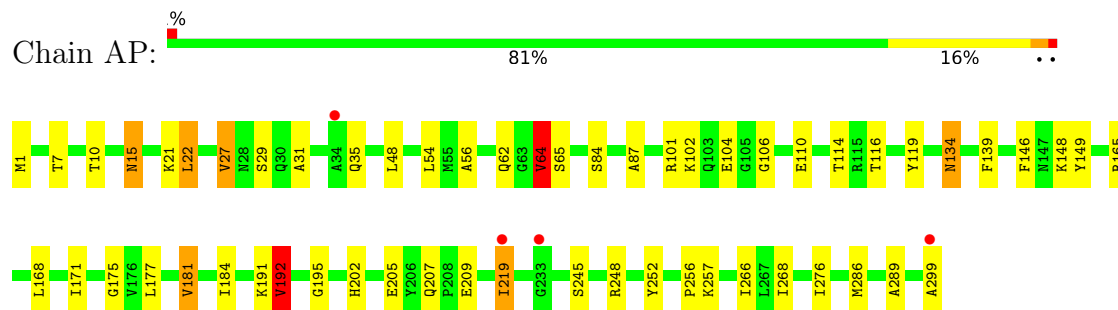
- Molecule 1: ORF48



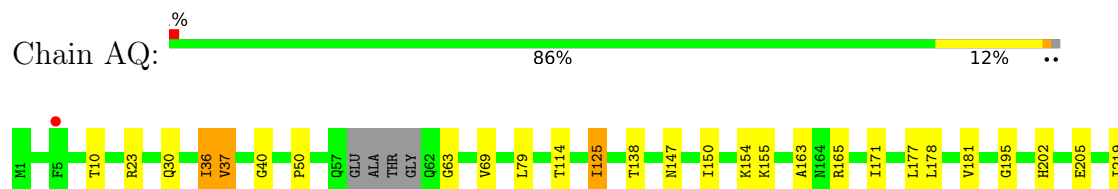
- Molecule 1: ORF48



- Molecule 1: ORF48

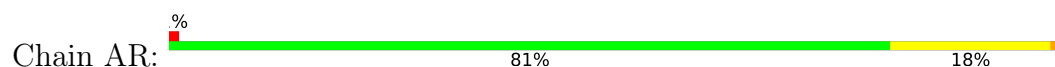


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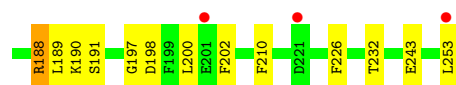
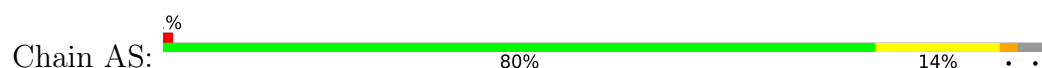




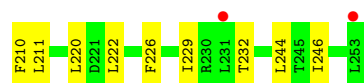
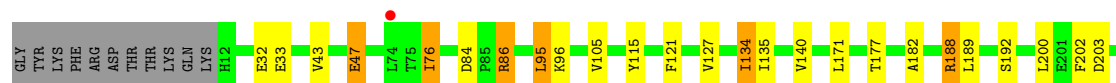
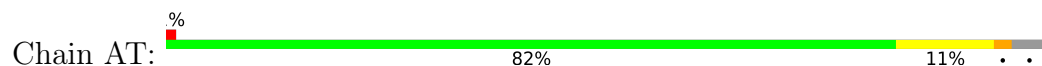
• Molecule 1: ORF48



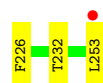
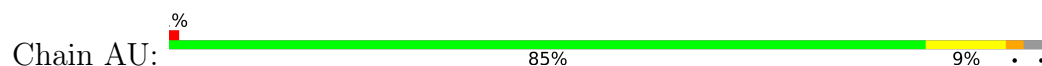
• Molecule 2: ORF46



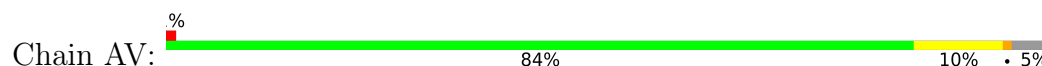
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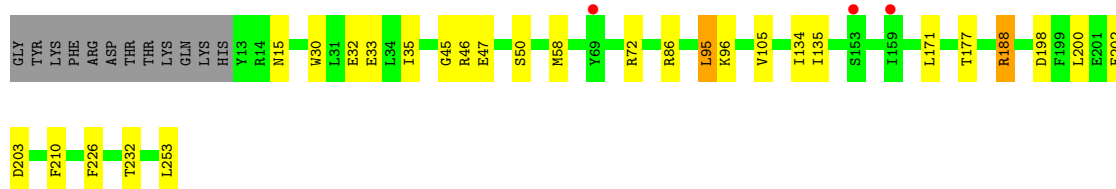


• Molecule 2: ORF46



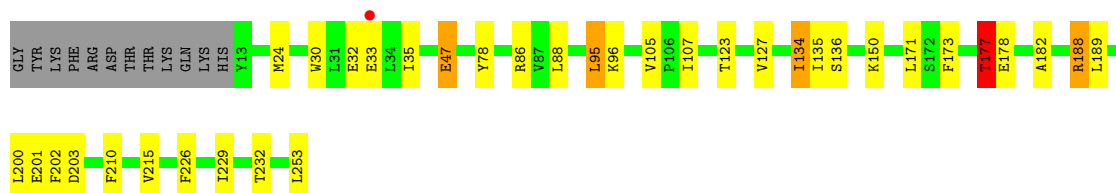
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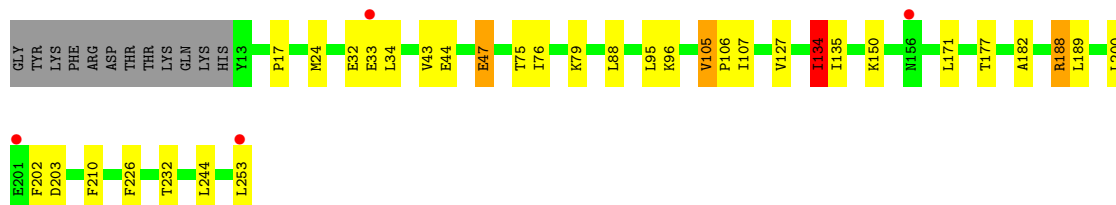
• Molecule 2: ORF46

Chain AW: 81% 12% • 5%



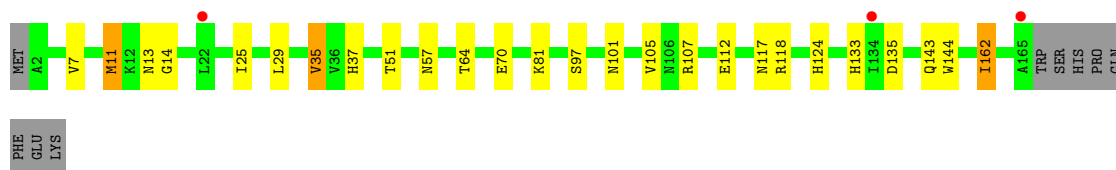
• Molecule 2: ORF46

Chain AX: 82% 12% • 5%



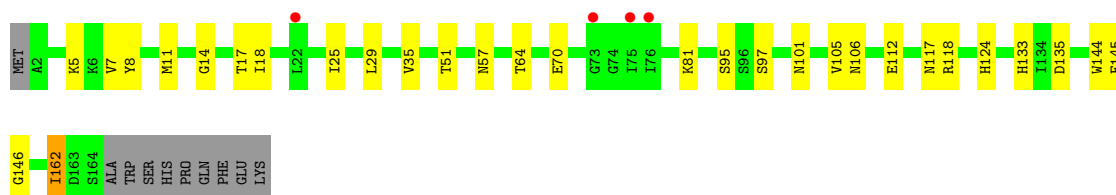
• Molecule 3: BPP

Chain BA: 80% 13% • 5%



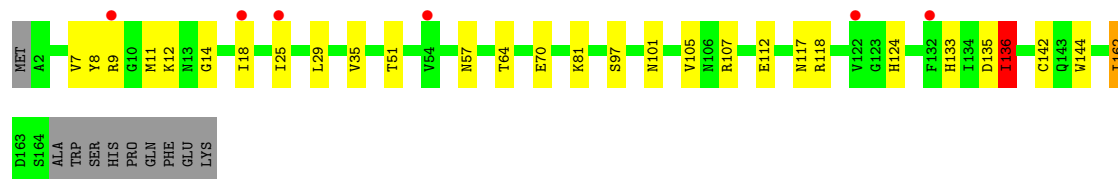
• Molecule 3: BPP

Chain BB: 77% 17% • 6%



• Molecule 3: BPP

Chain BC: 3% 77% 16% 6%



• Molecule 3: BPP

Chain BD: 2% 82% 13% 5%



• Molecule 3: BPP

Chain BE: 0% 83% 12% 5%



• Molecule 3: BPP

Chain BF: 0% 84% 10% 6%



• Molecule 3: BPP

Chain BG: 2% 83% 12% 5%



• Molecule 3: BPP

Chain BH: 0% 82% 12% 5%

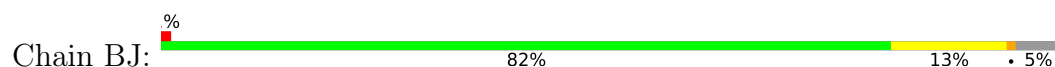


• Molecule 3: BPP

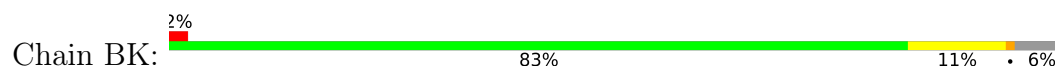
Chain BI: 2% 84% 10% 6%



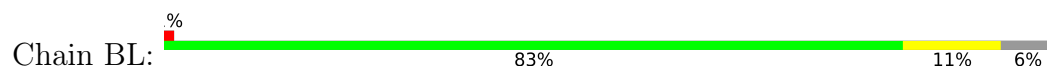
- Molecule 3: BPP



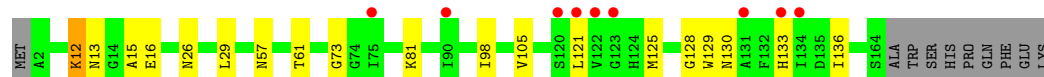
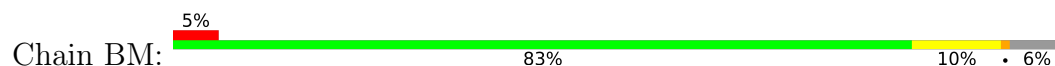
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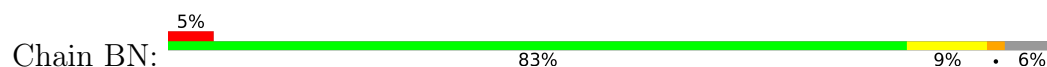
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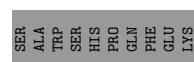
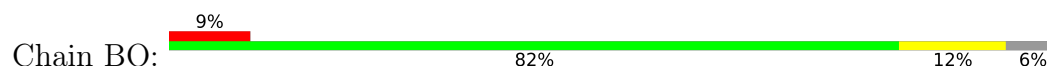
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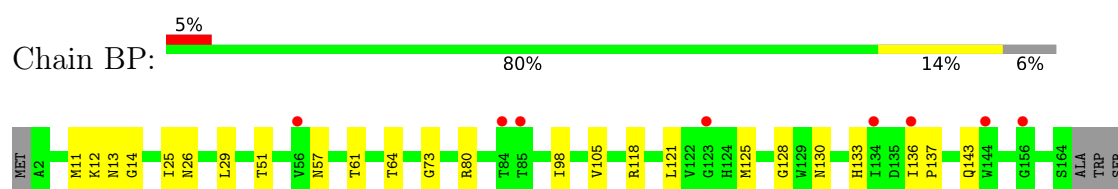
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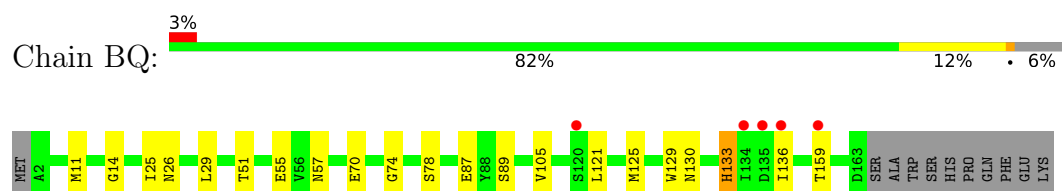
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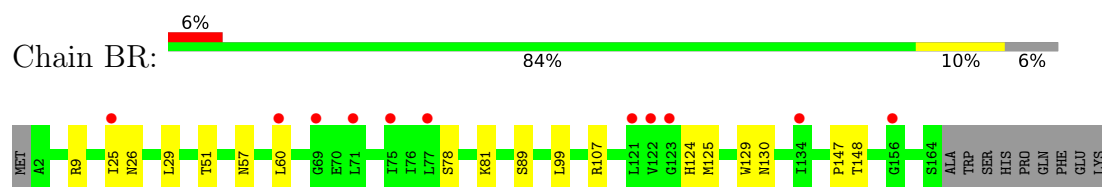
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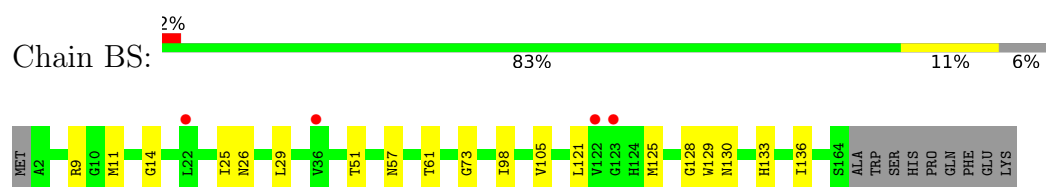
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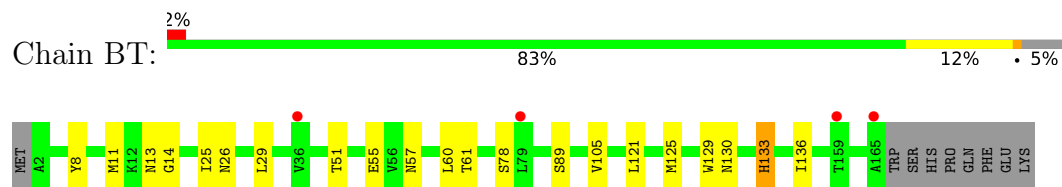
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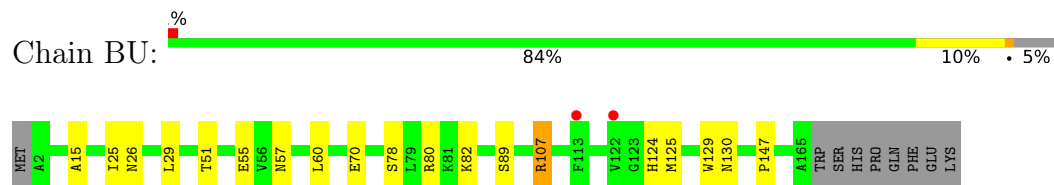
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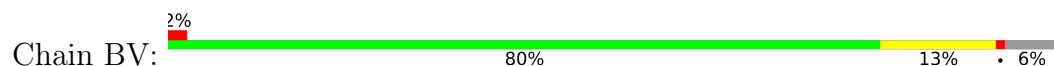
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• Molecule 3: BPP

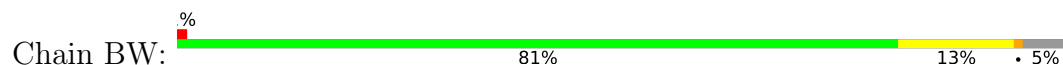


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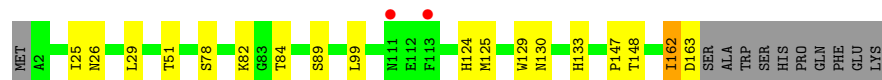
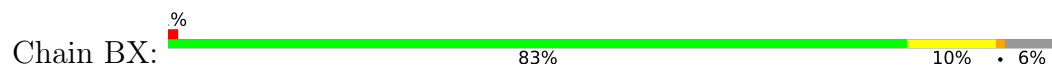




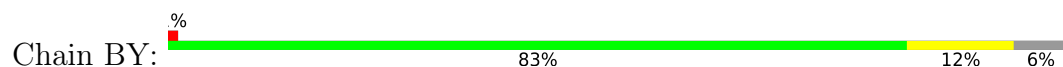
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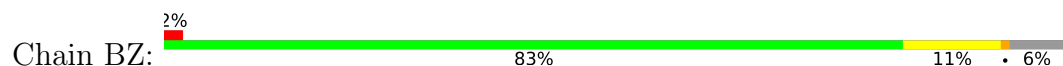
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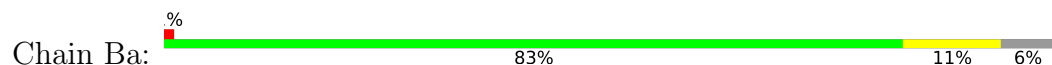
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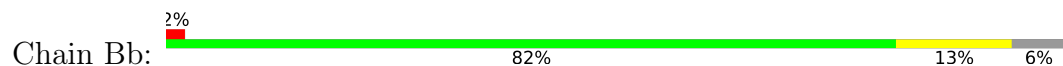
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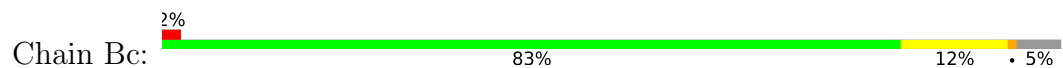
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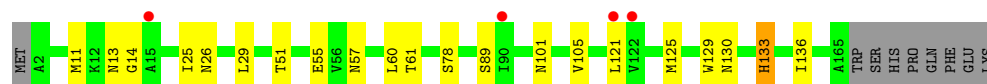


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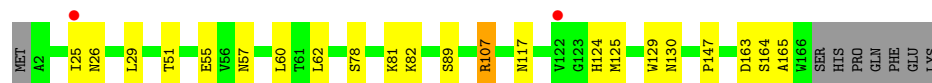
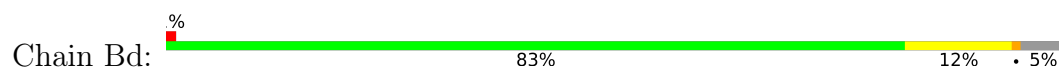


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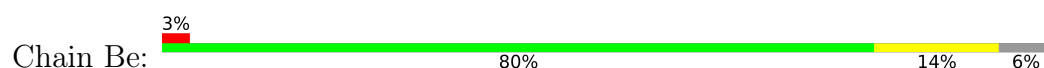




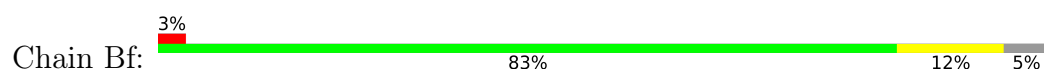
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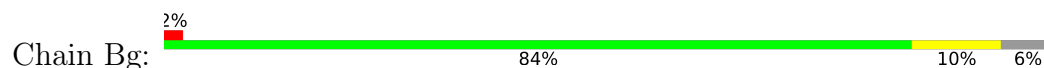
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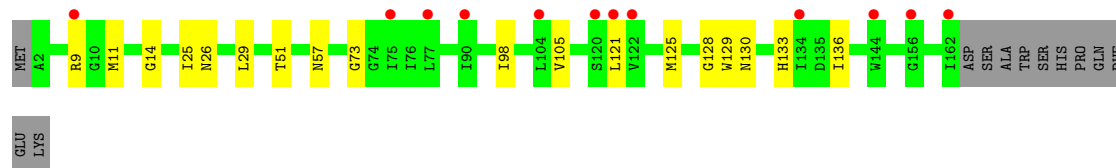
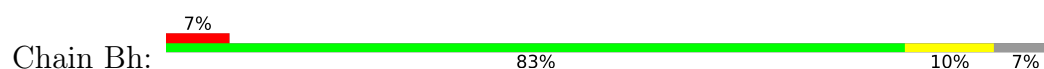
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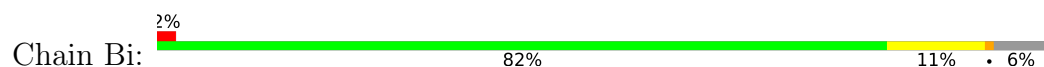
- Molecule 3: BPP



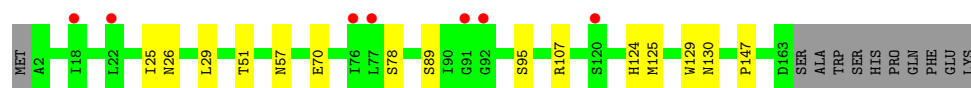
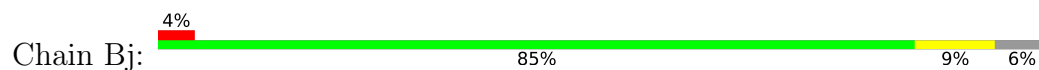
- Molecule 3: BPP



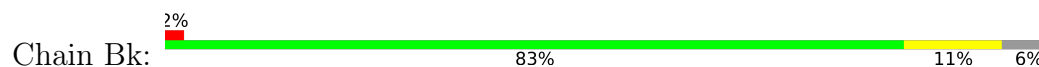
- Molecule 3: BPP



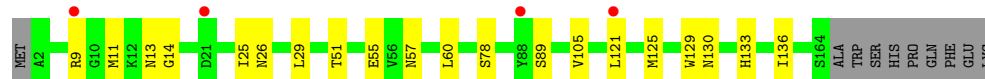
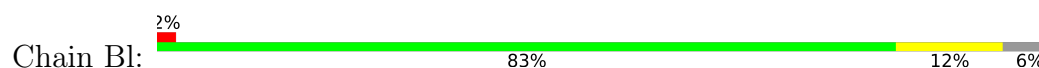
- Molecule 3: BPP



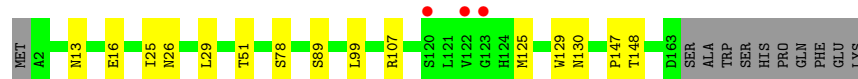
- Molecule 3: BPP



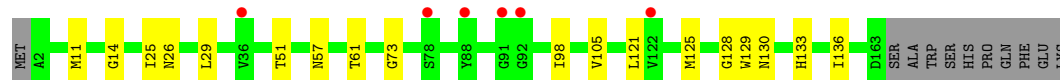
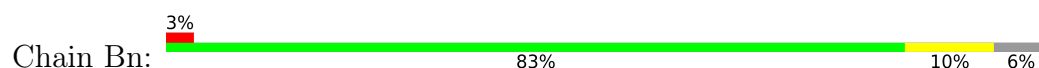
- Molecule 3: BPP



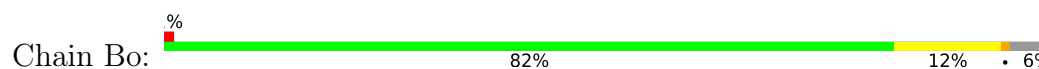
- Molecule 3: BPP



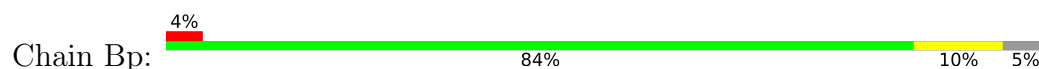
- Molecule 3: BPP



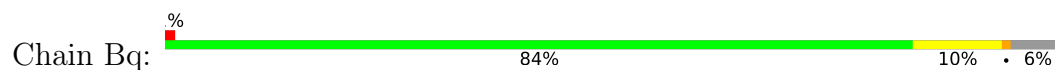
- Molecule 3: BPP



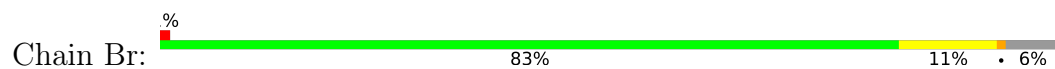
- Molecule 3: BPP



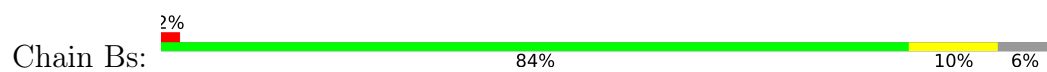
• Molecule 3: BPP



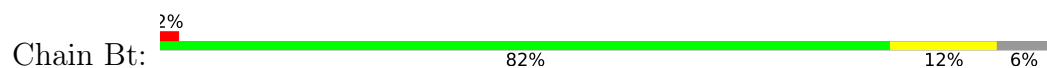
• Molecule 3: BPP



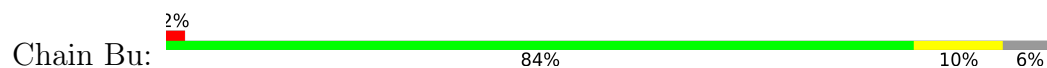
• Molecule 3: BPP



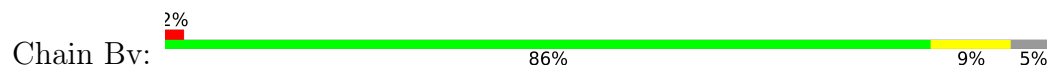
• Molecule 3: BPP



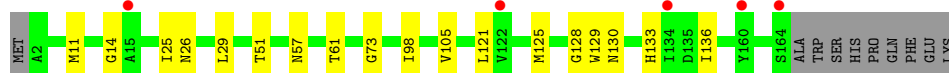
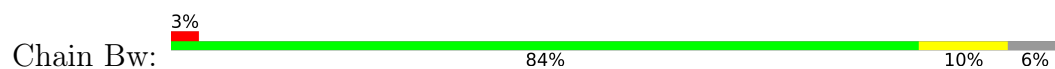
• Molecule 3: BPP



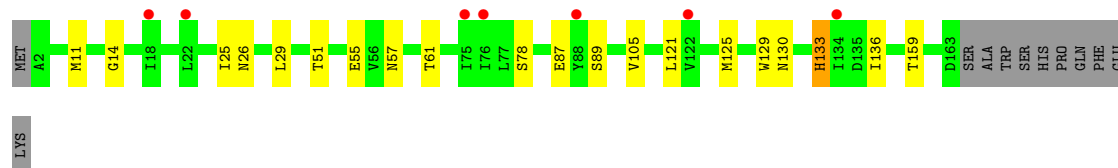
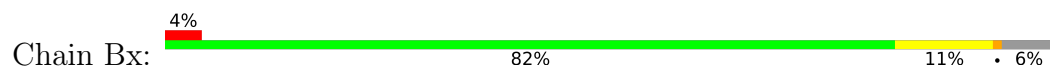
• Molecule 3: BPP



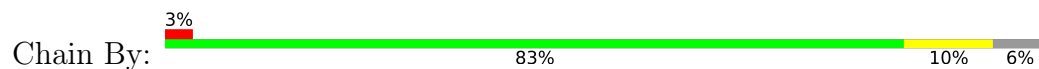
• Molecule 3: BPP



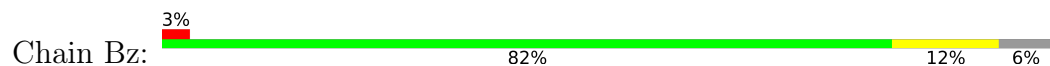
• Molecule 3: BPP



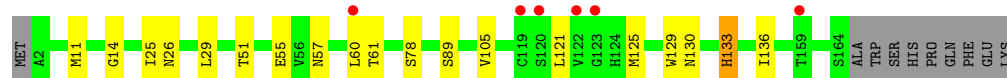
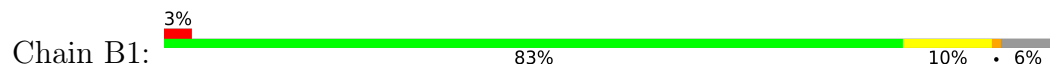
• Molecule 3: BPP



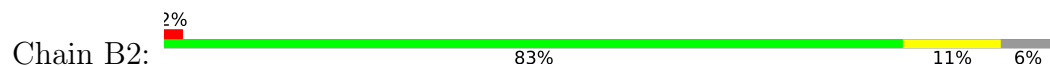
• Molecule 3: BPP



• Molecule 3: BPP



• Molecule 3: BPP



4 Data and refinement statistics

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) 99.4 (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)	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	1424 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å ²)	123.5	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 116.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	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.*

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 ⓘ

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	0.76	0/2444	1.23	9/3307 (0.3%)
1	AB	0.72	0/2398	1.20	6/3243 (0.2%)
1	AC	0.77	0/2444	1.20	9/3306 (0.3%)
1	AD	0.65	0/2448	1.09	4/3311 (0.1%)
1	AE	0.69	0/2390	1.11	5/3233 (0.2%)
1	AF	0.69	0/2444	1.12	3/3307 (0.1%)
1	AG	0.66	0/2441	1.08	3/3302 (0.1%)
1	AH	0.67	0/2396	1.10	3/3242 (0.1%)
1	AI	0.69	0/2444	1.11	5/3307 (0.2%)
1	AJ	0.66	0/2448	1.09	3/3311 (0.1%)
1	AK	0.71	1/2373 (0.0%)	1.11	4/3214 (0.1%)
1	AL	0.73	1/2437 (0.0%)	1.15	4/3298 (0.1%)
1	AM	0.68	1/2444 (0.0%)	1.08	4/3307 (0.1%)
1	AN	0.70	0/2381	1.12	4/3223 (0.1%)
1	AO	0.71	0/2448	1.14	5/3311 (0.2%)
1	AP	0.66	0/2437	1.07	4/3298 (0.1%)
1	AQ	0.67	0/2401	1.09	1/3250 (0.0%)
1	AR	0.71	0/2445	1.14	4/3307 (0.1%)
2	AS	0.70	0/1972	1.11	4/2669 (0.1%)
2	AT	0.71	0/1972	1.10	2/2670 (0.1%)
2	AU	0.71	0/1965	1.10	2/2661 (0.1%)
2	AV	0.68	0/1938	1.09	1/2625 (0.0%)
2	AW	0.65	0/1957	1.09	4/2649 (0.2%)
2	AX	0.69	0/1952	1.08	3/2643 (0.1%)
3	B1	0.62	0/1222	1.00	1/1655 (0.1%)
3	B2	0.65	0/1216	0.99	1/1647 (0.1%)
3	BA	0.66	1/1221 (0.1%)	1.03	1/1655 (0.1%)
3	BB	0.68	0/1216	1.04	2/1648 (0.1%)
3	BC	0.68	0/1216	1.03	2/1648 (0.1%)
3	BD	0.66	0/1221	1.00	2/1655 (0.1%)
3	BE	0.63	0/1221	0.99	1/1655 (0.1%)
3	BF	0.63	0/1216	0.99	0/1648
3	BG	0.65	0/1221	1.03	1/1655 (0.1%)
3	BH	0.65	0/1227	0.99	1/1662 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	BI	0.63	0/1216	1.00	0/1648
3	BJ	0.67	0/1221	1.03	3/1655 (0.2%)
3	BK	0.63	0/1216	0.99	1/1648 (0.1%)
3	BL	0.66	0/1216	1.01	1/1648 (0.1%)
3	BM	0.67	0/1216	1.02	2/1648 (0.1%)
3	BN	0.67	0/1210	1.02	0/1640
3	BO	0.67	0/1210	1.06	3/1640 (0.2%)
3	BP	0.68	0/1216	1.03	1/1648 (0.1%)
3	BQ	0.65	0/1216	1.00	1/1647 (0.1%)
3	BR	0.64	0/1216	1.00	0/1648
3	BS	0.65	0/1216	1.00	1/1648 (0.1%)
3	BT	0.66	0/1221	0.99	1/1655 (0.1%)
3	BU	0.64	0/1221	0.99	0/1655
3	BV	0.68	1/1216 (0.1%)	1.07	2/1648 (0.1%)
3	BW	0.66	0/1221	1.00	1/1655 (0.1%)
3	BX	0.62	0/1210	1.06	2/1640 (0.1%)
3	BY	0.65	0/1216	1.01	2/1648 (0.1%)
3	BZ	0.64	0/1216	1.00	0/1648
3	Ba	0.63	0/1216	1.00	0/1647
3	Bb	0.66	0/1216	1.00	2/1648 (0.1%)
3	Bc	0.65	0/1220	1.00	1/1654 (0.1%)
3	Bd	0.65	0/1231	1.01	1/1668 (0.1%)
3	Be	0.66	0/1216	1.01	1/1648 (0.1%)
3	Bf	0.67	0/1221	1.00	1/1655 (0.1%)
3	Bg	0.64	0/1216	1.01	2/1648 (0.1%)
3	Bh	0.66	0/1208	1.00	1/1636 (0.1%)
3	Bi	0.65	0/1210	1.00	1/1640 (0.1%)
3	Bj	0.66	0/1216	1.01	0/1647
3	Bk	0.66	0/1216	0.99	1/1648 (0.1%)
3	Bl	0.64	0/1216	1.00	1/1648 (0.1%)
3	Bm	0.66	0/1210	1.00	1/1640 (0.1%)
3	Bn	0.67	0/1216	0.99	1/1647 (0.1%)
3	Bo	0.65	0/1216	0.99	1/1647 (0.1%)
3	Bp	0.66	0/1227	0.98	0/1662
3	Bq	0.67	1/1222 (0.1%)	1.00	1/1655 (0.1%)
3	Br	0.65	0/1216	1.00	1/1648 (0.1%)
3	Bs	0.66	0/1216	1.00	0/1648
3	Bt	0.67	0/1210	1.00	1/1640 (0.1%)
3	Bu	0.66	0/1216	1.00	0/1647
3	Bv	0.66	0/1221	1.01	0/1655
3	Bw	0.67	0/1216	1.00	1/1648 (0.1%)
3	Bx	0.65	0/1216	1.01	1/1647 (0.1%)
3	By	0.64	0/1216	1.01	0/1647

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	Bz	0.63	0/1222	1.00	1/1655 (0.1%)
All	All	0.67	6/121148 (0.0%)	1.06	150/164062 (0.1%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AK	278	GLU	C-O	-7.96	1.17	1.24
3	BV	162	ILE	C-N	-7.56	1.22	1.33
1	AM	159	GLN	C-N	-6.06	1.25	1.33
1	AL	55	MET	SD-CE	5.74	1.93	1.79
3	Bq	11	MET	SD-CE	-5.67	1.65	1.79
3	BA	11	MET	SD-CE	-5.26	1.66	1.79

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BV	162	ILE	CB-CA-C	13.71	127.31	111.55
3	BX	162	ILE	CB-CA-C	11.01	126.99	112.24
1	AB	268	ILE	CB-CA-C	10.08	122.67	111.59
1	AD	162	GLU	CB-CG-CD	9.03	127.95	112.60
1	AH	268	ILE	CB-CA-C	8.96	121.44	111.59
1	AE	268	ILE	CB-CA-C	8.93	121.41	111.59
1	AK	192	VAL	CB-CA-C	8.92	119.24	110.94
1	AQ	268	ILE	CB-CA-C	8.84	121.31	111.59
3	BX	163	ASP	N-CA-CB	-8.64	95.81	110.50
1	AO	169	GLU	N-CA-C	8.45	120.27	111.14
3	BO	161	PRO	O-C-N	-8.29	112.88	123.00
1	AR	180	LYS	N-CA-C	8.07	119.71	111.07
1	AR	28	ASN	N-CA-C	8.07	122.52	111.39
1	AP	192	VAL	CB-CA-C	7.97	118.50	109.89
1	AM	194	ALA	N-CA-C	7.94	127.70	110.80
3	BO	161	PRO	CA-C-N	7.92	130.78	121.84
3	BO	161	PRO	C-N-CA	7.92	130.78	121.84
1	AF	28	ASN	N-CA-C	7.76	121.86	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	268	ILE	CB-CA-C	7.59	123.00	111.68
1	AC	194	ALA	N-CA-C	7.18	126.11	110.80
3	BM	12	LYS	N-CA-C	-7.11	99.51	110.10
1	AR	179	ALA	CB-CA-C	7.05	121.95	110.88
1	AJ	83	ALA	CB-CA-C	6.98	121.31	109.72
3	BC	105	VAL	N-CA-C	6.94	118.99	111.77
3	BA	105	VAL	N-CA-C	6.86	118.91	111.77
3	BB	105	VAL	N-CA-C	6.83	118.87	111.77
1	AO	28	ASN	N-CA-C	6.78	120.52	111.30
1	AA	192	VAL	CB-CA-C	6.76	123.67	111.36
1	AK	268	ILE	CB-CA-C	6.69	122.27	111.29
2	AW	177	THR	CA-C-N	6.50	129.47	120.63
2	AW	177	THR	C-N-CA	6.50	129.47	120.63
1	AG	192	VAL	CB-CA-C	6.49	123.17	111.36
1	AC	15	ASN	CA-CB-CG	6.43	119.03	112.60
1	AN	195	GLY	N-CA-C	6.34	128.20	113.18
1	AN	268	ILE	CB-CA-C	6.26	121.55	111.29
1	AR	15	ASN	CA-CB-CG	6.20	118.80	112.60
2	AW	188	ARG	CB-CA-C	6.18	120.02	110.14
1	AL	15	ASN	CA-CB-CG	6.17	118.77	112.60
1	AG	185	GLU	CA-C-N	6.16	128.86	120.54
1	AG	185	GLU	C-N-CA	6.16	128.86	120.54
1	AI	15	ASN	CA-CB-CG	6.11	118.71	112.60
3	Bd	164	SER	N-CA-C	6.09	119.32	110.42
1	AF	15	ASN	CA-CB-CG	6.07	118.67	112.60
1	AB	24	HIS	N-CA-C	6.05	117.54	111.07
1	AC	101	ARG	N-CA-C	6.05	118.37	109.24
1	AD	151	GLU	CB-CG-CD	5.95	122.72	112.60
1	AA	122	GLU	CA-C-N	5.92	129.28	120.87
1	AA	122	GLU	C-N-CA	5.92	129.28	120.87
1	AH	152	ASP	CA-CB-CG	5.90	118.50	112.60
3	BG	105	VAL	N-CA-C	5.87	117.81	112.29
1	AC	70	VAL	N-CA-C	5.81	117.33	111.00
2	AT	115	TYR	CB-CA-C	5.80	122.40	110.40
3	BJ	16	GLU	CA-C-N	5.80	128.05	120.28
3	BJ	16	GLU	C-N-CA	5.80	128.05	120.28
1	AB	268	ILE	N-CA-C	-5.73	103.81	110.05
3	BV	105	VAL	N-CA-C	5.70	117.64	112.29
3	Bk	105	VAL	N-CA-C	5.69	117.64	112.29
1	AP	268	ILE	N-CA-C	-5.68	101.71	109.55
3	BT	105	VAL	N-CA-C	5.67	117.55	112.17
3	Bw	105	VAL	N-CA-C	5.65	117.60	112.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	BS	105	VAL	N-CA-C	5.63	117.58	112.29
3	BP	105	VAL	N-CA-C	5.61	117.56	112.29
1	AO	109	ILE	CB-CA-C	5.60	116.47	111.71
3	BJ	105	VAL	N-CA-C	5.60	117.55	112.29
3	Bz	105	VAL	N-CA-C	5.59	117.55	112.29
1	AC	26	ASP	N-CA-C	5.58	117.56	108.63
1	AO	15	ASN	CA-CB-CG	5.57	118.17	112.60
3	BC	136	ILE	CB-CG1-CD1	5.57	125.49	113.80
3	Bm	16	GLU	CB-CG-CD	5.55	122.03	112.60
1	AA	288	ASP	N-CA-C	5.54	119.61	112.86
3	BY	105	VAL	N-CA-C	5.53	117.49	112.29
1	AD	194	ALA	N-CA-C	5.53	122.58	110.80
2	AU	188	ARG	CB-CA-C	5.51	118.95	110.14
1	AE	26	ASP	CA-C-N	5.50	127.60	120.56
1	AE	26	ASP	C-N-CA	5.50	127.60	120.56
2	AT	188	ARG	CB-CA-C	5.46	118.88	110.14
3	Bt	105	VAL	N-CA-C	5.45	117.42	112.29
3	BY	153	THR	CB-CA-C	5.44	115.56	110.17
1	AA	268	ILE	N-CA-C	-5.44	100.52	109.12
2	AS	198	ASP	N-CA-C	5.44	118.70	111.30
2	AW	134	ILE	N-CA-C	5.44	115.78	108.17
3	Bh	105	VAL	N-CA-C	5.42	117.39	112.29
3	Bb	153	THR	CB-CA-C	5.42	115.54	110.17
3	Bc	105	VAL	N-CA-C	5.42	117.32	112.17
3	Br	105	VAL	N-CA-C	5.42	117.32	112.17
1	AA	24	HIS	N-CA-C	5.41	117.60	111.11
3	BK	105	VAL	N-CA-C	5.41	117.31	112.17
1	AI	45	PHE	CA-CB-CG	5.40	119.20	113.80
3	BD	105	VAL	N-CA-C	5.39	117.35	112.29
3	Bf	105	VAL	N-CA-C	5.38	117.28	112.17
1	AA	70	VAL	N-CA-C	5.37	115.58	110.53
3	Be	105	VAL	N-CA-C	5.37	117.33	112.29
1	AI	152	ASP	CA-CB-CG	5.37	117.97	112.60
2	AS	188	ARG	CB-CA-C	5.36	118.71	110.14
3	Bi	105	VAL	N-CA-C	5.35	117.25	112.17
1	AK	195	GLY	N-CA-C	5.35	125.86	113.18
3	Bn	105	VAL	N-CA-C	5.35	117.32	112.29
3	BE	105	VAL	N-CA-C	5.34	117.25	112.17
1	AB	170	SER	N-CA-C	5.34	119.31	111.04
1	AO	194	ALA	N-CA-C	5.33	122.15	110.80
1	AC	24	HIS	N-CA-C	5.32	117.08	111.28
2	AS	75	THR	CB-CA-C	5.30	118.50	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AK	170	SER	N-CA-C	5.29	119.24	111.04
1	AA	246	TYR	N-CA-C	5.28	118.06	109.24
3	Bo	105	VAL	N-CA-C	5.28	117.19	112.17
2	AX	47	GLU	N-CA-C	5.28	117.94	111.82
3	Bq	105	VAL	N-CA-C	5.27	117.25	112.29
3	B1	105	VAL	N-CA-C	5.26	117.17	112.17
3	B2	105	VAL	N-CA-C	5.25	118.03	112.83
1	AN	165	ARG	CA-C-N	5.25	127.85	120.28
1	AN	165	ARG	C-N-CA	5.25	127.85	120.28
3	Bb	105	VAL	N-CA-C	5.25	117.22	112.29
2	AX	188	ARG	CB-CA-C	5.24	118.53	110.14
1	AF	195	GLY	N-CA-C	5.24	120.11	113.24
1	AE	17	ILE	CA-C-N	5.23	125.07	120.10
1	AE	17	ILE	C-N-CA	5.23	125.07	120.10
1	AM	164	ASN	CA-C-N	5.23	127.24	120.44
1	AM	164	ASN	C-N-CA	5.23	127.24	120.44
3	BM	105	VAL	N-CA-C	5.22	117.19	112.29
1	AC	158	GLU	CA-C-N	5.20	127.68	120.29
1	AC	158	GLU	C-N-CA	5.20	127.68	120.29
3	Bl	105	VAL	N-CA-C	5.20	117.11	112.17
1	AP	64	VAL	N-CA-CB	5.20	116.19	110.53
3	BD	153	THR	CB-CA-C	5.20	115.31	110.17
3	Bg	13	ASN	CA-C-N	5.19	125.71	120.00
3	Bg	13	ASN	C-N-CA	5.19	125.71	120.00
3	Bx	105	VAL	N-CA-C	5.19	117.10	112.17
3	BL	38	LYS	CG-CD-CE	5.18	123.22	111.30
2	AV	188	ARG	CB-CA-C	5.16	118.39	110.14
1	AH	192	VAL	CB-CA-C	5.14	120.71	111.36
1	AL	176	VAL	CA-C-N	5.13	127.11	120.44
1	AL	176	VAL	C-N-CA	5.13	127.11	120.44
3	BB	146	GLY	N-CA-C	-5.13	106.02	112.23
3	BH	105	VAL	N-CA-C	5.12	117.04	112.17
1	AM	268	ILE	N-CA-C	-5.11	102.50	109.55
1	AB	70	VAL	N-CA-C	5.10	115.32	110.53
1	AJ	24	HIS	N-CA-C	5.10	116.53	111.07
1	AJ	268	ILE	N-CA-C	-5.09	102.53	109.55
1	AB	101	ARG	N-CA-C	5.08	117.40	109.52
3	BQ	105	VAL	N-CA-C	5.08	117.00	112.17
1	AP	101	ARG	N-CA-C	5.08	117.53	109.50
1	AI	12	GLU	CB-CG-CD	5.06	121.21	112.60
1	AI	28	ASN	N-CA-C	5.05	121.56	110.80
1	AC	217	ASN	N-CA-C	5.05	118.74	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AL	26	ASP	CA-CB-CG	5.03	117.63	112.60
2	AS	72	ARG	N-CA-C	5.03	118.41	109.96
1	AD	101	ARG	N-CA-C	5.03	117.03	109.23
3	BW	105	VAL	N-CA-C	5.03	117.72	112.90
2	AU	217	ASN	CA-CB-CG	5.02	117.62	112.60
2	AX	134	ILE	N-CA-C	5.01	115.52	108.36

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 ⓘ

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	62	0
1	AB	2345	0	2295	37	0
1	AC	2389	0	2340	49	0
1	AD	2393	0	2344	31	0
1	AE	2336	0	2292	28	0
1	AF	2389	0	2333	29	0
1	AG	2386	0	2338	34	0
1	AH	2343	0	2280	26	0
1	AI	2389	0	2333	36	0
1	AJ	2393	0	2344	31	0
1	AK	2320	0	2246	38	0
1	AL	2382	0	2330	40	0
1	AM	2389	0	2333	27	0
1	AN	2328	0	2253	30	0
1	AO	2393	0	2344	32	0
1	AP	2382	0	2327	34	0
1	AQ	2347	0	2281	22	0
1	AR	2390	0	2335	38	0
2	AS	1932	0	1882	31	0
2	AT	1931	0	1886	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AU	1924	0	1879	20	0
2	AV	1899	0	1836	18	0
2	AW	1917	0	1865	33	0
2	AX	1913	0	1867	22	0
3	B1	1200	0	1182	15	0
3	B2	1194	0	1177	15	0
3	BA	1199	0	1176	22	0
3	BB	1194	0	1171	21	0
3	BC	1194	0	1171	22	0
3	BD	1199	0	1176	18	0
3	BE	1199	0	1176	16	0
3	BF	1194	0	1171	16	0
3	BG	1199	0	1176	17	0
3	BH	1205	0	1187	17	0
3	BI	1194	0	1171	18	0
3	BJ	1199	0	1176	17	0
3	BK	1194	0	1171	15	0
3	BL	1194	0	1171	13	0
3	BM	1194	0	1171	14	0
3	BN	1188	0	1166	15	0
3	BO	1188	0	1166	16	0
3	BP	1194	0	1171	22	0
3	BQ	1194	0	1177	16	0
3	BR	1194	0	1171	14	0
3	BS	1194	0	1171	15	0
3	BT	1199	0	1176	18	0
3	BU	1199	0	1176	20	0
3	BV	1194	0	1171	15	0
3	BW	1199	0	1176	17	0
3	BX	1188	0	1166	14	0
3	BY	1194	0	1171	13	0
3	BZ	1194	0	1171	19	0
3	Ba	1194	0	1177	15	0
3	Bb	1194	0	1171	14	0
3	Bc	1198	0	1173	17	0
3	Bd	1209	0	1186	15	0
3	Be	1194	0	1171	17	0
3	Bf	1199	0	1176	16	0
3	Bg	1194	0	1171	14	0
3	Bh	1186	0	1173	13	0
3	Bi	1188	0	1166	19	0
3	Bj	1194	0	1177	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Bk	1194	0	1171	13	0
3	Bl	1194	0	1171	14	0
3	Bm	1188	0	1166	11	0
3	Bn	1194	0	1177	14	0
3	Bo	1194	0	1177	16	0
3	Bp	1205	0	1187	15	0
3	Bq	1200	0	1182	13	0
3	Br	1194	0	1171	16	0
3	Bs	1194	0	1171	15	0
3	Bt	1188	0	1166	15	0
3	Bu	1194	0	1177	13	0
3	Bv	1199	0	1176	13	0
3	Bw	1194	0	1171	13	0
3	Bx	1194	0	1177	15	0
3	By	1194	0	1177	13	0
3	Bz	1200	0	1182	14	0
All	All	118740	0	116288	1180	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 5.

All (1180) 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
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
3:BA:143:GLN:HE22	3:Bg:95:SER:HB2	1.16	1.08
1:AO:21:LYS:HG3	1:AO:120:ILE:HG13	1.36	1.04
1:AR:21:LYS:HG2	1:AR:120:ILE:HD11	1.42	0.99
1:AI:108:TRP:HZ2	1:AK:125:ILE:CD1	1.71	0.98
2:AW:127:VAL:CG2	2:AW:134:ILE:HD11	1.92	0.95
2:AW:127:VAL:HG23	2:AW:134:ILE:HD11	0.95	0.95
2:AW:253:LEU:OXT	2:AX:96:LYS:HD2	1.66	0.95
1:AB:13:PRO:HA	1:AB:115:ARG:HE	1.29	0.95
1:AG:168:LEU:HD21	1:AH:168:LEU:HD11	1.49	0.94
1:AA:12:GLU:O	1:AA:115:ARG:HD3	1.71	0.91
1:AI:108:TRP:HZ2	1:AK:125:ILE:HD11	1.08	0.89
2:AV:253:LEU:OXT	2:AW:96:LYS:HD2	1.74	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AS:253:LEU:OXT	2:AT:96:LYS:HD2	1.77	0.84
1:AR:179:ALA:O	1:AR:182:ILE:HG22	1.78	0.83
1:AP:177:LEU:HD11	1:AQ:181:VAL:HG11	1.59	0.83
2:AS:96:LYS:HD2	2:AX:253:LEU:OXT	1.79	0.83
2:AV:188:ARG:O	2:AV:226:PHE:HD2	1.62	0.82
1:AB:12:GLU:O	1:AB:115:ARG:HD3	1.80	0.82
1:AA:49:GLN:HE21	1:AA:50:PRO:HD2	1.44	0.82
3:BC:7:VAL:HG13	3:BC:11:MET:HE1	1.62	0.81
2:AW:188:ARG:O	2:AW:226:PHE:HD2	1.63	0.81
1:AA:179:ALA:O	1:AA:182:ILE:HG22	1.81	0.80
1:AG:12:GLU:OE1	2:AS:150:LYS:HE2	1.81	0.80
1:AR:245:SER:HB2	1:AR:252:TYR:HB2	1.64	0.80
2:AU:188:ARG:O	2:AU:226:PHE:HD2	1.64	0.79
1:AC:202:HIS:HB3	1:AC:286:MET:HE1	1.65	0.79
1:AA:202:HIS:HB3	1:AA:286:MET:HE1	1.64	0.78
2:AT:188:ARG:O	2:AT:226:PHE:HD2	1.66	0.78
1:AA:165:ARG:HH22	1:AC:171:ILE:HG21	1.49	0.78
3:BA:143:GLN:NE2	3:Bg:95:SER:HB2	1.96	0.77
2:AS:188:ARG:O	2:AS:226:PHE:HD2	1.68	0.77
1:AA:202:HIS:CB	1:AA:286:MET:HE1	2.14	0.76
1:AD:191:LYS:HD3	1:AE:193:PRO:O	1.83	0.76
2:AX:188:ARG:O	2:AX:226:PHE:HD2	1.67	0.76
1:AM:104:GLU:HB2	1:AM:109:ILE:HD11	1.66	0.75
1:AG:245:SER:HB3	1:AG:252:TYR:HB2	1.68	0.75
1:AI:108:TRP:CH2	1:AK:125:ILE:CD1	2.62	0.75
1:AJ:12:GLU:OE1	2:AX:150:LYS:HE2	1.87	0.74
1:AA:13:PRO:HA	1:AA:115:ARG:HE	1.53	0.74
1:AJ:245:SER:HB3	1:AJ:252:TYR:HB2	1.67	0.74
1:AP:165:ARG:HH12	1:AR:171:ILE:HG22	1.50	0.74
3:BN:103:ASN:HD21	3:BN:141:VAL:HG12	1.52	0.73
1:AA:286:MET:HE3	1:AA:289:ALA:HB3	1.70	0.73
3:BP:12:LYS:HG2	3:BP:13:ASN:ND2	2.04	0.73
1:AA:15:ASN:HD22	1:AA:15:ASN:H	1.35	0.72
1:AP:165:ARG:HH12	1:AR:171:ILE:CG2	2.02	0.72
3:BJ:138:SER:HB2	3:BU:107:ARG:NH2	2.05	0.71
1:AA:11:THR:HG21	1:AA:39:ASN:OD1	1.91	0.71
3:BB:106:ASN:OD1	3:Bf:138:SER:HB2	1.90	0.71
3:BP:13:ASN:HA	3:BR:9:ARG:HH21	1.55	0.71
1:AJ:266:ILE:HD12	1:AJ:276:ILE:HD12	1.72	0.71
1:AO:245:SER:HB3	1:AO:252:TYR:HB2	1.73	0.71
1:AA:104:GLU:HB2	1:AA:109:ILE:HD11	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AM:245:SER:HB3	1:AM:252:TYR:HB2	1.74	0.70
1:AD:245:SER:HB3	1:AD:252:TYR:HB2	1.73	0.70
1:AR:21:LYS:CG	1:AR:120:ILE:HD11	2.19	0.70
1:AC:202:HIS:CB	1:AC:286:MET:HE1	2.21	0.70
1:AI:245:SER:HB3	1:AI:252:TYR:HB2	1.71	0.70
3:BV:84:THR:HB	3:BV:163:ASP:OD1	1.91	0.70
1:AE:245:SER:HB3	1:AE:252:TYR:HB2	1.74	0.70
3:BB:7:VAL:HG13	3:BB:11:MET:HE1	1.72	0.69
1:AH:245:SER:HB3	1:AH:252:TYR:HB2	1.74	0.69
1:AN:167:ILE:HG12	1:AN:168:LEU:N	2.06	0.69
3:BP:12:LYS:HG2	3:BP:13:ASN:HD22	1.57	0.69
3:BA:133:HIS:HD2	3:BB:124:HIS:ND1	1.90	0.69
2:AW:202:PHE:HB2	2:AW:210:PHE:HB2	1.75	0.69
3:BA:124:HIS:ND1	3:BC:133:HIS:HD2	1.91	0.69
1:AJ:177:LEU:HD11	1:AL:177:LEU:HD21	1.75	0.68
3:BN:93:GLU:HG2	3:Ba:76:ILE:HG12	1.75	0.68
1:AL:85:ASP:HA	1:AL:88:LEU:HD12	1.75	0.68
2:AS:80:LEU:HB3	2:AS:134:ILE:HD11	1.75	0.68
1:AP:245:SER:HB2	1:AP:252:TYR:HB2	1.74	0.68
3:BB:133:HIS:HD2	3:BC:124:HIS:ND1	1.91	0.68
3:BA:7:VAL:HG13	3:BA:11:MET:HE1	1.76	0.68
3:BZ:121:LEU:HD11	3:BZ:136:ILE:HD11	1.76	0.68
1:AI:15:ASN:ND2	2:AS:33:GLU:OE2	2.27	0.67
1:AN:245:SER:HB3	1:AN:252:TYR:HB2	1.76	0.67
3:BD:138:SER:HB2	3:Bd:107:ARG:NH2	2.10	0.67
1:AO:93:ARG:HA	1:AO:120:ILE:HG22	1.77	0.66
2:AW:127:VAL:CG2	2:AW:134:ILE:HD12	2.21	0.66
1:AC:16:ASN:HB3	1:AC:118:HIS:HE1	1.59	0.66
2:AS:80:LEU:O	2:AS:134:ILE:HG13	1.94	0.66
2:AW:253:LEU:OXT	2:AX:96:LYS:CD	2.41	0.66
1:AK:245:SER:HB3	1:AK:252:TYR:HB2	1.76	0.66
3:BW:121:LEU:HD11	3:BW:136:ILE:HD11	1.77	0.66
1:AM:12:GLU:OE1	2:AW:150:LYS:HE2	1.96	0.66
1:AL:245:SER:HB3	1:AL:252:TYR:HB2	1.77	0.65
3:Br:121:LEU:HD11	3:Br:136:ILE:HD11	1.78	0.65
1:AR:179:ALA:O	1:AR:182:ILE:CG2	2.44	0.65
1:AP:207:GLN:NE2	3:BP:13:ASN:OD1	2.29	0.65
1:AQ:245:SER:HB3	1:AQ:252:TYR:HB2	1.77	0.65
3:Bl:121:LEU:HD11	3:Bl:136:ILE:HD11	1.79	0.65
1:AB:202:HIS:HB3	1:AB:286:MET:HE1	1.79	0.65
3:BT:121:LEU:HD11	3:BT:136:ILE:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AD:167:ILE:HG12	1:AE:173:PRO:HG2	1.77	0.65
3:BN:121:LEU:HD11	3:BN:136:ILE:HD11	1.79	0.65
3:BE:121:LEU:HD11	3:BE:136:ILE:HD11	1.79	0.65
3:Bu:121:LEU:HD11	3:Bu:136:ILE:HD11	1.79	0.65
1:AA:192:VAL:O	1:AA:256:PRO:HG3	1.96	0.64
1:AM:15:ASN:HD22	1:AM:15:ASN:H	1.45	0.64
1:AP:15:ASN:H	1:AP:15:ASN:HD22	1.45	0.64
3:BH:121:LEU:HD11	3:BH:136:ILE:HD11	1.78	0.64
1:AB:245:SER:HB3	1:AB:252:TYR:HB2	1.79	0.64
1:AF:195:GLY:HA3	1:AF:257:LYS:HG2	1.80	0.64
1:AK:177:LEU:HD23	1:AL:177:LEU:HD22	1.80	0.64
1:AK:266:ILE:HD13	1:AK:276:ILE:HD12	1.80	0.64
3:Bc:121:LEU:HD11	3:Bc:136:ILE:HD11	1.78	0.64
3:BQ:121:LEU:HD11	3:BQ:136:ILE:HD11	1.80	0.64
1:AH:266:ILE:HD13	1:AH:276:ILE:HD12	1.79	0.64
2:AS:92:PHE:HZ	2:AS:134:ILE:CD1	2.10	0.63
3:BK:121:LEU:HD11	3:BK:136:ILE:HD11	1.80	0.63
3:Bi:121:LEU:HD11	3:Bi:136:ILE:HD11	1.79	0.63
1:AA:165:ARG:HH22	1:AC:171:ILE:CG2	2.11	0.63
3:BP:143:GLN:HE22	3:Bj:95:SER:HB2	1.63	0.63
3:Bx:121:LEU:HD11	3:Bx:136:ILE:HD11	1.79	0.63
1:AI:16:ASN:HB3	1:AI:118:HIS:HE1	1.62	0.63
3:B1:121:LEU:HD11	3:B1:136:ILE:HD11	1.79	0.63
3:Bf:121:LEU:HD11	3:Bf:136:ILE:HD11	1.80	0.63
3:Bo:121:LEU:HD11	3:Bo:136:ILE:HD11	1.81	0.63
1:AJ:15:ASN:HD22	1:AJ:15:ASN:H	1.44	0.63
1:AD:15:ASN:H	1:AD:15:ASN:HD22	1.45	0.62
1:AE:266:ILE:HD13	1:AE:276:ILE:HD12	1.80	0.62
1:AG:168:LEU:CD2	1:AH:168:LEU:HD11	2.26	0.62
1:AD:191:LYS:HE3	1:AE:243:SER:OG	2.00	0.62
2:AS:92:PHE:HZ	2:AS:134:ILE:HD13	1.63	0.62
1:AD:179:ALA:O	1:AD:182:ILE:HG22	2.00	0.62
1:AH:6:ILE:HB	1:AH:17:ILE:HD11	1.80	0.62
1:AC:257:LYS:O	1:AC:260:THR:HG22	1.99	0.62
1:AA:267:LEU:HD23	1:AA:268:ILE:O	1.99	0.61
1:AL:16:ASN:HB3	1:AL:118:HIS:HE1	1.65	0.61
1:AC:286:MET:HE3	1:AC:289:ALA:HB3	1.82	0.61
1:AQ:266:ILE:HD13	1:AQ:276:ILE:HD12	1.83	0.61
1:AN:266:ILE:HD13	1:AN:276:ILE:HD12	1.80	0.61
3:BA:25:ILE:HG23	3:BB:29:LEU:HD11	1.83	0.61
1:AG:15:ASN:H	1:AG:15:ASN:HD22	1.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AP:171:ILE:HD11	1:AQ:177:LEU:HD11	1.82	0.60
1:AR:21:LYS:HG2	1:AR:120:ILE:CD1	2.23	0.60
1:AC:4:HIS:HB2	1:AC:32:ILE:HG22	1.83	0.60
3:BA:29:LEU:HD11	3:BC:25:ILE:HG23	1.84	0.60
3:Br:9:ARG:HH22	3:Bs:13:ASN:HA	1.67	0.60
1:AR:101:ARG:NH1	1:AR:108:TRP:HE1	2.00	0.60
2:AT:202:PHE:HB2	2:AT:210:PHE:HB2	1.84	0.60
1:AG:188:VAL:HG21	1:AI:184:ILE:HD11	1.82	0.60
1:AP:1:MET:HE2	1:AP:31:ALA:HB2	1.82	0.59
1:AC:26:ASP:CB	1:AC:30:GLN:HE21	2.15	0.59
1:AD:191:LYS:NZ	1:AE:243:SER:HB2	2.16	0.59
1:AK:125:ILE:HG23	1:AK:126:TYR:N	2.16	0.59
3:BV:9:ARG:HH22	3:BW:13:ASN:H	1.48	0.59
3:BA:11:MET:HE3	3:BA:14:GLY:HA2	1.83	0.59
1:AC:24:HIS:CD2	1:AC:127:SER:HB3	2.37	0.59
1:AK:177:LEU:CD2	1:AL:177:LEU:HD22	2.33	0.59
3:BJ:118:ARG:HD2	3:BU:70:GLU:OE1	2.03	0.59
3:BJ:138:SER:HB2	3:BU:107:ARG:HH21	1.68	0.59
3:Bn:125:MET:HB2	3:Bn:130:ASN:HB2	1.85	0.59
3:BB:25:ILE:HG23	3:BC:29:LEU:HD11	1.85	0.59
1:AB:266:ILE:HD13	1:AB:276:ILE:HD12	1.84	0.59
1:AG:206:TYR:HD1	3:BG:13:ASN:HD22	1.50	0.59
1:AK:243:SER:HB3	1:AK:254:GLU:HB3	1.84	0.59
1:AP:219:ILE:HD13	3:Bf:14:GLY:HA3	1.85	0.59
1:AB:192:VAL:O	1:AB:256:PRO:HG3	2.03	0.59
1:AC:226:PHE:CZ	3:BB:18:ILE:HD11	2.38	0.58
1:AC:245:SER:HB3	1:AC:252:TYR:HB2	1.85	0.58
1:AG:266:ILE:HD13	1:AG:276:ILE:HD12	1.84	0.58
1:AA:164:ASN:HD22	1:AB:168:LEU:HG	1.67	0.58
1:AF:15:ASN:ND2	2:AT:33:GLU:OE2	2.32	0.58
1:AG:164:ASN:HD22	1:AH:168:LEU:HD23	1.68	0.58
1:AK:177:LEU:HD23	1:AL:177:LEU:CD2	2.34	0.58
1:AM:266:ILE:HD13	1:AM:276:ILE:HD12	1.85	0.58
2:AU:202:PHE:HB2	2:AU:210:PHE:HB2	1.85	0.58
1:AD:112:PHE:HA	1:AF:26:ASP:OD1	2.04	0.57
1:AH:243:SER:HB3	1:AH:254:GLU:HB3	1.85	0.57
3:BG:121:LEU:HD11	3:BG:136:ILE:HD11	1.87	0.57
1:AA:167:ILE:HG12	1:AB:173:PRO:HG2	1.86	0.57
2:AW:188:ARG:O	2:AW:226:PHE:CD2	2.53	0.57
1:AB:267:LEU:HD23	1:AB:268:ILE:O	2.05	0.57
1:AR:15:ASN:ND2	2:AV:33:GLU:OE2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AV:202:PHE:HB2	2:AV:210:PHE:HB2	1.86	0.57
1:AC:286:MET:HE3	1:AC:289:ALA:CB	2.35	0.57
1:AN:36:ILE:HD11	1:AN:79:LEU:CD2	2.34	0.57
3:BY:121:LEU:HD11	3:BY:136:ILE:HD11	1.87	0.57
2:AS:48:MET:HE1	2:AT:95:LEU:HD22	1.87	0.57
2:AS:96:LYS:CD	2:AX:253:LEU:OXT	2.52	0.57
1:AB:13:PRO:HA	1:AB:115:ARG:NE	2.11	0.57
1:AM:55:MET:HE3	1:AO:123:LYS:HE3	1.86	0.57
3:Bd:117:ASN:ND2	3:Bd:165:ALA:HB3	2.20	0.56
1:AP:195:GLY:HA3	1:AP:257:LYS:HE2	1.87	0.56
1:AQ:23:ARG:H	1:AQ:30:GLN:HE22	1.52	0.56
2:AS:253:LEU:OXT	2:AT:96:LYS:CD	2.51	0.56
2:AU:216:ASN:O	2:AU:220:LEU:HB2	2.05	0.56
2:AU:253:LEU:OXT	2:AV:96:LYS:HD2	2.05	0.56
3:Ba:125:MET:HB2	3:Ba:130:ASN:HB2	1.86	0.56
3:BO:115:PRO:HB3	3:BO:162:ILE:HA	1.87	0.56
1:AI:93:ARG:HA	1:AI:120:ILE:HG22	1.88	0.56
1:AL:93:ARG:HG2	1:AL:120:ILE:HD13	1.88	0.56
1:AR:266:ILE:HD13	1:AR:276:ILE:HD12	1.88	0.56
2:AV:253:LEU:OXT	2:AW:96:LYS:CD	2.52	0.56
1:AQ:36:ILE:HD11	1:AQ:79:LEU:HD23	1.88	0.56
1:AK:184:ILE:HD11	1:AL:185:GLU:HG3	1.88	0.56
2:AV:188:ARG:O	2:AV:226:PHE:CD2	2.53	0.56
3:Bw:121:LEU:HD11	3:Bw:136:ILE:HD11	1.88	0.56
3:BP:121:LEU:HD11	3:BP:136:ILE:HD11	1.88	0.56
2:AS:202:PHE:HB2	2:AS:210:PHE:HB2	1.87	0.56
3:BX:84:THR:O	3:BX:162:ILE:HG22	2.06	0.56
1:AA:257:LYS:O	1:AA:260:THR:HG22	2.06	0.55
1:AJ:102:LYS:HG2	1:AJ:109:ILE:HB	1.88	0.55
3:BC:11:MET:HE3	3:BC:14:GLY:HA2	1.87	0.55
1:AA:21:LYS:NZ	1:AR:15:ASN:HB2	2.21	0.55
1:AP:266:ILE:HD13	1:AP:276:ILE:HD12	1.86	0.55
1:AJ:299:ALA:O	1:AL:154:LYS:HE2	2.06	0.55
3:BC:64:THR:HA	3:BC:81:LYS:O	2.07	0.55
3:Bn:121:LEU:HD11	3:Bn:136:ILE:HD11	1.88	0.55
1:AA:38:GLU:OE1	1:AC:2:THR:HG22	2.06	0.55
2:AS:180:LEU:HB3	2:AS:191:SER:HB3	1.88	0.55
1:AC:194:ALA:H	1:AC:256:PRO:HA	1.70	0.55
1:AE:243:SER:HB3	1:AE:254:GLU:HB3	1.88	0.55
1:AF:266:ILE:HD13	1:AF:276:ILE:HD12	1.87	0.55
1:AR:103:GLN:HE21	1:AR:106:GLY:H	1.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AU:253:LEU:OXT	2:AV:96:LYS:CE	2.55	0.55
1:AC:19:ILE:HD11	2:AU:113:LEU:HD12	1.89	0.55
1:AG:12:GLU:OE1	2:AS:150:LYS:CE	2.55	0.55
1:AD:266:ILE:HD13	1:AD:276:ILE:HD12	1.87	0.55
2:AT:211:LEU:HD13	2:AT:220:LEU:HD21	1.89	0.55
3:BS:121:LEU:HD11	3:BS:136:ILE:HD11	1.89	0.55
3:Bt:121:LEU:HD11	3:Bt:136:ILE:HD11	1.89	0.55
1:AA:10:THR:HG21	1:AA:112:PHE:HE1	1.71	0.55
1:AC:10:THR:HG21	1:AC:112:PHE:HE1	1.71	0.55
1:AI:169:GLU:O	1:AI:176:VAL:HG22	2.07	0.55
3:BB:95:SER:HB2	3:Bf:143:GLN:HE22	1.71	0.55
3:BG:13:ASN:HA	3:BI:9:ARG:NH2	2.22	0.55
1:AD:299:ALA:O	1:AF:154:LYS:HE2	2.07	0.54
3:Bk:125:MET:HB2	3:Bk:130:ASN:HB2	1.89	0.54
1:AC:193:PRO:HB3	1:AC:254:GLU:O	2.07	0.54
1:AL:147:ASN:HA	1:AL:150:ILE:HG22	1.89	0.54
3:Bq:121:LEU:HD11	3:Bq:136:ILE:HD11	1.89	0.54
3:Bh:121:LEU:HD11	3:Bh:136:ILE:HD11	1.90	0.54
1:AB:23:ARG:HB2	1:AB:30:GLN:HE22	1.72	0.54
3:BA:13:ASN:HA	3:BC:9:ARG:NH2	2.23	0.54
3:BV:125:MET:HB2	3:BV:130:ASN:HB2	1.88	0.54
1:AO:15:ASN:ND2	2:AW:33:GLU:OE2	2.40	0.54
1:AR:243:SER:HB3	1:AR:254:GLU:HB3	1.90	0.54
3:BD:128:GLY:HA2	3:BF:147:PRO:HG3	1.90	0.54
3:BJ:121:LEU:HD11	3:BJ:136:ILE:HD11	1.89	0.54
1:AA:110:GLU:HB2	1:AC:29:SER:HB3	1.89	0.54
1:AB:179:ALA:O	1:AB:182:ILE:HG13	2.07	0.54
3:Be:121:LEU:HD11	3:Be:136:ILE:HD11	1.89	0.54
1:AI:261:LEU:HD11	1:AI:277:LYS:HB3	1.89	0.54
3:BD:121:LEU:HD11	3:BD:136:ILE:HD11	1.90	0.54
3:BH:95:SER:HB2	3:BW:143:GLN:HE22	1.72	0.54
1:AA:266:ILE:HD13	1:AA:276:ILE:HD12	1.89	0.54
1:AD:191:LYS:HZ1	1:AE:243:SER:HB2	1.73	0.54
3:BY:125:MET:HB2	3:BY:130:ASN:HB2	1.90	0.54
3:Bk:121:LEU:HD11	3:Bk:136:ILE:HD11	1.89	0.54
3:Bh:125:MET:HB2	3:Bh:130:ASN:HB2	1.91	0.53
1:AG:63:GLY:HA3	1:AG:90:PHE:HE2	1.74	0.53
3:BX:125:MET:HB2	3:BX:130:ASN:HB2	1.90	0.53
3:Bb:121:LEU:HD11	3:Bb:136:ILE:HD11	1.89	0.53
3:Bb:125:MET:HB2	3:Bb:130:ASN:HB2	1.90	0.53
3:Bl:9:ARG:HH22	3:Bm:13:ASN:HA	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:10:THR:OG1	1:AA:38:GLU:HG3	2.08	0.53
1:AN:36:ILE:HD11	1:AN:79:LEU:HD23	1.89	0.53
3:BM:121:LEU:HD11	3:BM:136:ILE:HD11	1.90	0.53
3:Bt:125:MET:HB2	3:Bt:130:ASN:HB2	1.90	0.53
1:AI:266:ILE:HD13	1:AI:276:ILE:HD12	1.89	0.53
3:Be:13:ASN:HA	3:Bg:9:ARG:HH21	1.73	0.53
1:AC:266:ILE:HD13	1:AC:276:ILE:HD12	1.89	0.53
1:AL:266:ILE:HD13	1:AL:276:ILE:HD12	1.88	0.53
2:AW:127:VAL:HG23	2:AW:134:ILE:HD13	1.72	0.53
3:BJ:125:MET:HB2	3:BJ:130:ASN:HB2	1.90	0.53
3:BM:125:MET:HB2	3:BM:130:ASN:HB2	1.91	0.53
3:BR:125:MET:HB2	3:BR:130:ASN:HB2	1.91	0.53
3:Bq:125:MET:HB2	3:Bq:130:ASN:HB2	1.91	0.53
1:AE:23:ARG:H	1:AE:30:GLN:HE22	1.57	0.53
1:AK:267:LEU:HD23	1:AK:268:ILE:O	2.08	0.53
3:BA:118:ARG:HD3	3:BA:135:ASP:OD2	2.09	0.53
2:AW:127:VAL:CG2	2:AW:134:ILE:HD13	2.34	0.53
3:Be:125:MET:HB2	3:Be:130:ASN:HB2	1.90	0.53
1:AC:219:ILE:HD13	1:AC:233:GLY:HA2	1.90	0.53
1:AL:16:ASN:HB3	1:AL:118:HIS:CE1	2.44	0.53
3:BA:133:HIS:CD2	3:BB:124:HIS:ND1	2.76	0.52
3:BD:125:MET:HB2	3:BD:130:ASN:HB2	1.90	0.52
3:BV:121:LEU:HD11	3:BV:136:ILE:HD11	1.92	0.52
3:Be:117:ASN:OD1	3:Be:164:SER:HB3	2.09	0.52
3:Bw:125:MET:HB2	3:Bw:130:ASN:HB2	1.91	0.52
3:By:125:MET:HB2	3:By:130:ASN:HB2	1.91	0.52
1:AH:274:LEU:HD11	3:Bp:8:TYR:CE2	2.45	0.52
3:BL:125:MET:HB2	3:BL:130:ASN:HB2	1.90	0.52
1:AI:16:ASN:HB3	1:AI:118:HIS:CE1	2.44	0.52
1:AN:36:ILE:HD13	1:AN:100:PHE:CZ	2.44	0.52
3:Bd:62:LEU:HD12	3:Bd:82:LYS:HE2	1.91	0.52
3:Bj:125:MET:HB2	3:Bj:130:ASN:HB2	1.91	0.52
1:AI:36:ILE:HG22	1:AI:43:LYS:HB3	1.92	0.52
1:AJ:219:ILE:HD13	3:BZ:14:GLY:HA3	1.91	0.52
1:AL:15:ASN:ND2	2:AX:33:GLU:OE2	2.39	0.52
3:BG:125:MET:HB2	3:BG:130:ASN:HB2	1.92	0.52
3:BP:125:MET:HB2	3:BP:130:ASN:HB2	1.90	0.52
1:AD:54:LEU:HB3	1:AD:65:SER:HB3	1.92	0.52
1:AM:120:ILE:HD12	2:AX:17:PRO:HG3	1.92	0.52
1:AO:266:ILE:HD13	1:AO:276:ILE:HD12	1.91	0.52
2:AW:253:LEU:OXT	2:AX:96:LYS:CE	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BB:64:THR:HA	3:BB:81:LYS:O	2.10	0.52
3:Bs:125:MET:HB2	3:Bs:130:ASN:HB2	1.91	0.52
1:AE:1:MET:HA	1:AE:28:ASN:HB3	1.92	0.52
3:Be:163:ASP:O	3:Be:164:SER:HB2	2.09	0.52
3:Bq:43:THR:HG23	3:Bs:49:THR:HB	1.92	0.52
1:AB:10:THR:HG21	1:AB:112:PHE:HE1	1.74	0.52
1:AC:10:THR:HG21	1:AC:112:PHE:CE1	2.45	0.52
2:AW:173:PHE:HB2	2:AW:201:GLU:HB2	1.91	0.52
3:B2:125:MET:HB2	3:B2:130:ASN:HB2	1.90	0.52
1:AH:23:ARG:H	1:AH:30:GLN:HE22	1.56	0.52
3:BA:35:VAL:HG22	3:BA:37:HIS:CE1	2.44	0.52
3:BF:125:MET:HB2	3:BF:130:ASN:HB2	1.91	0.52
1:AK:177:LEU:HD11	1:AL:178:LEU:HD23	1.92	0.51
2:AT:171:LEU:HD11	2:AT:229:ILE:HD11	1.92	0.51
3:Bm:125:MET:HB2	3:Bm:130:ASN:HB2	1.91	0.51
1:AL:198:PHE:HB3	1:AL:253:VAL:HG23	1.92	0.51
3:BS:125:MET:HB2	3:BS:130:ASN:HB2	1.91	0.51
3:Bg:125:MET:HB2	3:Bg:130:ASN:HB2	1.91	0.51
1:AA:21:LYS:HZ2	1:AR:15:ASN:HB2	1.75	0.51
1:AH:91:VAL:HG11	1:AH:123:LYS:HG3	1.92	0.51
1:AP:181:VAL:HA	1:AP:184:ILE:HG22	1.92	0.51
3:BA:7:VAL:HG13	3:BA:11:MET:CE	2.40	0.51
3:BG:13:ASN:HA	3:BI:9:ARG:HH21	1.76	0.51
3:Bp:125:MET:HB2	3:Bp:130:ASN:HB2	1.92	0.51
1:AA:157:TRP:HZ3	1:AB:161:VAL:HG23	1.76	0.51
3:Bz:121:LEU:HD11	3:Bz:136:ILE:HD11	1.92	0.51
1:AA:205:GLU:OE2	1:AA:248:ARG:HD3	2.10	0.51
2:AX:24:MET:HE2	2:AX:107:ILE:HG12	1.92	0.51
3:BD:13:ASN:HA	3:BF:9:ARG:NH2	2.25	0.51
1:AK:195:GLY:HA3	1:AK:257:LYS:HG2	1.92	0.51
3:Bv:125:MET:HB2	3:Bv:130:ASN:HB2	1.91	0.51
1:AN:23:ARG:HB2	1:AN:26:ASP:HB2	1.93	0.51
1:AR:86:ASN:O	1:AR:89:GLN:HG2	2.11	0.51
3:BJ:25:ILE:HG23	3:BK:29:LEU:HD11	1.93	0.51
1:AA:12:GLU:OE2	2:AU:150:LYS:HE2	2.11	0.51
1:AC:147:ASN:HA	1:AC:150:ILE:HG22	1.93	0.51
1:AR:93:ARG:HA	1:AR:120:ILE:HG22	1.92	0.51
1:AH:177:LEU:HD11	1:AI:177:LEU:HD22	1.93	0.51
1:AQ:286:MET:HE3	1:AQ:289:ALA:HB3	1.93	0.51
3:Bd:78:SER:HB2	3:Bd:89:SER:HB3	1.93	0.51
3:Bz:125:MET:HB2	3:Bz:130:ASN:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AO:205:GLU:OE2	1:AO:248:ARG:HD3	2.11	0.50
1:AR:101:ARG:HH11	1:AR:108:TRP:HE1	1.57	0.50
3:BR:78:SER:HB2	3:BR:89:SER:HB3	1.93	0.50
3:Bv:78:SER:HB2	3:Bv:89:SER:HB3	1.93	0.50
1:AA:245:SER:HB3	1:AA:252:TYR:HB2	1.93	0.50
1:AL:205:GLU:OE2	1:AL:248:ARG:HD3	2.12	0.50
1:AQ:163:ALA:HB3	1:AR:182:ILE:HD11	1.93	0.50
3:BW:62:LEU:HD12	3:BW:82:LYS:HE3	1.92	0.50
1:AB:103:GLN:HG3	1:AB:108:TRP:CD2	2.46	0.50
1:AM:274:LEU:HD11	3:Bi:8:TYR:CE2	2.46	0.50
1:AN:14:ASN:HB3	1:AN:17:ILE:HD12	1.92	0.50
3:BP:13:ASN:HA	3:BR:9:ARG:NH2	2.24	0.50
3:Bm:78:SER:HB2	3:Bm:89:SER:HB3	1.94	0.50
1:AF:15:ASN:HB2	1:AG:21:LYS:NZ	2.26	0.50
1:AK:164:ASN:ND2	1:AL:182:ILE:HD13	2.26	0.50
3:BU:125:MET:HB2	3:BU:130:ASN:HB2	1.91	0.50
3:BX:78:SER:HB2	3:BX:89:SER:HB3	1.94	0.50
3:B2:78:SER:HB2	3:B2:89:SER:HB3	1.94	0.50
1:AB:91:VAL:HG11	1:AB:123:LYS:HG3	1.93	0.50
3:BI:125:MET:HB2	3:BI:130:ASN:HB2	1.92	0.50
1:AA:219:ILE:HD13	3:Bc:14:GLY:HA3	1.94	0.50
1:AE:104:GLU:HB3	1:AE:109:ILE:HD12	1.93	0.50
3:BB:133:HIS:CD2	3:BC:124:HIS:ND1	2.76	0.50
3:BV:57:ASN:HB2	3:BW:51:THR:HA	1.92	0.50
3:Bd:125:MET:HB2	3:Bd:130:ASN:HB2	1.93	0.50
1:AF:24:HIS:CG	1:AF:127:SER:HB3	2.47	0.50
3:Ba:78:SER:HB2	3:Ba:89:SER:HB3	1.94	0.50
1:AB:110:GLU:OE2	1:AB:113:SER:HB3	2.12	0.50
3:BU:78:SER:HB2	3:BU:89:SER:HB3	1.94	0.50
1:AA:73:ASP:OD2	1:AA:76:ASN:HB2	2.11	0.50
1:AA:146:PHE:CD2	1:AB:150:ILE:HD12	2.47	0.50
1:AC:73:ASP:OD2	1:AC:76:ASN:HB2	2.12	0.50
1:AF:268:ILE:HB	1:AF:272:THR:HG23	1.94	0.50
1:AN:141:GLU:HA	1:AN:144:ARG:HG2	1.94	0.50
3:BG:25:ILE:HG23	3:BH:29:LEU:HD11	1.93	0.50
3:BM:29:LEU:HD11	3:BO:25:ILE:HG23	1.94	0.50
3:BN:103:ASN:HD21	3:BN:141:VAL:CG1	2.24	0.50
1:AA:188:VAL:HA	1:AA:192:VAL:HG12	1.93	0.49
2:AV:46:ARG:O	2:AW:96:LYS:NZ	2.44	0.49
3:Bj:78:SER:HB2	3:Bj:89:SER:HB3	1.94	0.49
1:AC:205:GLU:OE2	1:AC:248:ARG:HD3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AN:50:PRO:HG2	1:AN:69:VAL:HB	1.94	0.49
1:AO:112:PHE:HB3	1:AP:29:SER:HB3	1.93	0.49
1:AH:50:PRO:HG2	1:AH:69:VAL:HB	1.93	0.49
1:AO:167:ILE:HA	1:AO:171:ILE:HD12	1.94	0.49
3:BZ:125:MET:HB2	3:BZ:130:ASN:HB2	1.93	0.49
3:Bg:78:SER:HB2	3:Bg:89:SER:HB3	1.94	0.49
1:AC:192:VAL:O	1:AC:256:PRO:HG3	2.11	0.49
1:AF:23:ARG:HG3	1:AF:24:HIS:N	2.27	0.49
2:AU:171:LEU:HB2	2:AU:203:ASP:HB2	1.92	0.49
2:AV:171:LEU:HB2	2:AV:203:ASP:HB2	1.93	0.49
3:BP:118:ARG:HG2	3:BP:137:PRO:HA	1.95	0.49
3:Bq:25:ILE:HG23	3:Br:29:LEU:HD11	1.94	0.49
1:AA:202:HIS:HD2	1:AA:204:SER:H	1.57	0.49
1:AG:102:LYS:HG2	1:AG:109:ILE:HB	1.93	0.49
1:AI:26:ASP:CG	1:AI:30:GLN:HE21	2.21	0.49
1:AQ:50:PRO:HG2	1:AQ:69:VAL:HB	1.95	0.49
2:AS:188:ARG:O	2:AS:226:PHE:CD2	2.58	0.49
3:BC:118:ARG:HD3	3:BC:135:ASP:OD2	2.12	0.49
3:BD:13:ASN:HA	3:BF:9:ARG:HH21	1.78	0.49
3:Be:29:LEU:HD11	3:Bg:25:ILE:HG23	1.95	0.49
1:AF:104:GLU:HB2	1:AF:109:ILE:HD11	1.95	0.49
1:AH:267:LEU:HD23	1:AH:268:ILE:O	2.13	0.49
1:AL:58:GLU:HG3	1:AL:58:GLU:O	2.13	0.49
1:AP:54:LEU:HB3	1:AP:65:SER:HB3	1.94	0.49
1:AQ:267:LEU:HD23	1:AQ:268:ILE:O	2.13	0.49
1:AA:12:GLU:O	1:AA:115:ARG:CD	2.55	0.49
1:AO:24:HIS:CG	1:AO:127:SER:HB3	2.47	0.49
3:Bu:11:MET:HE3	3:Bu:14:GLY:HA2	1.95	0.49
3:By:78:SER:HB2	3:By:89:SER:HB3	1.93	0.49
1:AB:257:LYS:O	1:AB:260:THR:HG22	2.13	0.49
1:AC:169:GLU:HG3	1:AC:176:VAL:HG23	1.94	0.49
1:AC:202:HIS:HD2	1:AC:204:SER:H	1.60	0.49
1:AG:171:ILE:HD11	1:AH:177:LEU:HG	1.95	0.49
1:AH:286:MET:HE3	1:AH:289:ALA:HB3	1.95	0.49
1:AN:167:ILE:HD11	1:AO:178:LEU:CD1	2.42	0.49
1:AN:267:LEU:HD23	1:AN:268:ILE:O	2.12	0.49
1:AP:56:ALA:HB2	1:AP:64:VAL:HG22	1.94	0.49
2:AT:127:VAL:HG23	2:AT:134:ILE:CD1	2.43	0.49
3:Bw:57:ASN:HB2	3:Bx:51:THR:HA	1.95	0.49
1:AB:146:PHE:HD1	1:AC:150:ILE:HG13	1.77	0.49
1:AF:169:GLU:O	1:AF:176:VAL:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AK:50:PRO:HG2	1:AK:69:VAL:HB	1.94	0.49
3:BH:125:MET:HB2	3:BH:130:ASN:HB2	1.95	0.49
3:Bl:57:ASN:HB2	3:Bm:51:THR:HA	1.94	0.49
1:AA:101:ARG:HD2	1:AA:108:TRP:CE2	2.48	0.49
1:AJ:177:LEU:CD1	1:AL:177:LEU:HD11	2.43	0.49
1:AM:50:PRO:HB3	1:AM:100:PHE:CE2	2.48	0.49
3:BA:124:HIS:ND1	3:BC:133:HIS:CD2	2.77	0.49
3:Bk:25:ILE:HG23	3:Bl:29:LEU:HD11	1.95	0.49
1:AA:286:MET:HE3	1:AA:289:ALA:CB	2.40	0.48
1:AC:19:ILE:HG12	1:AC:118:HIS:HB2	1.95	0.48
1:AJ:190:GLU:HG3	1:AJ:191:LYS:HD2	1.95	0.48
3:BS:29:LEU:HD11	3:BU:25:ILE:HG23	1.94	0.48
1:AK:286:MET:HE3	1:AK:289:ALA:HB3	1.95	0.48
2:AS:96:LYS:CE	2:AX:253:LEU:OXT	2.61	0.48
2:AW:182:ALA:HB3	2:AW:189:LEU:HB3	1.94	0.48
3:Bq:61:THR:HB	3:Br:55:GLU:HG3	1.95	0.48
1:AJ:11:THR:HB	2:AX:150:LYS:NZ	2.27	0.48
3:Bn:128:GLY:HA2	3:Bp:147:PRO:HG3	1.94	0.48
3:Bt:11:MET:HE3	3:Bt:14:GLY:HA2	1.95	0.48
3:Bt:29:LEU:HD11	3:Bv:25:ILE:HG23	1.95	0.48
1:AA:192:VAL:C	1:AA:256:PRO:HG3	2.38	0.48
1:AE:267:LEU:HD23	1:AE:268:ILE:O	2.14	0.48
1:AK:125:ILE:HG23	1:AK:126:TYR:CD1	2.48	0.48
1:AK:168:LEU:HA	1:AK:173:PRO:HG3	1.96	0.48
3:BA:101:ASN:HA	3:BA:144:TRP:O	2.14	0.48
1:AD:181:VAL:HA	1:AD:184:ILE:HG22	1.95	0.48
1:AL:268:ILE:HB	1:AL:272:THR:HG23	1.96	0.48
3:BD:73:GLY:HA3	3:BD:98:ILE:HD11	1.95	0.48
3:BL:78:SER:HB2	3:BL:89:SER:HB3	1.94	0.48
3:BO:125:MET:HB2	3:BO:130:ASN:HB2	1.95	0.48
3:BQ:25:ILE:HG23	3:BR:29:LEU:HD11	1.95	0.48
3:BT:57:ASN:HB2	3:BU:51:THR:HA	1.94	0.48
3:BU:80:ARG:HH12	3:BU:82:LYS:HE3	1.78	0.48
3:BZ:57:ASN:HB2	3:Ba:51:THR:HA	1.95	0.48
3:Bc:57:ASN:HB2	3:Bd:51:THR:HA	1.96	0.48
3:Bh:29:LEU:HD11	3:Bj:25:ILE:HG23	1.94	0.48
3:Bo:125:MET:HB2	3:Bo:130:ASN:HB2	1.96	0.48
3:Bp:78:SER:HB2	3:Bp:89:SER:HB3	1.94	0.48
1:AE:286:MET:HE3	1:AE:289:ALA:HB3	1.95	0.48
1:AO:27:VAL:HG12	1:AO:28:ASN:HD22	1.78	0.48
3:Bh:57:ASN:HB2	3:Bi:51:THR:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AE:50:PRO:HG2	1:AE:69:VAL:HB	1.94	0.48
1:AM:146:PHE:HZ	1:AO:157:TRP:HB2	1.78	0.48
1:AQ:125:ILE:C	1:AQ:125:ILE:HD13	2.39	0.48
3:BF:78:SER:HB2	3:BF:89:SER:HB3	1.94	0.48
3:Bw:29:LEU:HD11	3:By:25:ILE:HG23	1.95	0.48
3:Bz:29:LEU:HD11	3:B2:25:ILE:HG23	1.95	0.48
1:AI:268:ILE:HB	1:AI:272:THR:HG23	1.96	0.48
3:Br:125:MET:HB2	3:Br:130:ASN:HB2	1.96	0.48
3:Bs:78:SER:HB2	3:Bs:89:SER:HB3	1.94	0.48
3:Bt:25:ILE:HG23	3:Bu:29:LEU:HD11	1.96	0.48
1:AA:49:GLN:HE21	1:AA:50:PRO:CD	2.22	0.48
1:AC:219:ILE:CD1	1:AC:233:GLY:HA2	2.44	0.48
1:AM:202:HIS:HB3	1:AM:286:MET:HE1	1.96	0.48
1:AN:286:MET:HE3	1:AN:289:ALA:HB3	1.96	0.48
3:Bz:25:ILE:HG23	3:B1:29:LEU:HD11	1.96	0.48
3:BA:35:VAL:HG22	3:BA:37:HIS:NE2	2.29	0.47
3:BS:57:ASN:HB2	3:BT:51:THR:HA	1.95	0.47
3:Bf:11:MET:HE3	3:Bf:14:GLY:HA2	1.97	0.47
3:Bi:125:MET:HB2	3:Bi:130:ASN:HB2	1.96	0.47
3:Br:57:ASN:HB2	3:Bs:51:THR:HA	1.95	0.47
1:AI:181:VAL:HA	1:AI:184:ILE:HG22	1.95	0.47
3:BD:57:ASN:HB2	3:BE:51:THR:HA	1.96	0.47
3:Bt:57:ASN:HB2	3:Bu:51:THR:HA	1.96	0.47
3:Bt:73:GLY:HA3	3:Bt:98:ILE:HD11	1.96	0.47
1:AF:245:SER:OG	1:AF:252:TYR:HB2	2.15	0.47
1:AG:50:PRO:HG2	1:AG:69:VAL:HB	1.94	0.47
1:AM:48:LEU:HG	1:AM:102:LYS:HB2	1.96	0.47
1:AO:268:ILE:HB	1:AO:272:THR:HG23	1.95	0.47
3:BB:145:PHE:O	3:BC:124:HIS:HE1	1.97	0.47
3:BG:57:ASN:HB2	3:BH:51:THR:HA	1.96	0.47
3:BI:78:SER:HB2	3:BI:89:SER:HB3	1.96	0.47
3:Be:57:ASN:HB2	3:Bf:51:THR:HA	1.95	0.47
1:AG:202:HIS:HB3	1:AG:286:MET:HE1	1.97	0.47
1:AK:125:ILE:HG23	1:AK:126:TYR:H	1.79	0.47
3:BE:78:SER:HB2	3:BE:89:SER:HB3	1.97	0.47
3:BO:78:SER:HB2	3:BO:89:SER:HB3	1.95	0.47
3:BV:29:LEU:HD11	3:BX:25:ILE:HG23	1.97	0.47
3:Bb:25:ILE:HG23	3:Bc:29:LEU:HD11	1.96	0.47
3:Bu:78:SER:HB2	3:Bu:89:SER:HB3	1.96	0.47
1:AA:202:HIS:HB2	1:AA:286:MET:HE1	1.92	0.47
1:AE:164:ASN:OD1	1:AF:182:ILE:HD13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AU:182:ALA:HB3	2:AU:189:LEU:HB3	1.97	0.47
3:BQ:70:GLU:CD	3:Bi:118:ARG:HD2	2.40	0.47
3:Bh:73:GLY:HA3	3:Bh:98:ILE:HD11	1.96	0.47
3:Bn:73:GLY:HA3	3:Bn:98:ILE:HD11	1.96	0.47
1:AB:13:PRO:CA	1:AB:115:ARG:HE	2.13	0.47
1:AI:205:GLU:OE2	1:AI:248:ARG:HD3	2.15	0.47
1:AO:14:ASN:HB3	1:AO:17:ILE:HG13	1.97	0.47
1:AP:202:HIS:HB3	1:AP:286:MET:HE1	1.96	0.47
1:AR:268:ILE:HB	1:AR:272:THR:HG23	1.96	0.47
2:AX:44:GLU:HB2	2:AX:75:THR:HG23	1.96	0.47
3:BB:118:ARG:HD3	3:BB:135:ASP:OD2	2.13	0.47
3:BM:73:GLY:HA3	3:BM:98:ILE:HD11	1.96	0.47
3:BN:125:MET:HB2	3:BN:130:ASN:HB2	1.97	0.47
3:BT:125:MET:HB2	3:BT:130:ASN:HB2	1.96	0.47
3:BY:57:ASN:HB2	3:BZ:51:THR:HA	1.97	0.47
3:Bb:29:LEU:HD11	3:Bd:25:ILE:HG23	1.96	0.47
3:Bc:125:MET:HB2	3:Bc:130:ASN:HB2	1.96	0.47
3:Bq:29:LEU:HD11	3:Bs:25:ILE:HG23	1.96	0.47
1:AA:11:THR:HB	2:AU:150:LYS:NZ	2.30	0.47
1:AB:205:GLU:OE2	1:AB:248:ARG:HD3	2.14	0.47
2:AS:253:LEU:OXT	2:AT:96:LYS:CE	2.63	0.47
2:AT:188:ARG:O	2:AT:226:PHE:CD2	2.57	0.47
3:BH:11:MET:HE3	3:BH:14:GLY:HA2	1.96	0.47
3:BS:61:THR:HB	3:BT:55:GLU:HG3	1.97	0.47
3:Bb:73:GLY:HA3	3:Bb:98:ILE:HD11	1.97	0.47
3:Bw:73:GLY:HA3	3:Bw:98:ILE:HD11	1.96	0.47
1:AG:56:ALA:HB2	1:AG:64:VAL:HG22	1.96	0.47
2:AS:182:ALA:HB3	2:AS:189:LEU:HB3	1.96	0.47
2:AT:84:ASP:OD2	2:AT:86:ARG:HG3	2.15	0.47
3:BD:29:LEU:HD11	3:BF:25:ILE:HG23	1.97	0.47
3:BH:25:ILE:HG23	3:BI:29:LEU:HD11	1.96	0.47
3:BK:11:MET:HE3	3:BK:14:GLY:HA2	1.96	0.47
3:BK:125:MET:HB2	3:BK:130:ASN:HB2	1.96	0.47
3:Bh:25:ILE:HG23	3:Bi:29:LEU:HD11	1.97	0.47
1:AB:21:LYS:HG2	1:AB:120:ILE:CG2	2.45	0.47
1:AG:54:LEU:HB3	1:AG:65:SER:HB3	1.97	0.47
1:AJ:274:LEU:HD11	3:BZ:8:TYR:HE2	1.79	0.47
1:AM:102:LYS:HG2	1:AM:109:ILE:HD12	1.97	0.47
3:BB:5:LYS:HE3	3:BB:17:THR:HG23	1.97	0.47
3:BY:25:ILE:HG23	3:BZ:29:LEU:HD11	1.97	0.47
3:Bu:125:MET:HB2	3:Bu:130:ASN:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:49:GLN:NE2	1:AA:50:PRO:HD2	2.21	0.47
1:AK:1:MET:HA	1:AK:28:ASN:HB3	1.97	0.47
1:AN:36:ILE:CD1	1:AN:100:PHE:HZ	2.28	0.47
3:BA:64:THR:HA	3:BA:81:LYS:O	2.15	0.47
3:BQ:125:MET:HB2	3:BQ:130:ASN:HB2	1.96	0.47
3:Bn:25:ILE:HG23	3:Bo:29:LEU:HD11	1.97	0.47
3:B1:57:ASN:HB2	3:B2:51:THR:HA	1.97	0.47
1:AD:205:GLU:OE2	1:AD:248:ARG:HD3	2.15	0.46
1:AM:134:ASN:HD22	1:AM:134:ASN:H	1.63	0.46
1:AR:205:GLU:OE2	1:AR:248:ARG:HD3	2.15	0.46
3:BC:101:ASN:HA	3:BC:144:TRP:O	2.15	0.46
3:BN:57:ASN:HB2	3:BO:51:THR:HA	1.97	0.46
3:Bi:78:SER:HB2	3:Bi:89:SER:HB3	1.97	0.46
3:Bn:29:LEU:HD11	3:Bp:25:ILE:HG23	1.96	0.46
3:Bz:73:GLY:HA3	3:Bz:98:ILE:HD11	1.97	0.46
1:AC:232:PHE:CZ	3:BC:18:ILE:HD11	2.50	0.46
1:AG:11:THR:HB	2:AS:150:LYS:NZ	2.30	0.46
1:AG:165:ARG:HH22	1:AI:171:ILE:CG2	2.28	0.46
1:AJ:146:PHE:HZ	1:AL:157:TRP:HB2	1.79	0.46
1:AL:102:LYS:HG2	1:AL:109:ILE:HD12	1.97	0.46
1:AM:205:GLU:OE2	1:AM:248:ARG:HD3	2.16	0.46
2:AT:171:LEU:HB2	2:AT:203:ASP:HB2	1.97	0.46
2:AX:182:ALA:HB3	2:AX:189:LEU:HB3	1.97	0.46
3:BP:64:THR:CG2	3:BP:80:ARG:HE	2.28	0.46
3:BY:29:LEU:HD11	3:Ba:25:ILE:HG23	1.95	0.46
3:Bf:125:MET:HB2	3:Bf:130:ASN:HB2	1.97	0.46
3:Bi:57:ASN:HB2	3:Bj:51:THR:HA	1.97	0.46
3:B1:125:MET:HB2	3:B1:130:ASN:HB2	1.96	0.46
1:AD:165:ARG:HH22	1:AF:171:ILE:CG2	2.28	0.46
1:AG:11:THR:HB	2:AS:150:LYS:HZ3	1.80	0.46
1:AP:22:LEU:HD11	1:AP:119:TYR:CD1	2.50	0.46
3:BP:73:GLY:HA3	3:BP:98:ILE:HD11	1.96	0.46
3:BT:78:SER:HB2	3:BT:89:SER:HB3	1.98	0.46
3:B1:78:SER:HB2	3:B1:89:SER:HB3	1.98	0.46
1:AC:268:ILE:HB	1:AC:272:THR:HG23	1.97	0.46
1:AI:202:HIS:HB3	1:AI:286:MET:HE1	1.97	0.46
1:AN:167:ILE:HG12	1:AN:168:LEU:H	1.80	0.46
2:AT:182:ALA:HB3	2:AT:189:LEU:HB3	1.97	0.46
3:BE:125:MET:HB2	3:BE:130:ASN:HB2	1.96	0.46
3:BJ:29:LEU:HD11	3:BL:25:ILE:HG23	1.96	0.46
3:BK:57:ASN:HB2	3:BL:51:THR:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BP:25:ILE:HG23	3:BQ:29:LEU:HD11	1.97	0.46
3:BY:11:MET:HE3	3:BY:14:GLY:HA2	1.96	0.46
3:Bc:11:MET:HE3	3:Bc:14:GLY:HA2	1.97	0.46
3:Be:11:MET:HE3	3:Be:14:GLY:HA2	1.97	0.46
3:Bl:125:MET:HB2	3:Bl:130:ASN:HB2	1.96	0.46
3:Bo:57:ASN:HB2	3:Bp:51:THR:HA	1.98	0.46
3:Bx:125:MET:HB2	3:Bx:130:ASN:HB2	1.96	0.46
1:AB:146:PHE:O	1:AB:150:ILE:HG12	2.14	0.46
1:AQ:205:GLU:OE2	1:AQ:248:ARG:HD3	2.16	0.46
2:AS:188:ARG:NH1	2:AS:190:LYS:HE3	2.30	0.46
3:BN:78:SER:HB2	3:BN:89:SER:HB3	1.97	0.46
3:BP:57:ASN:HB2	3:BQ:51:THR:HA	1.96	0.46
3:Bk:29:LEU:HD11	3:Bm:25:ILE:HG23	1.97	0.46
3:Bk:73:GLY:HA3	3:Bk:98:ILE:HD11	1.98	0.46
1:AB:73:ASP:OD2	1:AB:76:ASN:HB2	2.15	0.46
1:AF:205:GLU:OE2	1:AF:248:ARG:HD3	2.15	0.46
3:BA:51:THR:HA	3:BC:57:ASN:HB2	1.98	0.46
3:BG:29:LEU:HD11	3:Bl:25:ILE:HG23	1.98	0.46
3:BG:73:GLY:HA3	3:BG:98:ILE:HD11	1.98	0.46
3:BV:73:GLY:HA3	3:BV:98:ILE:HD11	1.97	0.46
3:BW:57:ASN:HB2	3:BX:51:THR:HA	1.97	0.46
3:BW:125:MET:HB2	3:BW:130:ASN:HB2	1.96	0.46
3:Bh:11:MET:HE3	3:Bh:14:GLY:HA2	1.98	0.46
3:Bo:78:SER:HB2	3:Bo:89:SER:HB3	1.97	0.46
3:Bz:11:MET:HE3	3:Bz:14:GLY:HA2	1.98	0.46
1:AA:15:ASN:H	1:AA:15:ASN:ND2	2.08	0.46
1:AA:101:ARG:HD3	1:AA:111:GLN:NE2	2.31	0.46
1:AG:146:PHE:HZ	1:AI:157:TRP:HB2	1.81	0.46
3:BY:73:GLY:HA3	3:BY:98:ILE:HD11	1.97	0.46
3:Bc:25:ILE:HG23	3:Bd:29:LEU:HD11	1.98	0.46
3:Bf:78:SER:HB2	3:Bf:89:SER:HB3	1.97	0.46
1:AG:192:VAL:O	1:AG:256:PRO:HG3	2.16	0.46
1:AL:202:HIS:HB3	1:AL:286:MET:HE1	1.97	0.46
2:AS:188:ARG:HH12	2:AS:190:LYS:HE3	1.80	0.46
3:BM:57:ASN:HB2	3:BN:51:THR:HA	1.97	0.46
3:Bk:57:ASN:HB2	3:Bl:51:THR:HA	1.97	0.46
3:Bl:11:MET:HE3	3:Bl:14:GLY:HA2	1.98	0.46
1:AA:48:LEU:HD23	1:AA:102:LYS:HB2	1.97	0.46
1:AD:202:HIS:HB3	1:AD:286:MET:HE1	1.97	0.46
1:AP:134:ASN:C	1:AP:134:ASN:HD22	2.23	0.46
2:AS:24:MET:HE2	2:AS:107:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AX:188:ARG:O	2:AX:226:PHE:CD2	2.58	0.46
3:BF:26:ASN:HA	3:BF:29:LEU:HD12	1.98	0.46
3:BM:26:ASN:HA	3:BM:29:LEU:HD12	1.97	0.46
3:BW:25:ILE:HG23	3:BX:29:LEU:HD11	1.98	0.46
3:Bw:25:ILE:HG23	3:Bx:29:LEU:HD11	1.98	0.46
1:AB:276:ILE:HG12	1:AB:281:VAL:HG22	1.97	0.46
1:AC:16:ASN:HB3	1:AC:118:HIS:CE1	2.45	0.46
1:AG:205:GLU:OE2	1:AG:248:ARG:HD3	2.16	0.46
1:AN:179:ALA:O	1:AN:182:ILE:HG13	2.16	0.46
2:AU:188:ARG:O	2:AU:226:PHE:CD2	2.55	0.46
3:BY:61:THR:HB	3:BZ:55:GLU:HG3	1.98	0.46
3:Bb:57:ASN:HB2	3:Bc:51:THR:HA	1.97	0.46
3:Bq:73:GLY:HA3	3:Bq:98:ILE:HD11	1.98	0.46
1:AC:16:ASN:HB2	2:AU:30:TRP:HZ2	1.82	0.45
1:AM:185:GLU:HB3	1:AO:184:ILE:HD11	1.98	0.45
2:AV:45:GLY:O	2:AV:72:ARG:HD2	2.16	0.45
3:BJ:57:ASN:HB2	3:BK:51:THR:HA	1.96	0.45
3:BZ:11:MET:HE3	3:BZ:14:GLY:HA2	1.97	0.45
3:Bd:26:ASN:HA	3:Bd:29:LEU:HD12	1.98	0.45
3:Bn:51:THR:HA	3:Bp:57:ASN:HB2	1.98	0.45
1:AB:165:ARG:NH2	1:AB:170:SER:OG	2.49	0.45
1:AD:15:ASN:H	1:AD:15:ASN:ND2	2.13	0.45
1:AJ:56:ALA:HB2	1:AJ:64:VAL:HG22	1.98	0.45
3:BN:11:MET:HE3	3:BN:14:GLY:HA2	1.97	0.45
3:Br:11:MET:HE3	3:Br:14:GLY:HA2	1.99	0.45
3:Br:78:SER:HB2	3:Br:89:SER:HB3	1.99	0.45
1:AB:10:THR:HG21	1:AB:112:PHE:CE1	2.50	0.45
1:AD:103:GLN:HG2	1:AD:108:TRP:HD1	1.81	0.45
1:AJ:202:HIS:HB3	1:AJ:286:MET:HE1	1.98	0.45
1:AJ:274:LEU:HD11	3:BZ:8:TYR:CE2	2.52	0.45
1:AL:169:GLU:O	1:AL:176:VAL:HG22	2.16	0.45
1:AP:177:LEU:CD1	1:AQ:181:VAL:HG11	2.39	0.45
1:AR:168:LEU:HD12	1:AR:179:ALA:HB2	1.99	0.45
2:AU:253:LEU:OXT	2:AV:96:LYS:HE3	2.16	0.45
2:AW:171:LEU:HD11	2:AW:229:ILE:HD11	1.98	0.45
3:BB:11:MET:HE3	3:BB:14:GLY:HA2	1.98	0.45
3:BE:130:ASN:HA	3:BF:129:TRP:HB3	1.98	0.45
3:BH:57:ASN:HB2	3:BI:51:THR:HA	1.99	0.45
3:BO:26:ASN:HA	3:BO:29:LEU:HD12	1.98	0.45
3:BV:25:ILE:HG23	3:BW:29:LEU:HD11	1.98	0.45
3:BV:130:ASN:HA	3:BW:129:TRP:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BW:130:ASN:HA	3:BX:129:TRP:HB3	1.99	0.45
3:Bl:130:ASN:HA	3:Bm:129:TRP:HB3	1.98	0.45
3:Bu:130:ASN:HA	3:Bv:129:TRP:HB3	1.98	0.45
1:AF:225:GLY:HA3	3:BE:10:GLY:HA2	1.99	0.45
1:AH:36:ILE:HG13	1:AH:100:PHE:HZ	1.81	0.45
1:AO:15:ASN:HB2	1:AP:21:LYS:NZ	2.32	0.45
3:BA:118:ARG:HH21	3:Bg:70:GLU:CD	2.24	0.45
3:BD:25:ILE:HG23	3:BE:29:LEU:HD11	1.97	0.45
3:BH:78:SER:HB2	3:BH:89:SER:HB3	1.97	0.45
3:Bp:26:ASN:HA	3:Bp:29:LEU:HD12	1.98	0.45
3:Bs:26:ASN:HA	3:Bs:29:LEU:HD12	1.99	0.45
1:AG:164:ASN:ND2	1:AH:168:LEU:HD23	2.30	0.45
1:AM:194:ALA:H	1:AM:256:PRO:HA	1.82	0.45
1:AM:219:ILE:HD13	3:Bi:14:GLY:HA3	1.98	0.45
1:AO:286:MET:HE3	1:AO:289:ALA:HB3	1.98	0.45
3:BE:11:MET:HE3	3:BE:14:GLY:HA2	1.98	0.45
3:BI:26:ASN:HA	3:BI:29:LEU:HD12	1.98	0.45
3:BL:26:ASN:HA	3:BL:29:LEU:HD12	1.99	0.45
3:BS:25:ILE:HG23	3:BT:29:LEU:HD11	1.98	0.45
3:Bc:130:ASN:HA	3:Bd:129:TRP:HB3	1.98	0.45
3:Be:73:GLY:HA3	3:Be:98:ILE:HD11	1.97	0.45
3:Bf:57:ASN:HB2	3:Bg:51:THR:HA	1.99	0.45
3:Bx:78:SER:HB2	3:Bx:89:SER:HB3	1.98	0.45
1:AA:1:MET:HB2	1:AA:29:SER:O	2.16	0.45
1:AQ:195:GLY:HA3	1:AQ:257:LYS:HG3	1.98	0.45
3:BC:7:VAL:HG13	3:BC:11:MET:CE	2.39	0.45
3:B1:130:ASN:HA	3:B2:129:TRP:HB3	1.98	0.45
1:AA:112:PHE:HA	1:AC:26:ASP:OD2	2.17	0.45
1:AF:23:ARG:HB3	1:AF:26:ASP:OD2	2.16	0.45
1:AO:22:LEU:HD22	1:AO:30:GLN:HB3	1.99	0.45
2:AW:171:LEU:HB2	2:AW:203:ASP:HB2	1.97	0.45
3:BP:143:GLN:NE2	3:Bj:95:SER:HB2	2.29	0.45
3:BQ:130:ASN:HA	3:BR:129:TRP:HB3	1.99	0.45
3:BS:11:MET:HE3	3:BS:14:GLY:HA2	1.97	0.45
3:BU:26:ASN:HA	3:BU:29:LEU:HD12	1.98	0.45
3:BZ:78:SER:HB2	3:BZ:89:SER:HB3	1.99	0.45
3:Bb:61:THR:HB	3:Bc:55:GLU:HG3	1.98	0.45
3:Be:25:ILE:HG23	3:Bf:29:LEU:HD11	1.98	0.45
3:Bn:57:ASN:HB2	3:Bo:51:THR:HA	1.98	0.45
3:Bu:25:ILE:HG23	3:Bv:29:LEU:HD11	1.97	0.45
1:AJ:168:LEU:O	1:AJ:171:ILE:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AR:202:HIS:HB3	1:AR:286:MET:HE1	1.98	0.45
2:AS:92:PHE:CZ	2:AS:134:ILE:CD1	2.96	0.45
3:BP:29:LEU:HD11	3:BR:25:ILE:HG23	1.99	0.45
3:Bm:26:ASN:HA	3:Bm:29:LEU:HD12	1.98	0.45
1:AL:286:MET:HE3	1:AL:289:ALA:HB3	1.99	0.45
1:AN:205:GLU:OE2	1:AN:248:ARG:HD3	2.17	0.45
1:AO:16:ASN:HB3	1:AO:118:HIS:HE1	1.81	0.45
1:AR:166:GLU:O	1:AR:170:SER:HB2	2.17	0.45
3:BG:51:THR:HA	3:BI:57:ASN:HB2	1.99	0.45
3:Bb:26:ASN:HA	3:Bb:29:LEU:HD12	1.99	0.45
3:Bg:26:ASN:HA	3:Bg:29:LEU:HD12	1.99	0.45
3:Bt:130:ASN:HA	3:Bu:129:TRP:HB3	1.99	0.45
3:Bx:57:ASN:HB2	3:By:51:THR:HA	1.99	0.45
3:Bz:130:ASN:HA	3:B1:129:TRP:HB3	1.99	0.45
1:AJ:12:GLU:OE1	2:AX:150:LYS:CE	2.61	0.45
1:AM:56:ALA:HB2	1:AM:64:VAL:HB	1.98	0.45
1:AO:16:ASN:HB3	1:AO:118:HIS:CE1	2.52	0.45
1:AR:286:MET:HE3	1:AR:289:ALA:HB3	1.99	0.45
3:BH:130:ASN:HA	3:BI:129:TRP:HB3	1.99	0.45
3:BJ:26:ASN:HA	3:BJ:29:LEU:HD12	1.99	0.45
3:BY:130:ASN:HA	3:BZ:129:TRP:HB3	1.99	0.45
3:Bf:130:ASN:HA	3:Bg:129:TRP:HB3	1.99	0.45
3:Bz:61:THR:HB	3:B1:55:GLU:HG3	1.99	0.45
1:AA:10:THR:HG21	1:AA:112:PHE:CE1	2.52	0.44
1:AB:207:GLN:NE2	3:Bc:13:ASN:OD1	2.49	0.44
1:AI:164:ASN:HA	1:AI:167:ILE:HD12	1.99	0.44
1:AI:286:MET:HE3	1:AI:289:ALA:HB3	1.98	0.44
1:AK:36:ILE:HG13	1:AK:100:PHE:HZ	1.83	0.44
1:AP:149:TYR:CE1	1:AQ:154:LYS:HG2	2.52	0.44
3:BD:11:MET:HE3	3:BD:14:GLY:HA2	2.00	0.44
3:BG:61:THR:HB	3:BH:55:GLU:HG3	2.00	0.44
3:BJ:11:MET:HE3	3:BJ:14:GLY:HA2	1.99	0.44
3:BT:130:ASN:HA	3:BU:129:TRP:HB3	1.98	0.44
3:BX:26:ASN:HA	3:BX:29:LEU:HD12	1.99	0.44
3:Bh:130:ASN:HA	3:Bi:129:TRP:HB3	2.00	0.44
3:B1:25:ILE:HG23	3:B2:29:LEU:HD11	1.99	0.44
1:AA:95:GLU:HG3	1:AA:118:HIS:NE2	2.32	0.44
1:AK:205:GLU:OE2	1:AK:248:ARG:HD3	2.18	0.44
3:BA:13:ASN:HA	3:BC:9:ARG:HH22	1.81	0.44
3:BD:130:ASN:HA	3:BE:129:TRP:HB3	1.99	0.44
3:BP:11:MET:HE3	3:BP:14:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AD:146:PHE:O	1:AD:150:ILE:HG12	2.17	0.44
1:AD:192:VAL:O	1:AD:256:PRO:HG3	2.18	0.44
1:AE:10:THR:HG22	1:AE:114:THR:HA	1.99	0.44
1:AL:15:ASN:HB2	1:AM:21:LYS:NZ	2.33	0.44
1:AM:11:THR:HB	2:AW:150:LYS:NZ	2.32	0.44
1:AP:168:LEU:HB3	1:AR:172:ASP:OD1	2.18	0.44
1:AQ:10:THR:HG22	1:AQ:114:THR:HA	1.99	0.44
1:AR:165:ARG:O	1:AR:169:GLU:HG2	2.18	0.44
3:BM:15:ALA:HB1	3:BO:7:VAL:HG12	1.99	0.44
3:Bb:130:ASN:HA	3:Bc:129:TRP:HB3	2.00	0.44
3:Bc:26:ASN:HA	3:Bc:29:LEU:HD12	1.99	0.44
3:Bq:11:MET:HE3	3:Bq:14:GLY:HA2	1.99	0.44
1:AC:44:ASN:ND2	1:AC:46:GLU:OE2	2.50	0.44
1:AL:24:HIS:CG	1:AL:127:SER:HB3	2.53	0.44
1:AL:102:LYS:HB2	1:AL:102:LYS:HE2	1.84	0.44
1:AM:128:GLN:HB3	1:AN:126:TYR:CZ	2.53	0.44
3:Ba:26:ASN:HA	3:Ba:29:LEU:HD12	2.00	0.44
3:Bk:61:THR:HB	3:Bl:55:GLU:HG3	1.99	0.44
3:B1:11:MET:HE3	3:B1:14:GLY:HA2	1.99	0.44
1:AN:239:ASN:HD22	1:AO:244:LEU:HB2	1.82	0.44
3:BE:26:ASN:HA	3:BE:29:LEU:HD12	2.00	0.44
3:BK:78:SER:HB2	3:BK:89:SER:HB3	1.98	0.44
3:BM:130:ASN:HA	3:BN:129:TRP:HB3	2.00	0.44
3:BR:26:ASN:HA	3:BR:29:LEU:HD12	2.00	0.44
3:BV:11:MET:HE3	3:BV:14:GLY:HA2	1.99	0.44
3:Bh:9:ARG:HH22	3:Bi:13:ASN:HA	1.82	0.44
3:Bx:25:ILE:HG23	3:By:29:LEU:HD11	2.00	0.44
1:AB:21:LYS:HG2	1:AB:120:ILE:HG23	2.00	0.44
1:AH:10:THR:HG22	1:AH:114:THR:HA	1.99	0.44
3:BB:101:ASN:HA	3:BB:144:TRP:O	2.17	0.44
3:BC:136:ILE:HG13	3:BC:142:CYS:SG	2.58	0.44
3:BK:25:ILE:HG23	3:BL:29:LEU:HD11	1.99	0.44
3:BQ:78:SER:HB2	3:BQ:89:SER:HB3	1.99	0.44
3:BT:25:ILE:HG23	3:BU:29:LEU:HD11	2.00	0.44
3:Bf:25:ILE:HG23	3:Bg:29:LEU:HD11	2.00	0.44
3:Bk:26:ASN:HA	3:Bk:29:LEU:HD12	2.00	0.44
3:Bz:57:ASN:HB2	3:B1:51:THR:HA	1.99	0.44
1:AA:101:ARG:HH11	1:AA:108:TRP:NE1	2.15	0.44
1:AD:50:PRO:HG2	1:AD:69:VAL:HB	1.99	0.44
1:AG:31:ALA:HA	1:AG:82:VAL:HA	2.00	0.44
1:AJ:213:THR:HG21	3:BZ:12:LYS:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AV:58:MET:HE3	2:AV:58:MET:HB3	1.90	0.44
3:BE:57:ASN:HB2	3:BF:51:THR:HA	1.98	0.44
3:BG:130:ASN:HA	3:BH:129:TRP:HB3	1.99	0.44
3:BN:130:ASN:HA	3:BO:129:TRP:HB3	1.99	0.44
3:BP:26:ASN:HA	3:BP:29:LEU:HD12	2.00	0.44
3:BP:130:ASN:HA	3:BQ:129:TRP:HB3	2.00	0.44
3:BQ:57:ASN:HB2	3:BR:51:THR:HA	1.99	0.44
3:Bf:26:ASN:HA	3:Bf:29:LEU:HD12	1.99	0.44
3:Bl:78:SER:HB2	3:Bl:89:SER:HB3	1.98	0.44
3:Bu:57:ASN:HB2	3:Bv:51:THR:HA	2.00	0.44
3:B2:26:ASN:HA	3:B2:29:LEU:HD12	1.99	0.44
1:AC:62:GLN:HG2	1:AE:125:ILE:HG22	2.00	0.44
1:AC:108:TRP:CH2	1:AE:125:ILE:HD11	2.53	0.44
1:AF:202:HIS:HB3	1:AF:286:MET:HE1	1.99	0.44
1:AG:274:LEU:HD11	3:BT:8:TYR:HE2	1.83	0.44
1:AH:239:ASN:HD22	1:AI:244:LEU:HB2	1.82	0.44
3:BC:8:TYR:O	3:BC:11:MET:HB3	2.18	0.44
3:BD:61:THR:HB	3:BE:55:GLU:HG3	2.00	0.44
3:BG:11:MET:HE3	3:BG:14:GLY:HA2	2.00	0.44
3:BM:129:TRP:HB3	3:BO:130:ASN:HA	2.00	0.44
3:BS:73:GLY:HA3	3:BS:98:ILE:HD11	2.00	0.44
3:Bi:25:ILE:HG23	3:Bj:29:LEU:HD11	2.00	0.44
3:Bv:26:ASN:HA	3:Bv:29:LEU:HD12	2.00	0.44
3:Bw:61:THR:HB	3:Bx:55:GLU:HG3	2.00	0.44
1:AJ:22:LEU:HD22	1:AJ:30:GLN:HB3	1.99	0.44
3:BN:25:ILE:HG23	3:BO:29:LEU:HD11	2.00	0.44
3:BP:51:THR:HA	3:BR:57:ASN:HB2	2.00	0.44
3:BT:26:ASN:HA	3:BT:29:LEU:HD12	2.00	0.44
1:AA:44:ASN:ND2	1:AA:46:GLU:OE2	2.50	0.43
1:AJ:136:TRP:HB2	1:AL:142:LEU:HD11	1.99	0.43
1:AP:171:ILE:HG12	1:AQ:177:LEU:CD1	2.48	0.43
3:BK:130:ASN:HA	3:BL:129:TRP:HB3	1.99	0.43
3:BV:128:GLY:HA2	3:BX:147:PRO:HG3	2.00	0.43
3:Bi:130:ASN:HA	3:Bj:129:TRP:HB3	1.99	0.43
3:Bl:25:ILE:HG23	3:Bm:29:LEU:HD11	2.00	0.43
3:Bt:115:PRO:HA	3:Bt:162:ILE:HG13	2.00	0.43
3:By:26:ASN:HA	3:By:29:LEU:HD12	1.99	0.43
1:AF:15:ASN:HB2	1:AG:21:LYS:HZ1	1.83	0.43
1:AH:205:GLU:OE2	1:AH:248:ARG:HD3	2.18	0.43
1:AK:184:ILE:HD11	1:AL:185:GLU:CG	2.48	0.43
1:AK:202:HIS:HB3	1:AK:286:MET:HE1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AM:11:THR:HB	2:AW:150:LYS:HZ1	1.81	0.43
3:BD:13:ASN:HB3	3:BD:16:GLU:HB2	1.99	0.43
3:BS:130:ASN:HA	3:BT:129:TRP:HB3	2.01	0.43
3:BY:128:GLY:HA2	3:Ba:147:PRO:HG3	2.00	0.43
3:Bq:130:ASN:HA	3:Br:129:TRP:HB3	1.99	0.43
3:Bx:130:ASN:HA	3:By:129:TRP:HB3	1.99	0.43
3:B2:99:LEU:HA	3:B2:148:THR:HG23	2.00	0.43
1:AE:205:GLU:OE2	1:AE:248:ARG:HD3	2.18	0.43
1:AK:239:ASN:HD22	1:AL:244:LEU:HB2	1.84	0.43
2:AX:171:LEU:HB2	2:AX:203:ASP:HB2	2.00	0.43
3:BP:61:THR:HB	3:BQ:55:GLU:HG3	2.01	0.43
3:BW:11:MET:HE3	3:BW:14:GLY:HA2	1.98	0.43
3:BY:26:ASN:HA	3:BY:29:LEU:HD12	2.00	0.43
3:Bt:51:THR:HA	3:Bv:57:ASN:HB2	1.99	0.43
3:Bx:26:ASN:HA	3:Bx:29:LEU:HD12	2.00	0.43
1:AA:157:TRP:CZ3	1:AB:161:VAL:HG23	2.53	0.43
1:AK:23:ARG:H	1:AK:30:GLN:HE22	1.66	0.43
1:AO:202:HIS:HB3	1:AO:286:MET:HE1	1.99	0.43
3:BJ:130:ASN:HA	3:BK:129:TRP:HB3	2.00	0.43
3:BM:13:ASN:HB3	3:BM:16:GLU:HB2	2.00	0.43
3:Bk:130:ASN:HA	3:Bl:129:TRP:HB3	1.99	0.43
3:Bw:130:ASN:HA	3:Bx:129:TRP:HB3	1.99	0.43
1:AB:12:GLU:O	1:AB:115:ARG:CD	2.59	0.43
1:AE:195:GLY:HA3	1:AE:257:LYS:HB3	2.00	0.43
1:AM:237:ILE:HG21	3:Bi:12:LYS:HE3	2.00	0.43
1:AN:36:ILE:HD11	1:AN:79:LEU:HD21	2.01	0.43
1:AO:132:ASP:HB3	1:AO:137:TRP:CD1	2.53	0.43
1:AR:192:VAL:O	1:AR:256:PRO:HG3	2.19	0.43
2:AV:50:SER:HB3	2:AW:123:THR:HG22	2.00	0.43
2:AW:135:ILE:HG23	2:AW:135:ILE:O	2.17	0.43
3:BZ:26:ASN:HA	3:BZ:29:LEU:HD12	2.00	0.43
3:Br:130:ASN:HA	3:Bs:129:TRP:HB3	1.99	0.43
1:AA:93:ARG:HB2	2:AV:15:ASN:HD22	1.84	0.43
1:AB:13:PRO:HB3	1:AB:115:ARG:HH21	1.84	0.43
1:AB:242:VAL:HG12	1:AB:255:MET:HG2	1.99	0.43
1:AK:36:ILE:HD12	1:AK:114:THR:HG21	2.00	0.43
1:AO:54:LEU:HB3	1:AO:65:SER:HB3	2.00	0.43
1:AP:192:VAL:O	1:AP:256:PRO:HG3	2.18	0.43
1:AP:205:GLU:OE2	1:AP:248:ARG:HD3	2.19	0.43
3:BG:26:ASN:HA	3:BG:29:LEU:HD12	2.00	0.43
3:BJ:61:THR:HB	3:BK:55:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Bo:130:ASN:HA	3:Bp:129:TRP:HB3	2.00	0.43
3:Bv:13:ASN:HB3	3:Bv:16:GLU:HB2	2.00	0.43
1:AC:223:THR:HG23	1:AC:279:THR:CG2	2.48	0.43
1:AF:286:MET:HE3	1:AF:289:ALA:HB3	1.99	0.43
1:AI:194:ALA:H	1:AI:256:PRO:HA	1.84	0.43
2:AS:105:VAL:HA	2:AS:106:PRO:HD3	1.90	0.43
3:BV:129:TRP:HB3	3:BX:130:ASN:HA	2.00	0.43
3:Bk:11:MET:HE3	3:Bk:14:GLY:HA2	2.01	0.43
1:AA:146:PHE:HZ	1:AC:157:TRP:HB2	1.83	0.43
1:AD:134:ASN:N	1:AD:134:ASN:HD22	2.16	0.43
1:AD:177:LEU:CD2	1:AE:181:VAL:HG21	2.48	0.43
1:AF:54:LEU:HB3	1:AF:65:SER:HB3	2.01	0.43
1:AI:54:LEU:HB3	1:AI:65:SER:HB3	2.01	0.43
1:AJ:54:LEU:HB3	1:AJ:65:SER:HB2	2.01	0.43
2:AT:121:PHE:HA	2:AT:140:VAL:HG12	2.00	0.43
3:BE:25:ILE:HG23	3:BF:29:LEU:HD11	1.99	0.43
3:BM:61:THR:HB	3:BN:55:GLU:HG3	2.00	0.43
3:Be:130:ASN:HA	3:Bf:129:TRP:HB3	2.00	0.43
3:Bj:26:ASN:HA	3:Bj:29:LEU:HD12	2.01	0.43
3:Bl:26:ASN:HA	3:Bl:29:LEU:HD12	1.99	0.43
3:Bt:61:THR:HB	3:Bu:55:GLU:HG3	2.01	0.43
1:AJ:165:ARG:HH12	1:AL:171:ILE:CG2	2.32	0.43
1:AK:10:THR:HG22	1:AK:114:THR:HA	2.00	0.43
1:AN:54:LEU:HD21	1:AN:87:ALA:HA	2.00	0.43
3:BW:78:SER:HB2	3:BW:89:SER:HB3	2.00	0.43
3:Bc:78:SER:HB2	3:Bc:89:SER:HB3	1.99	0.43
1:AH:202:HIS:HB3	1:AH:286:MET:HE1	2.00	0.43
1:AJ:177:LEU:HD11	1:AL:177:LEU:HD11	2.01	0.43
3:BC:112:GLU:O	3:BC:162:ILE:HD11	2.19	0.43
3:Be:61:THR:HB	3:Bf:55:GLU:HG3	2.01	0.43
3:Bh:26:ASN:HA	3:Bh:29:LEU:HD12	2.01	0.43
1:AA:21:LYS:O	1:AR:115:ARG:NH2	2.52	0.42
1:AA:180:LYS:NZ	1:AB:185:GLU:CD	2.77	0.42
1:AC:19:ILE:HD11	2:AU:113:LEU:CD1	2.48	0.42
1:AI:112:PHE:HB3	1:AJ:29:SER:HB2	2.00	0.42
1:AP:48:LEU:HD21	1:AP:110:GLU:HG3	2.01	0.42
2:AW:35:ILE:HD13	2:AW:95:LEU:HG	2.01	0.42
3:Ba:99:LEU:HA	3:Ba:148:THR:HG23	2.01	0.42
3:Bn:61:THR:HB	3:Bo:55:GLU:HG3	2.01	0.42
3:Bw:26:ASN:HA	3:Bw:29:LEU:HD12	2.00	0.42
3:Bz:129:TRP:HB3	3:B2:130:ASN:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:134:ASN:HD22	1:AA:134:ASN:H	1.68	0.42
1:AA:268:ILE:HG22	1:AA:270:ASP:OD1	2.19	0.42
1:AC:202:HIS:HB2	1:AC:286:MET:HE1	1.98	0.42
2:AX:127:VAL:HG23	2:AX:134:ILE:CD1	2.50	0.42
3:BJ:51:THR:HA	3:BL:57:ASN:HB2	2.00	0.42
3:Bn:26:ASN:HA	3:Bn:29:LEU:HD12	2.01	0.42
3:Bn:51:THR:HG22	3:Bp:57:ASN:HD22	1.84	0.42
3:Bq:26:ASN:HA	3:Bq:29:LEU:HD12	2.01	0.42
3:Br:26:ASN:HA	3:Br:29:LEU:HD12	2.01	0.42
1:AH:207:GLN:NE2	3:BT:13:ASN:OD1	2.53	0.42
1:AL:186:LYS:O	1:AL:190:GLU:HG2	2.19	0.42
1:AP:191:LYS:HE2	1:AQ:254:GLU:OE1	2.19	0.42
1:AQ:37:VAL:HG13	1:AQ:40:GLY:H	1.84	0.42
3:BA:112:GLU:O	3:BA:162:ILE:HD11	2.19	0.42
3:BD:26:ASN:HA	3:BD:29:LEU:HD12	2.00	0.42
3:BE:61:THR:HB	3:BF:55:GLU:HG3	2.02	0.42
3:BJ:73:GLY:HA3	3:BJ:98:ILE:HD11	1.99	0.42
3:BK:26:ASN:HA	3:BK:29:LEU:HD12	2.00	0.42
3:BS:26:ASN:HA	3:BS:29:LEU:HD12	2.01	0.42
3:BV:26:ASN:HA	3:BV:29:LEU:HD12	2.01	0.42
3:Bb:11:MET:HE3	3:Bb:14:GLY:HA2	2.00	0.42
3:Bx:11:MET:HE3	3:Bx:14:GLY:HA2	2.01	0.42
3:Bz:26:ASN:HA	3:Bz:29:LEU:HD12	2.01	0.42
1:AE:202:HIS:HB3	1:AE:286:MET:HE1	2.01	0.42
1:AG:22:LEU:HD22	1:AG:30:GLN:HB3	2.02	0.42
1:AG:274:LEU:HD11	3:BT:8:TYR:CE2	2.54	0.42
1:AI:225:GLY:HA3	3:BH:10:GLY:HA2	2.01	0.42
1:AJ:15:ASN:H	1:AJ:15:ASN:ND2	2.15	0.42
1:AR:23:ARG:HB3	1:AR:26:ASP:OD2	2.19	0.42
3:BJ:13:ASN:HB3	3:BJ:16:GLU:HB2	2.01	0.42
3:BQ:26:ASN:HA	3:BQ:29:LEU:HD12	2.01	0.42
3:Bb:129:TRP:HB3	3:Bd:130:ASN:HA	2.02	0.42
3:Bi:11:MET:HE3	3:Bi:14:GLY:HA2	2.01	0.42
1:AC:26:ASP:HB2	1:AC:30:GLN:HE21	1.84	0.42
1:AE:36:ILE:HD12	1:AE:114:THR:HG21	2.02	0.42
1:AF:168:LEU:HD21	1:AF:179:ALA:HB2	2.01	0.42
1:AP:299:ALA:O	1:AR:154:LYS:HE2	2.19	0.42
1:AR:147:ASN:O	1:AR:150:ILE:HG22	2.19	0.42
2:AS:35:ILE:HD13	2:AS:95:LEU:HG	2.02	0.42
3:Be:26:ASN:HA	3:Be:29:LEU:HD12	2.00	0.42
3:Bi:26:ASN:HA	3:Bi:29:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Bo:26:ASN:HA	3:Bo:29:LEU:HD12	2.02	0.42
3:Bo:87:GLU:HG2	3:Bo:159:THR:HG22	2.02	0.42
3:Br:7:VAL:HB	3:Bs:19:ASN:HB2	2.01	0.42
1:AD:157:TRP:HZ3	1:AE:161:VAL:HG13	1.84	0.42
2:AW:78:TYR:CZ	2:AW:136:SER:HB3	2.54	0.42
3:BB:57:ASN:HB2	3:BC:51:THR:HA	2.01	0.42
3:BJ:128:GLY:HA2	3:BL:147:PRO:HG3	2.01	0.42
3:BT:11:MET:HE3	3:BT:14:GLY:HA2	2.02	0.42
3:Bq:57:ASN:HB2	3:Br:51:THR:HA	2.01	0.42
3:Bu:26:ASN:HA	3:Bu:29:LEU:HD12	2.01	0.42
3:Bw:128:GLY:HA2	3:By:147:PRO:HG3	2.02	0.42
1:AO:128:GLN:HA	1:AO:129:PRO:HD3	1.88	0.42
3:BD:51:THR:HA	3:BF:57:ASN:HB2	2.01	0.42
3:BT:61:THR:HB	3:BU:55:GLU:HG3	2.02	0.42
3:Bc:61:THR:HB	3:Bd:55:GLU:HG3	2.02	0.42
1:AI:101:ARG:HB3	1:AI:111:GLN:HG3	2.00	0.42
1:AJ:205:GLU:OE2	1:AJ:248:ARG:HD3	2.20	0.42
1:AM:286:MET:HE3	1:AM:289:ALA:HB3	2.02	0.42
1:AP:146:PHE:HZ	1:AR:157:TRP:HB2	1.85	0.42
2:AT:47:GLU:H	2:AT:47:GLU:HG2	1.04	0.42
2:AT:192:SER:HB3	2:AT:222:LEU:HD13	2.01	0.42
3:BM:13:ASN:HA	3:BO:9:ARG:NH2	2.35	0.42
3:Bk:9:ARG:HH22	3:Bl:13:ASN:HA	1.84	0.42
3:Bt:26:ASN:HA	3:Bt:29:LEU:HD12	2.01	0.42
3:Bt:51:THR:HG22	3:Bv:57:ASN:HD22	1.85	0.42
3:Bw:11:MET:HE3	3:Bw:14:GLY:HA2	2.01	0.42
1:AD:146:PHE:HZ	1:AF:157:TRP:HB2	1.84	0.42
1:AK:23:ARG:HB2	1:AK:26:ASP:HB2	2.02	0.42
1:AK:125:ILE:CG2	1:AK:126:TYR:N	2.82	0.42
1:AR:16:ASN:HB2	2:AV:30:TRP:HZ2	1.84	0.42
2:AW:47:GLU:H	2:AW:47:GLU:HG2	1.00	0.42
3:BB:7:VAL:HG13	3:BB:11:MET:CE	2.45	0.42
3:BE:95:SER:HB2	3:Bc:101:ASN:OD1	2.20	0.42
3:BG:129:TRP:HB3	3:BI:130:ASN:HA	2.02	0.42
3:BH:26:ASN:HA	3:BH:29:LEU:HD12	2.01	0.42
3:BW:133:HIS:HD2	3:BX:124:HIS:ND1	2.18	0.42
3:Bh:129:TRP:HB3	3:Bj:130:ASN:HA	2.02	0.42
3:Bm:99:LEU:HA	3:Bm:148:THR:HG23	2.01	0.42
1:AA:204:SER:HB2	1:AA:289:ALA:HB2	2.01	0.42
1:AE:23:ARG:HB2	1:AE:26:ASP:HB2	2.02	0.42
1:AE:239:ASN:HD22	1:AF:244:LEU:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AH:158:GLU:HA	1:AH:161:VAL:HG12	2.02	0.42
1:AL:202:HIS:CE1	1:AL:251:VAL:HG23	2.55	0.42
1:AO:24:HIS:HB3	1:AO:124:SER:HB3	2.01	0.42
2:AW:177:THR:HG22	2:AW:178:GLU:H	1.85	0.42
3:B1:133:HIS:HB3	3:B2:124:HIS:HB3	2.02	0.42
1:AA:24:HIS:CD2	1:AA:126:TYR:O	2.73	0.41
1:AJ:171:ILE:HG12	1:AK:177:LEU:HD22	2.01	0.41
1:AN:23:ARG:H	1:AN:30:GLN:HE22	1.68	0.41
2:AU:44:GLU:HB2	2:AU:75:THR:HG23	2.02	0.41
3:BF:99:LEU:HA	3:BF:148:THR:HG23	2.03	0.41
3:BK:61:THR:HB	3:BL:55:GLU:HG3	2.02	0.41
3:BP:51:THR:HG22	3:BR:57:ASN:HD22	1.85	0.41
3:BU:80:ARG:NH1	3:BU:82:LYS:HE3	2.34	0.41
3:Bt:129:TRP:HB3	3:Bv:130:ASN:HA	2.02	0.41
1:AN:54:LEU:HD13	1:AN:65:SER:HB3	2.01	0.41
1:AO:168:LEU:HD21	1:AO:178:LEU:HD23	2.02	0.41
1:AQ:202:HIS:HB3	1:AQ:286:MET:HE1	2.01	0.41
3:BJ:129:TRP:HB3	3:BL:130:ASN:HA	2.01	0.41
3:Bz:128:GLY:HA2	3:B2:147:PRO:HG3	2.01	0.41
1:AC:148:LYS:HA	1:AC:151:GLU:HG2	2.02	0.41
1:AJ:11:THR:HB	2:AX:150:LYS:HZ1	1.83	0.41
1:AL:24:HIS:CD2	1:AL:127:SER:HB3	2.55	0.41
1:AN:162:GLU:O	1:AN:166:GLU:HB2	2.20	0.41
1:AP:10:THR:HG22	1:AP:114:THR:HA	2.02	0.41
2:AW:24:MET:HE2	2:AW:107:ILE:HG12	2.02	0.41
3:BX:99:LEU:HA	3:BX:148:THR:HG23	2.02	0.41
3:BZ:61:THR:HB	3:Ba:55:GLU:HG3	2.03	0.41
3:Be:9:ARG:HH22	3:Bf:13:ASN:HA	1.86	0.41
3:Bo:11:MET:HE3	3:Bo:14:GLY:HA2	2.01	0.41
3:Bt:128:GLY:HA2	3:Bv:147:PRO:HG3	2.02	0.41
1:AC:108:TRP:CH2	1:AE:125:ILE:CD1	3.03	0.41
1:AL:190:GLU:HG3	1:AL:191:LYS:HD2	2.02	0.41
1:AO:61:GLY:H	1:AO:64:VAL:HG22	1.85	0.41
1:AP:171:ILE:CD1	1:AQ:177:LEU:HD11	2.48	0.41
1:AR:36:ILE:HD12	1:AR:114:THR:HG21	2.01	0.41
2:AS:44:GLU:HB2	2:AS:75:THR:HG23	2.02	0.41
3:BB:112:GLU:O	3:BB:162:ILE:HD11	2.20	0.41
3:BQ:11:MET:HE3	3:BQ:14:GLY:HA2	2.02	0.41
3:Br:133:HIS:HB3	3:Bs:124:HIS:HB3	2.02	0.41
1:AD:219:ILE:HD13	3:BW:14:GLY:HA3	2.01	0.41
1:AK:257:LYS:O	1:AK:260:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AO:169:GLU:O	1:AO:176:VAL:HG22	2.20	0.41
2:AU:35:ILE:HD13	2:AU:95:LEU:HG	2.01	0.41
2:AX:105:VAL:HA	2:AX:106:PRO:HD3	1.90	0.41
3:BD:129:TRP:HB3	3:BF:130:ASN:HA	2.01	0.41
3:BQ:70:GLU:OE1	3:BQ:74:GLY:HA2	2.20	0.41
3:BS:51:THR:HA	3:BU:57:ASN:HB2	2.03	0.41
3:BW:26:ASN:HA	3:BW:29:LEU:HD12	2.01	0.41
3:BZ:130:ASN:HA	3:Ba:129:TRP:HB3	2.02	0.41
3:Bi:133:HIS:HB3	3:Bj:124:HIS:HB3	2.03	0.41
3:Bo:61:THR:HB	3:Bp:55:GLU:HG3	2.01	0.41
3:Br:133:HIS:HD2	3:Bs:124:HIS:ND1	2.19	0.41
1:AA:2:THR:HG21	1:AR:10:THR:HB	2.02	0.41
1:AN:6:ILE:HD11	1:AN:18:GLY:H	1.86	0.41
1:AR:16:ASN:HB3	1:AR:118:HIS:HE1	1.85	0.41
2:AS:108:ILE:HG12	2:AS:116:THR:HG23	2.02	0.41
2:AU:253:LEU:OXT	2:AV:96:LYS:CD	2.67	0.41
3:BQ:87:GLU:HG2	3:BQ:159:THR:HG22	2.02	0.41
3:BZ:133:HIS:HB3	3:Ba:124:HIS:HB3	2.03	0.41
3:Bo:25:ILE:HG23	3:Bp:29:LEU:HD11	2.02	0.41
3:Bw:51:THR:HA	3:By:57:ASN:HB2	2.01	0.41
3:Bx:61:THR:HB	3:By:55:GLU:HG3	2.03	0.41
1:AF:62:GLN:HB2	1:AH:122:GLU:HB2	2.03	0.41
1:AG:248:ARG:HG3	3:BI:9:ARG:HB3	2.03	0.41
2:AU:192:SER:HB3	2:AU:222:LEU:HD13	2.03	0.41
3:Bb:51:THR:HA	3:Bd:57:ASN:HB2	2.03	0.41
3:Bn:130:ASN:HA	3:Bo:129:TRP:HB3	2.02	0.41
1:AD:22:LEU:HD22	1:AD:30:GLN:HB3	2.03	0.41
1:AH:165:ARG:NH2	1:AH:170:SER:OG	2.53	0.41
2:AU:47:GLU:H	2:AU:47:GLU:HG2	1.16	0.41
3:BD:51:THR:HG22	3:BF:57:ASN:HD22	1.85	0.41
3:BQ:133:HIS:HB3	3:BR:124:HIS:HB3	2.03	0.41
3:BY:51:THR:HA	3:Ba:57:ASN:HB2	2.02	0.41
1:AC:232:PHE:O	3:BC:9:ARG:HA	2.21	0.41
1:AJ:286:MET:HE3	1:AJ:289:ALA:HB3	2.02	0.41
1:AN:91:VAL:HG11	1:AN:123:LYS:HB2	2.03	0.41
1:AN:202:HIS:HB3	1:AN:286:MET:HE1	2.02	0.41
1:AO:165:ARG:O	1:AO:169:GLU:HB3	2.20	0.41
1:AP:84:SER:H	1:AP:87:ALA:HB3	1.86	0.41
1:AR:31:ALA:HB2	1:AR:82:VAL:HG22	2.03	0.41
2:AW:210:PHE:CE1	2:AW:215:VAL:HG22	2.56	0.41
3:BG:128:GLY:HA2	3:BI:147:PRO:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BH:61:THR:HB	3:BI:55:GLU:HG3	2.03	0.41
3:BV:124:HIS:ND1	3:BX:133:HIS:HD2	2.19	0.41
3:BW:84:THR:OG1	3:BX:82:LYS:NZ	2.54	0.41
3:Bk:129:TRP:HB3	3:Bm:130:ASN:HA	2.02	0.41
3:Bs:99:LEU:HA	3:Bs:148:THR:HG23	2.02	0.41
3:By:13:ASN:HB3	3:By:16:GLU:HB2	2.02	0.41
3:B1:26:ASN:HA	3:B1:29:LEU:HD12	2.01	0.41
1:AA:6:ILE:HD12	1:AA:8:LEU:HD21	2.01	0.41
1:AD:56:ALA:HB2	1:AD:64:VAL:HG13	2.02	0.41
1:AD:151:GLU:HG3	1:AD:152:ASP:N	2.34	0.41
1:AI:16:ASN:HB2	2:AS:30:TRP:HZ2	1.86	0.41
1:AI:49:GLN:NE2	1:AI:68:SER:OG	2.54	0.41
1:AJ:167:ILE:H	1:AJ:167:ILE:HG13	1.63	0.41
1:AK:22:LEU:HB3	1:AK:30:GLN:OE1	2.21	0.41
1:AQ:147:ASN:HA	1:AQ:150:ILE:HG12	2.03	0.41
2:AU:134:ILE:C	2:AU:134:ILE:HD12	2.46	0.41
2:AX:43:VAL:HG22	2:AX:76:ILE:HG23	2.03	0.41
3:BP:128:GLY:HA2	3:BR:147:PRO:HG3	2.02	0.41
3:BY:51:THR:HG22	3:Ba:57:ASN:HD22	1.86	0.41
3:BZ:133:HIS:HD2	3:Ba:124:HIS:ND1	2.19	0.41
3:Be:128:GLY:HA2	3:Bg:147:PRO:HG3	2.02	0.41
3:Bh:51:THR:HA	3:Bj:57:ASN:HB2	2.02	0.41
3:Bh:128:GLY:HA2	3:Bj:147:PRO:HG3	2.03	0.41
3:Bo:7:VAL:HB	3:Bp:19:ASN:HB2	2.04	0.41
3:Bo:133:HIS:HD2	3:Bp:124:HIS:ND1	2.19	0.41
1:AA:101:ARG:HH11	1:AA:108:TRP:HE1	1.69	0.40
1:AB:149:TYR:CZ	1:AC:154:LYS:HG2	2.56	0.40
1:AD:151:GLU:CG	1:AD:152:ASP:N	2.84	0.40
1:AE:37:VAL:HG13	1:AE:40:GLY:H	1.86	0.40
1:AF:16:ASN:HB3	1:AF:118:HIS:HE1	1.86	0.40
1:AG:219:ILE:HG22	3:BU:15:ALA:HB2	2.02	0.40
2:AX:202:PHE:HB2	2:AX:210:PHE:HB2	2.02	0.40
3:BH:133:HIS:HD2	3:BI:124:HIS:ND1	2.19	0.40
3:BK:133:HIS:HD2	3:BL:124:HIS:ND1	2.20	0.40
3:BM:16:GLU:OE2	3:BO:9:ARG:NH1	2.55	0.40
3:BS:51:THR:HG22	3:BU:57:ASN:HD22	1.86	0.40
3:BS:129:TRP:HB3	3:BU:130:ASN:HA	2.02	0.40
3:Bb:128:GLY:HA2	3:Bd:147:PRO:HG3	2.03	0.40
3:Bn:11:MET:HE3	3:Bn:14:GLY:HA2	2.02	0.40
3:Br:25:ILE:HG23	3:Bs:29:LEU:HD11	2.02	0.40
3:Bw:129:TRP:HB3	3:By:130:ASN:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Bz:51:THR:HG22	3:B2:57:ASN:HD22	1.86	0.40
1:AB:46:GLU:OE1	1:AB:75:LYS:HG2	2.21	0.40
1:AD:299:ALA:O	1:AF:154:LYS:CE	2.68	0.40
1:AF:24:HIS:CD2	1:AF:127:SER:HB3	2.56	0.40
1:AG:286:MET:HE3	1:AG:289:ALA:HB3	2.02	0.40
1:AL:225:GLY:HA3	3:BK:10:GLY:HA2	2.03	0.40
1:AM:167:ILE:H	1:AM:167:ILE:HG13	1.72	0.40
1:AM:274:LEU:HD11	3:Bi:8:TYR:HE2	1.86	0.40
1:AN:7:THR:HG23	1:AN:35:GLN:HB3	2.03	0.40
1:AP:7:THR:HG23	1:AP:35:GLN:HB3	2.02	0.40
1:AP:286:MET:HE3	1:AP:289:ALA:HB3	2.03	0.40
3:BL:99:LEU:HA	3:BL:148:THR:HG23	2.03	0.40
3:BM:128:GLY:HA2	3:BO:147:PRO:HG3	2.03	0.40
3:BR:99:LEU:HA	3:BR:148:THR:HG23	2.04	0.40
3:BS:128:GLY:HA2	3:BU:147:PRO:HG3	2.03	0.40
3:BT:133:HIS:HB3	3:BU:124:HIS:HB3	2.03	0.40
3:BZ:25:ILE:HG23	3:Ba:29:LEU:HD11	2.02	0.40
3:Bb:78:SER:HB2	3:Bb:89:SER:HB3	2.01	0.40
3:Bq:128:GLY:HA2	3:Bs:147:PRO:HG3	2.02	0.40
3:Bq:129:TRP:HB3	3:Bs:130:ASN:HA	2.03	0.40
3:Bz:51:THR:HA	3:B2:57:ASN:HB2	2.02	0.40
1:AC:48:LEU:HD23	1:AC:102:LYS:HB2	2.03	0.40
1:AG:102:LYS:HE2	1:AG:110:GLU:HG2	2.03	0.40
1:AI:61:GLY:H	1:AI:64:VAL:HG22	1.87	0.40
1:AK:36:ILE:HD11	1:AK:79:LEU:HD21	2.04	0.40
1:AL:261:LEU:HD21	1:AL:275:VAL:HG12	2.04	0.40
1:AO:16:ASN:HB2	2:AW:30:TRP:HZ2	1.86	0.40
2:AS:152:GLN:NE2	2:AS:160:GLU:OE1	2.55	0.40
2:AT:43:VAL:HG13	2:AT:76:ILE:HG22	2.03	0.40
2:AV:35:ILE:HD13	2:AV:95:LEU:HG	2.03	0.40
3:BT:133:HIS:HD2	3:BU:124:HIS:ND1	2.20	0.40
3:Bn:129:TRP:HB3	3:Bp:130:ASN:HA	2.02	0.40
3:Bx:133:HIS:HD2	3:By:124:HIS:ND1	2.20	0.40
3:B1:61:THR:HB	3:B2:55:GLU:HG3	2.03	0.40
3:BA:57:ASN:HB2	3:BB:51:THR:HA	2.03	0.40
3:BB:8:TYR:O	3:BB:11:MET:HB3	2.22	0.40
3:BE:133:HIS:HD2	3:BF:124:HIS:ND1	2.19	0.40
3:BG:55:GLU:HG3	3:BI:61:THR:HB	2.04	0.40
3:BH:133:HIS:HB3	3:BI:124:HIS:HB3	2.04	0.40
3:BI:99:LEU:HA	3:BI:148:THR:HG23	2.04	0.40
3:BN:133:HIS:HD2	3:BO:124:HIS:ND1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:BV:78:SER:HB2	3:BV:89:SER:HB3	2.04	0.40
3:Bu:61:THR:HB	3:Bv:55:GLU:HG3	2.03	0.40
3:Bx:87:GLU:HG2	3:Bx:159:THR:HG22	2.04	0.40
3:B1:133:HIS:HD2	3:B2:124:HIS:ND1	2.19	0.40
1:AF:101:ARG:HB3	1:AF:111:GLN:HG3	2.03	0.40
1:AH:248:ARG:HG3	3:BS:9:ARG:HB3	2.04	0.40
1:AI:128:GLN:HA	1:AI:129:PRO:HD3	2.01	0.40
1:AN:123:LYS:HD3	1:AN:125:ILE:HD11	2.04	0.40
1:AN:207:GLN:NE2	3:Bi:13:ASN:OD1	2.53	0.40
3:BN:133:HIS:HB3	3:BO:124:HIS:HB3	2.03	0.40
3:BO:99:LEU:HA	3:BO:148:THR:HG23	2.03	0.40
3:Bc:133:HIS:HD2	3:Bd:124:HIS:ND1	2.19	0.40
3:Be:51:THR:HA	3:Bg:57:ASN:HB2	2.03	0.40
3:Be:129:TRP:HB3	3:Bg:130:ASN:HA	2.02	0.40
3:Bk:128:GLY:HA2	3:Bm:147:PRO:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	18	51
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%)	18	51
1	AE	287/299 (96%)	268 (93%)	19 (7%)	0	100	100
1	AF	297/299 (99%)	277 (93%)	19 (6%)	1 (0%)	36	67
1	AG	297/299 (99%)	278 (94%)	14 (5%)	5 (2%)	7	34
1	AH	290/299 (97%)	271 (93%)	18 (6%)	1 (0%)	36	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AI	297/299 (99%)	275 (93%)	20 (7%)	2 (1%)	18	51
1	AJ	297/299 (99%)	275 (93%)	20 (7%)	2 (1%)	18	51
1	AK	289/299 (97%)	270 (93%)	19 (7%)	0	100	100
1	AL	296/299 (99%)	276 (93%)	19 (6%)	1 (0%)	36	67
1	AM	297/299 (99%)	276 (93%)	19 (6%)	2 (1%)	18	51
1	AN	290/299 (97%)	270 (93%)	20 (7%)	0	100	100
1	AO	297/299 (99%)	276 (93%)	20 (7%)	1 (0%)	36	67
1	AP	297/299 (99%)	281 (95%)	13 (4%)	3 (1%)	12	43
1	AQ	291/299 (97%)	269 (92%)	21 (7%)	1 (0%)	36	67
1	AR	297/299 (99%)	277 (93%)	17 (6%)	3 (1%)	12	43
2	AS	240/253 (95%)	215 (90%)	24 (10%)	1 (0%)	30	62
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	43	73

All (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
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

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Mol	Chain	Res	Type
1	AI	235	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	242 (93%)	18 (7%)	14	40
1	AB	255/261 (98%)	243 (95%)	12 (5%)	23	48
1	AC	260/261 (100%)	245 (94%)	15 (6%)	18	44
1	AD	261/261 (100%)	248 (95%)	13 (5%)	22	47
1	AE	256/261 (98%)	247 (96%)	9 (4%)	32	54
1	AF	260/261 (100%)	250 (96%)	10 (4%)	29	53
1	AG	259/261 (99%)	252 (97%)	7 (3%)	39	59
1	AH	254/261 (97%)	244 (96%)	10 (4%)	28	52
1	AI	260/261 (100%)	246 (95%)	14 (5%)	20	45
1	AJ	261/261 (100%)	248 (95%)	13 (5%)	22	47
1	AK	250/261 (96%)	240 (96%)	10 (4%)	28	52
1	AL	259/261 (99%)	242 (93%)	17 (7%)	15	41
1	AM	260/261 (100%)	250 (96%)	10 (4%)	29	53
1	AN	250/261 (96%)	238 (95%)	12 (5%)	23	47
1	AO	261/261 (100%)	252 (97%)	9 (3%)	32	55
1	AP	258/261 (99%)	243 (94%)	15 (6%)	18	44
1	AQ	254/261 (97%)	244 (96%)	10 (4%)	28	52
1	AR	260/261 (100%)	252 (97%)	8 (3%)	35	57
2	AS	212/229 (93%)	203 (96%)	9 (4%)	26	50
2	AT	212/229 (93%)	199 (94%)	13 (6%)	17	43
2	AU	209/229 (91%)	201 (96%)	8 (4%)	29	53
2	AV	204/229 (89%)	193 (95%)	11 (5%)	20	45
2	AW	209/229 (91%)	200 (96%)	9 (4%)	26	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AX	209/229 (91%)	196 (94%)	13 (6%)	16	42
3	B1	133/142 (94%)	131 (98%)	2 (2%)	57	69
3	B2	132/142 (93%)	129 (98%)	3 (2%)	44	63
3	BA	132/142 (93%)	126 (96%)	6 (4%)	24	48
3	BB	132/142 (93%)	127 (96%)	5 (4%)	29	53
3	BC	132/142 (93%)	124 (94%)	8 (6%)	17	43
3	BD	132/142 (93%)	130 (98%)	2 (2%)	57	69
3	BE	132/142 (93%)	130 (98%)	2 (2%)	57	69
3	BF	132/142 (93%)	130 (98%)	2 (2%)	57	69
3	BG	132/142 (93%)	130 (98%)	2 (2%)	57	69
3	BH	133/142 (94%)	130 (98%)	3 (2%)	44	63
3	BI	132/142 (93%)	131 (99%)	1 (1%)	73	76
3	BJ	132/142 (93%)	130 (98%)	2 (2%)	57	69
3	BK	132/142 (93%)	130 (98%)	2 (2%)	57	69
3	BL	132/142 (93%)	129 (98%)	3 (2%)	44	63
3	BM	132/142 (93%)	129 (98%)	3 (2%)	44	63
3	BN	131/142 (92%)	127 (97%)	4 (3%)	35	57
3	BO	131/142 (92%)	128 (98%)	3 (2%)	44	63
3	BP	132/142 (93%)	131 (99%)	1 (1%)	73	76
3	BQ	132/142 (93%)	131 (99%)	1 (1%)	73	76
3	BR	132/142 (93%)	129 (98%)	3 (2%)	44	63
3	BS	132/142 (93%)	131 (99%)	1 (1%)	73	76
3	BT	132/142 (93%)	130 (98%)	2 (2%)	57	69
3	BU	132/142 (93%)	130 (98%)	2 (2%)	57	69
3	BV	132/142 (93%)	129 (98%)	3 (2%)	44	63
3	BW	132/142 (93%)	128 (97%)	4 (3%)	36	57
3	BX	131/142 (92%)	131 (100%)	0	100	100
3	BY	132/142 (93%)	129 (98%)	3 (2%)	44	63
3	BZ	132/142 (93%)	130 (98%)	2 (2%)	57	69
3	Ba	132/142 (93%)	129 (98%)	3 (2%)	44	63
3	Bb	132/142 (93%)	130 (98%)	2 (2%)	57	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Bc	131/142 (92%)	129 (98%)	2 (2%)	57	69
3	Bd	132/142 (93%)	128 (97%)	4 (3%)	36	57
3	Be	132/142 (93%)	130 (98%)	2 (2%)	57	69
3	Bf	132/142 (93%)	130 (98%)	2 (2%)	57	69
3	Bg	132/142 (93%)	130 (98%)	2 (2%)	57	69
3	Bh	131/142 (92%)	130 (99%)	1 (1%)	73	76
3	Bi	131/142 (92%)	130 (99%)	1 (1%)	73	76
3	Bj	132/142 (93%)	130 (98%)	2 (2%)	57	69
3	Bk	132/142 (93%)	130 (98%)	2 (2%)	57	69
3	Bl	132/142 (93%)	130 (98%)	2 (2%)	57	69
3	Bm	131/142 (92%)	130 (99%)	1 (1%)	73	76
3	Bn	132/142 (93%)	131 (99%)	1 (1%)	73	76
3	Bo	132/142 (93%)	131 (99%)	1 (1%)	73	76
3	Bp	133/142 (94%)	130 (98%)	3 (2%)	44	63
3	Bq	133/142 (94%)	132 (99%)	1 (1%)	73	76
3	Br	132/142 (93%)	130 (98%)	2 (2%)	57	69
3	Bs	132/142 (93%)	130 (98%)	2 (2%)	57	69
3	Bt	131/142 (92%)	129 (98%)	2 (2%)	57	69
3	Bu	132/142 (93%)	131 (99%)	1 (1%)	73	76
3	Bv	132/142 (93%)	130 (98%)	2 (2%)	57	69
3	Bw	132/142 (93%)	131 (99%)	1 (1%)	73	76
3	Bx	132/142 (93%)	131 (99%)	1 (1%)	73	76
3	By	132/142 (93%)	129 (98%)	3 (2%)	44	63
3	Bz	133/142 (94%)	129 (97%)	4 (3%)	36	57
All	All	13018/13740 (95%)	12618 (97%)	400 (3%)	35	57

All (400) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	15	ASN
1	AA	27	VAL
1	AA	37	VAL
1	AA	49	GLN
1	AA	62	GLN

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Mol	Chain	Res	Type
1	AA	64	VAL
1	AA	101	ARG
1	AA	103	GLN
1	AA	134	ASN
1	AA	139	PHE
1	AA	171	ILE
1	AA	186	LYS
1	AA	219	ILE
1	AA	248	ARG
1	AA	250	LYS
1	AA	267	LEU
1	AA	272	THR
1	AA	286	MET
1	AB	37	VAL
1	AB	75	LYS
1	AB	125	ILE
1	AB	151	GLU
1	AB	171	ILE
1	AB	177	LEU
1	AB	187	ILE
1	AB	219	ILE
1	AB	248	ARG
1	AB	267	LEU
1	AB	277	LYS
1	AB	298	VAL
1	AC	2	THR
1	AC	19	ILE
1	AC	27	VAL
1	AC	37	VAL
1	AC	44	ASN
1	AC	62	GLN
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	219	ILE
1	AC	248	ARG
1	AC	267	LEU
1	AD	15	ASN
1	AD	20	VAL

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Mol	Chain	Res	Type
1	AD	27	VAL
1	AD	49	GLN
1	AD	62	GLN
1	AD	75	LYS
1	AD	116	THR
1	AD	134	ASN
1	AD	140	LYS
1	AD	144	ARG
1	AD	167	ILE
1	AD	178	LEU
1	AD	191	LYS
1	AE	6	ILE
1	AE	37	VAL
1	AE	79	LEU
1	AE	125	ILE
1	AE	171	ILE
1	AE	187	ILE
1	AE	189	ASN
1	AE	219	ILE
1	AE	277	LYS
1	AF	2	THR
1	AF	6	ILE
1	AF	91	VAL
1	AF	116	THR
1	AF	120	ILE
1	AF	158	GLU
1	AF	168	LEU
1	AF	178	LEU
1	AF	216	LYS
1	AF	267	LEU
1	AG	15	ASN
1	AG	27	VAL
1	AG	49	GLN
1	AG	62	GLN
1	AG	102	LYS
1	AG	103	GLN
1	AG	134	ASN
1	AH	37	VAL
1	AH	89	GLN
1	AH	125	ILE
1	AH	155	LYS
1	AH	165	ARG

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Mol	Chain	Res	Type
1	AH	168	LEU
1	AH	169	GLU
1	AH	171	ILE
1	AH	219	ILE
1	AH	277	LYS
1	AI	2	THR
1	AI	12	GLU
1	AI	27	VAL
1	AI	30	GLN
1	AI	62	GLN
1	AI	75	LYS
1	AI	108	TRP
1	AI	168	LEU
1	AI	177	LEU
1	AI	178	LEU
1	AI	184	ILE
1	AI	189	ASN
1	AI	219	ILE
1	AI	267	LEU
1	AJ	15	ASN
1	AJ	27	VAL
1	AJ	28	ASN
1	AJ	62	GLN
1	AJ	88	LEU
1	AJ	102	LYS
1	AJ	116	THR
1	AJ	134	ASN
1	AJ	139	PHE
1	AJ	140	LYS
1	AJ	148	LYS
1	AJ	154	LYS
1	AJ	186	LYS
1	AK	37	VAL
1	AK	89	GLN
1	AK	154	LYS
1	AK	155	LYS
1	AK	165	ARG
1	AK	171	ILE
1	AK	177	LEU
1	AK	219	ILE
1	AK	277	LYS
1	AK	298	VAL

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Mol	Chain	Res	Type
1	AL	2	THR
1	AL	6	ILE
1	AL	27	VAL
1	AL	58	GLU
1	AL	62	GLN
1	AL	102	LYS
1	AL	108	TRP
1	AL	120	ILE
1	AL	178	LEU
1	AL	182	ILE
1	AL	185	GLU
1	AL	186	LYS
1	AL	219	ILE
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
1	AM	116	THR
1	AM	120	ILE
1	AM	134	ASN
1	AM	178	LEU
1	AM	219	ILE
1	AN	17	ILE
1	AN	37	VAL
1	AN	43	LYS
1	AN	89	GLN
1	AN	167	ILE
1	AN	168	LEU
1	AN	171	ILE
1	AN	177	LEU
1	AN	178	LEU
1	AN	184	ILE
1	AN	219	ILE
1	AN	277	LYS
1	AO	23	ARG
1	AO	27	VAL
1	AO	62	GLN

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Mol	Chain	Res	Type
1	AO	116	THR
1	AO	159	GLN
1	AO	170	SER
1	AO	177	LEU
1	AO	219	ILE
1	AO	267	LEU
1	AP	15	ASN
1	AP	22	LEU
1	AP	27	VAL
1	AP	62	GLN
1	AP	64	VAL
1	AP	102	LYS
1	AP	104	GLU
1	AP	116	THR
1	AP	134	ASN
1	AP	139	PHE
1	AP	148	LYS
1	AP	181	VAL
1	AP	192	VAL
1	AP	209	GLU
1	AP	219	ILE
1	AQ	36	ILE
1	AQ	37	VAL
1	AQ	125	ILE
1	AQ	138	THR
1	AQ	155	LYS
1	AQ	165	ARG
1	AQ	171	ILE
1	AQ	178	LEU
1	AQ	219	ILE
1	AQ	298	VAL
1	AR	2	THR
1	AR	62	GLN
1	AR	116	THR
1	AR	150	ILE
1	AR	168	LEU
1	AR	178	LEU
1	AR	219	ILE
1	AR	267	LEU
2	AS	32	GLU
2	AS	47	GLU
2	AS	86	ARG

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Mol	Chain	Res	Type
2	AS	95	LEU
2	AS	105	VAL
2	AS	177	THR
2	AS	200	LEU
2	AS	232	THR
2	AS	243	GLU
2	AT	32	GLU
2	AT	47	GLU
2	AT	76	ILE
2	AT	86	ARG
2	AT	95	LEU
2	AT	105	VAL
2	AT	134	ILE
2	AT	135	ILE
2	AT	177	THR
2	AT	200	LEU
2	AT	232	THR
2	AT	244	LEU
2	AT	246	ILE
2	AU	32	GLU
2	AU	47	GLU
2	AU	76	ILE
2	AU	95	LEU
2	AU	177	THR
2	AU	200	LEU
2	AU	220	LEU
2	AU	232	THR
2	AV	32	GLU
2	AV	47	GLU
2	AV	86	ARG
2	AV	95	LEU
2	AV	105	VAL
2	AV	134	ILE
2	AV	135	ILE
2	AV	177	THR
2	AV	198	ASP
2	AV	200	LEU
2	AV	232	THR
2	AW	32	GLU
2	AW	47	GLU
2	AW	86	ARG
2	AW	88	LEU

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Mol	Chain	Res	Type
2	AW	95	LEU
2	AW	105	VAL
2	AW	177	THR
2	AW	200	LEU
2	AW	232	THR
2	AX	32	GLU
2	AX	34	LEU
2	AX	47	GLU
2	AX	79	LYS
2	AX	88	LEU
2	AX	95	LEU
2	AX	105	VAL
2	AX	134	ILE
2	AX	135	ILE
2	AX	177	THR
2	AX	200	LEU
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	BA	162	ILE
3	BB	35	VAL
3	BB	70	GLU
3	BB	97	SER
3	BB	117	ASN
3	BB	162	ILE
3	BC	12	LYS
3	BC	35	VAL
3	BC	70	GLU
3	BC	97	SER
3	BC	107	ARG
3	BC	117	ASN
3	BC	136	ILE
3	BC	162	ILE
3	BD	81	LYS
3	BD	133	HIS
3	BE	60	LEU
3	BE	133	HIS
3	BF	60	LEU

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Mol	Chain	Res	Type
3	BF	107	ARG
3	BG	5	LYS
3	BG	81	LYS
3	BH	12	LYS
3	BH	60	LEU
3	BH	133	HIS
3	BI	107	ARG
3	BJ	81	LYS
3	BJ	133	HIS
3	BK	60	LEU
3	BK	133	HIS
3	BL	60	LEU
3	BL	81	LYS
3	BL	107	ARG
3	BM	12	LYS
3	BM	81	LYS
3	BM	133	HIS
3	BN	60	LEU
3	BN	103	ASN
3	BN	133	HIS
3	BN	141	VAL
3	BO	5	LYS
3	BO	60	LEU
3	BO	107	ARG
3	BP	133	HIS
3	BQ	133	HIS
3	BR	60	LEU
3	BR	81	LYS
3	BR	107	ARG
3	BS	133	HIS
3	BT	60	LEU
3	BT	133	HIS
3	BU	60	LEU
3	BU	107	ARG
3	BV	81	LYS
3	BV	133	HIS
3	BV	162	ILE
3	BW	9	ARG
3	BW	12	LYS
3	BW	60	LEU
3	BW	133	HIS
3	BY	12	LYS

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Mol	Chain	Res	Type
3	BY	81	LYS
3	BY	133	HIS
3	BZ	60	LEU
3	BZ	133	HIS
3	Ba	60	LEU
3	Ba	81	LYS
3	Ba	107	ARG
3	Bb	81	LYS
3	Bb	133	HIS
3	Bc	60	LEU
3	Bc	133	HIS
3	Bd	60	LEU
3	Bd	81	LYS
3	Bd	107	ARG
3	Bd	163	ASP
3	Be	81	LYS
3	Be	133	HIS
3	Bf	60	LEU
3	Bf	133	HIS
3	Bg	60	LEU
3	Bg	107	ARG
3	Bh	133	HIS
3	Bi	133	HIS
3	Bj	70	GLU
3	Bj	107	ARG
3	Bk	81	LYS
3	Bk	133	HIS
3	Bl	60	LEU
3	Bl	133	HIS
3	Bm	107	ARG
3	Bn	133	HIS
3	Bo	133	HIS
3	Bp	60	LEU
3	Bp	107	ARG
3	Bp	162	ILE
3	Bq	133	HIS
3	Br	60	LEU
3	Br	133	HIS
3	Bs	81	LYS
3	Bs	107	ARG
3	Bt	81	LYS
3	Bt	133	HIS

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Mol	Chain	Res	Type
3	Bu	133	HIS
3	Bv	60	LEU
3	Bv	107	ARG
3	Bw	133	HIS
3	Bx	133	HIS
3	By	60	LEU
3	By	107	ARG
3	By	116	ARG
3	Bz	12	LYS
3	Bz	81	LYS
3	Bz	117	ASN
3	Bz	133	HIS
3	B1	60	LEU
3	B1	133	HIS
3	B2	12	LYS
3	B2	60	LEU
3	B2	81	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (395) 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	103	GLN
1	AA	134	ASN
1	AA	164	ASN
1	AA	202	HIS
1	AA	217	ASN
1	AA	280	GLN
1	AB	30	GLN
1	AC	24	HIS
1	AC	30	GLN
1	AC	44	ASN
1	AC	159	GLN
1	AC	189	ASN
1	AC	202	HIS
1	AC	280	GLN
1	AD	15	ASN
1	AD	28	ASN

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Mol	Chain	Res	Type
1	AD	89	GLN
1	AD	134	ASN
1	AD	217	ASN
1	AD	280	GLN
1	AE	49	GLN
1	AE	86	ASN
1	AE	118	HIS
1	AE	239	ASN
1	AE	280	GLN
1	AF	62	GLN
1	AF	76	ASN
1	AF	111	GLN
1	AF	128	GLN
1	AG	15	ASN
1	AG	28	ASN
1	AG	62	GLN
1	AG	86	ASN
1	AG	89	GLN
1	AG	164	ASN
1	AG	217	ASN
1	AG	280	GLN
1	AH	30	GLN
1	AH	49	GLN
1	AH	57	GLN
1	AH	86	ASN
1	AH	103	GLN
1	AH	239	ASN
1	AI	24	HIS
1	AI	30	GLN
1	AI	49	GLN
1	AI	57	GLN
1	AI	62	GLN
1	AI	89	GLN
1	AJ	15	ASN
1	AJ	28	ASN
1	AJ	49	GLN
1	AJ	62	GLN
1	AJ	86	ASN
1	AJ	217	ASN
1	AJ	239	ASN
1	AJ	280	GLN
1	AK	49	GLN

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Mol	Chain	Res	Type
1	AK	86	ASN
1	AK	118	HIS
1	AK	147	ASN
1	AK	164	ASN
1	AK	239	ASN
1	AK	280	GLN
1	AL	24	HIS
1	AL	62	GLN
1	AL	76	ASN
1	AL	86	ASN
1	AL	118	HIS
1	AL	128	GLN
1	AM	15	ASN
1	AM	28	ASN
1	AM	62	GLN
1	AM	128	GLN
1	AM	134	ASN
1	AM	189	ASN
1	AM	217	ASN
1	AM	239	ASN
1	AM	280	GLN
1	AN	49	GLN
1	AN	86	ASN
1	AN	118	HIS
1	AN	147	ASN
1	AN	239	ASN
1	AN	280	GLN
1	AO	15	ASN
1	AO	24	HIS
1	AO	28	ASN
1	AO	30	GLN
1	AO	49	GLN
1	AO	62	GLN
1	AO	111	GLN
1	AO	147	ASN
1	AP	15	ASN
1	AP	16	ASN
1	AP	62	GLN
1	AP	217	ASN
1	AP	239	ASN
1	AP	280	GLN
1	AQ	30	GLN

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Mol	Chain	Res	Type
1	AQ	49	GLN
1	AQ	86	ASN
1	AQ	118	HIS
1	AQ	239	ASN
1	AR	24	HIS
1	AR	57	GLN
1	AR	128	GLN
1	AR	280	GLN
2	AS	66	ASN
2	AS	126	ASN
2	AS	205	GLN
2	AT	102	GLN
2	AT	152	GLN
2	AT	217	ASN
2	AU	15	ASN
2	AU	89	GLN
2	AU	102	GLN
2	AU	126	ASN
2	AU	217	ASN
2	AV	15	ASN
2	AV	102	GLN
2	AV	126	ASN
2	AV	152	GLN
2	AV	212	ASN
2	AV	217	ASN
2	AW	59	GLN
2	AW	126	ASN
2	AW	152	GLN
2	AW	217	ASN
2	AX	15	ASN
2	AX	59	GLN
2	AX	66	ASN
2	AX	102	GLN
2	AX	110	ASN
2	AX	152	GLN
3	BA	26	ASN
3	BA	101	ASN
3	BA	133	HIS
3	BA	143	GLN
3	BB	13	ASN
3	BB	26	ASN
3	BB	133	HIS

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Mol	Chain	Res	Type
3	BC	19	ASN
3	BC	26	ASN
3	BC	101	ASN
3	BC	133	HIS
3	BD	19	ASN
3	BD	130	ASN
3	BD	133	HIS
3	BE	13	ASN
3	BE	19	ASN
3	BE	53	ASN
3	BE	101	ASN
3	BE	106	ASN
3	BE	130	ASN
3	BE	133	HIS
3	BF	34	ASN
3	BF	57	ASN
3	BF	103	ASN
3	BF	130	ASN
3	BG	19	ASN
3	BG	26	ASN
3	BG	34	ASN
3	BG	130	ASN
3	BG	133	HIS
3	BH	19	ASN
3	BH	53	ASN
3	BH	101	ASN
3	BH	130	ASN
3	BH	133	HIS
3	BI	34	ASN
3	BI	57	ASN
3	BI	103	ASN
3	BI	130	ASN
3	BJ	19	ASN
3	BJ	34	ASN
3	BJ	130	ASN
3	BJ	133	HIS
3	BK	19	ASN
3	BK	53	ASN
3	BK	101	ASN
3	BK	106	ASN
3	BK	130	ASN
3	BK	133	HIS

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Mol	Chain	Res	Type
3	BL	34	ASN
3	BL	57	ASN
3	BL	103	ASN
3	BL	130	ASN
3	BM	19	ASN
3	BM	26	ASN
3	BM	130	ASN
3	BM	133	HIS
3	BN	19	ASN
3	BN	53	ASN
3	BN	57	ASN
3	BN	101	ASN
3	BN	103	ASN
3	BN	130	ASN
3	BN	133	HIS
3	BO	13	ASN
3	BO	34	ASN
3	BO	57	ASN
3	BO	133	HIS
3	BP	19	ASN
3	BP	130	ASN
3	BP	133	HIS
3	BP	143	GLN
3	BQ	13	ASN
3	BQ	19	ASN
3	BQ	53	ASN
3	BQ	101	ASN
3	BQ	106	ASN
3	BQ	130	ASN
3	BQ	133	HIS
3	BR	57	ASN
3	BR	103	ASN
3	BR	130	ASN
3	BS	19	ASN
3	BS	34	ASN
3	BS	130	ASN
3	BS	133	HIS
3	BT	19	ASN
3	BT	34	ASN
3	BT	53	ASN
3	BT	101	ASN
3	BT	106	ASN

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Mol	Chain	Res	Type
3	BT	130	ASN
3	BT	133	HIS
3	BU	34	ASN
3	BU	57	ASN
3	BU	103	ASN
3	BU	130	ASN
3	BU	133	HIS
3	BV	19	ASN
3	BV	130	ASN
3	BV	133	HIS
3	BW	19	ASN
3	BW	53	ASN
3	BW	101	ASN
3	BW	130	ASN
3	BW	133	HIS
3	BW	143	GLN
3	BX	34	ASN
3	BX	57	ASN
3	BX	103	ASN
3	BX	130	ASN
3	BX	133	HIS
3	BY	19	ASN
3	BY	130	ASN
3	BY	133	HIS
3	BZ	19	ASN
3	BZ	53	ASN
3	BZ	57	ASN
3	BZ	101	ASN
3	BZ	106	ASN
3	BZ	130	ASN
3	BZ	133	HIS
3	Ba	34	ASN
3	Ba	57	ASN
3	Ba	103	ASN
3	Ba	130	ASN
3	Bb	19	ASN
3	Bb	130	ASN
3	Bb	133	HIS
3	Bc	19	ASN
3	Bc	53	ASN
3	Bc	57	ASN
3	Bc	106	ASN

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Mol	Chain	Res	Type
3	Bc	130	ASN
3	Bc	133	HIS
3	Bd	34	ASN
3	Bd	57	ASN
3	Bd	103	ASN
3	Bd	130	ASN
3	Be	19	ASN
3	Be	130	ASN
3	Be	133	HIS
3	Bf	19	ASN
3	Bf	53	ASN
3	Bf	101	ASN
3	Bf	106	ASN
3	Bf	130	ASN
3	Bf	133	HIS
3	Bf	143	GLN
3	Bg	19	ASN
3	Bg	34	ASN
3	Bg	57	ASN
3	Bg	103	ASN
3	Bg	106	ASN
3	Bg	130	ASN
3	Bh	19	ASN
3	Bh	130	ASN
3	Bh	133	HIS
3	Bi	19	ASN
3	Bi	34	ASN
3	Bi	53	ASN
3	Bi	101	ASN
3	Bi	106	ASN
3	Bi	130	ASN
3	Bi	133	HIS
3	Bj	34	ASN
3	Bj	57	ASN
3	Bj	103	ASN
3	Bj	130	ASN
3	Bk	19	ASN
3	Bk	26	ASN
3	Bk	130	ASN
3	Bk	133	HIS
3	Bl	13	ASN
3	Bl	19	ASN

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Mol	Chain	Res	Type
3	Bl	53	ASN
3	Bl	57	ASN
3	Bl	101	ASN
3	Bl	106	ASN
3	Bl	130	ASN
3	Bl	133	HIS
3	Bm	34	ASN
3	Bm	57	ASN
3	Bm	103	ASN
3	Bm	130	ASN
3	Bn	19	ASN
3	Bn	34	ASN
3	Bn	133	HIS
3	Bo	19	ASN
3	Bo	53	ASN
3	Bo	101	ASN
3	Bo	130	ASN
3	Bo	133	HIS
3	Bp	19	ASN
3	Bp	57	ASN
3	Bp	103	ASN
3	Bp	130	ASN
3	Bp	133	HIS
3	Bq	19	ASN
3	Bq	34	ASN
3	Bq	130	ASN
3	Bq	133	HIS
3	Br	19	ASN
3	Br	53	ASN
3	Br	101	ASN
3	Br	130	ASN
3	Br	133	HIS
3	Bs	34	ASN
3	Bs	53	ASN
3	Bs	57	ASN
3	Bs	103	ASN
3	Bs	130	ASN
3	Bt	19	ASN
3	Bt	130	ASN
3	Bt	133	HIS
3	Bu	13	ASN
3	Bu	19	ASN

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Mol	Chain	Res	Type
3	Bu	53	ASN
3	Bu	101	ASN
3	Bu	106	ASN
3	Bu	130	ASN
3	Bu	133	HIS
3	Bv	57	ASN
3	Bv	103	ASN
3	Bv	130	ASN
3	Bw	19	ASN
3	Bw	34	ASN
3	Bw	130	ASN
3	Bw	133	HIS
3	Bx	13	ASN
3	Bx	19	ASN
3	Bx	53	ASN
3	Bx	101	ASN
3	Bx	106	ASN
3	Bx	130	ASN
3	Bx	133	HIS
3	By	13	ASN
3	By	34	ASN
3	By	57	ASN
3	By	103	ASN
3	By	130	ASN
3	Bz	19	ASN
3	Bz	130	ASN
3	Bz	133	HIS
3	B1	19	ASN
3	B1	53	ASN
3	B1	57	ASN
3	B1	101	ASN
3	B1	130	ASN
3	B1	133	HIS
3	B2	19	ASN
3	B2	34	ASN
3	B2	57	ASN
3	B2	103	ASN
3	B2	130	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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, 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%)	-0.08	2 (0%) 84 65	84, 119, 162, 188	0
1	AB	294/299 (98%)	0.07	7 (2%) 59 41	94, 149, 206, 237	0
1	AC	299/299 (100%)	0.07	8 (2%) 56 38	95, 124, 160, 180	0
1	AD	299/299 (100%)	-0.16	2 (0%) 84 65	86, 128, 175, 206	0
1	AE	291/299 (97%)	0.02	4 (1%) 73 51	89, 159, 213, 249	0
1	AF	299/299 (100%)	-0.03	7 (2%) 61 42	90, 132, 167, 183	0
1	AG	299/299 (100%)	-0.22	4 (1%) 75 53	95, 133, 180, 203	0
1	AH	294/299 (98%)	-0.00	4 (1%) 73 51	103, 176, 237, 261	0
1	AI	299/299 (100%)	-0.08	1 (0%) 90 78	94, 135, 163, 180	0
1	AJ	299/299 (100%)	-0.19	2 (0%) 84 65	88, 121, 160, 183	0
1	AK	293/299 (97%)	-0.15	1 (0%) 90 78	94, 140, 229, 254	0
1	AL	298/299 (99%)	-0.05	6 (2%) 65 44	92, 122, 157, 172	0
1	AM	299/299 (100%)	-0.20	2 (0%) 84 65	85, 124, 188, 230	0
1	AN	294/299 (98%)	0.01	2 (0%) 84 65	92, 156, 235, 269	0
1	AO	299/299 (100%)	0.02	3 (1%) 79 58	91, 129, 164, 182	0
1	AP	299/299 (100%)	-0.08	4 (1%) 75 53	92, 129, 171, 193	0
1	AQ	295/299 (98%)	0.01	2 (0%) 84 65	111, 172, 217, 240	0
1	AR	299/299 (100%)	0.01	4 (1%) 75 53	95, 138, 197, 218	0
2	AS	242/253 (95%)	-0.01	3 (1%) 76 54	84, 124, 195, 234	0
2	AT	242/253 (95%)	-0.03	3 (1%) 76 54	88, 122, 191, 233	0
2	AU	242/253 (95%)	-0.05	3 (1%) 76 54	83, 121, 188, 235	0
2	AV	241/253 (95%)	0.05	3 (1%) 76 54	82, 125, 205, 257	0
2	AW	241/253 (95%)	-0.09	1 (0%) 88 74	83, 125, 200, 246	0
2	AX	241/253 (95%)	-0.06	4 (1%) 69 47	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%)	0.12	6 (3%) 45 31	134, 174, 213, 233	0
3	B2	162/173 (93%)	0.08	4 (2%) 58 40	106, 137, 159, 179	0
3	BA	164/173 (94%)	0.08	3 (1%) 67 46	103, 260, 278, 283	0
3	BB	163/173 (94%)	0.06	4 (2%) 58 40	112, 254, 272, 279	0
3	BC	163/173 (94%)	0.04	6 (3%) 45 31	113, 261, 278, 280	0
3	BD	164/173 (94%)	0.01	4 (2%) 59 41	112, 160, 181, 206	0
3	BE	164/173 (94%)	-0.05	1 (0%) 85 68	112, 157, 189, 219	0
3	BF	163/173 (94%)	0.03	2 (1%) 76 54	118, 183, 239, 258	0
3	BG	164/173 (94%)	-0.08	3 (1%) 67 46	97, 159, 203, 216	0
3	BH	164/173 (94%)	0.03	1 (0%) 85 68	102, 148, 177, 214	0
3	BI	163/173 (94%)	0.01	3 (1%) 67 46	99, 177, 221, 229	0
3	BJ	164/173 (94%)	0.10	1 (0%) 85 68	106, 179, 218, 232	0
3	BK	163/173 (94%)	0.09	4 (2%) 58 40	107, 171, 210, 235	0
3	BL	163/173 (94%)	0.07	1 (0%) 85 68	116, 190, 228, 239	0
3	BM	163/173 (94%)	0.33	9 (5%) 30 23	133, 280, 292, 295	0
3	BN	162/173 (93%)	0.37	8 (4%) 35 26	149, 265, 278, 282	0
3	BO	162/173 (93%)	0.67	16 (9%) 13 15	147, 276, 292, 295	0
3	BP	163/173 (94%)	0.20	8 (4%) 35 26	162, 274, 286, 288	0
3	BQ	162/173 (93%)	0.23	5 (3%) 51 35	176, 241, 272, 278	0
3	BR	163/173 (94%)	0.34	11 (6%) 24 20	179, 271, 290, 294	0
3	BS	163/173 (94%)	0.02	4 (2%) 58 40	163, 198, 224, 233	0
3	BT	164/173 (94%)	0.13	4 (2%) 59 41	149, 196, 218, 227	0
3	BU	164/173 (94%)	0.12	2 (1%) 76 54	148, 204, 241, 256	0
3	BV	163/173 (94%)	-0.14	3 (1%) 67 46	125, 150, 191, 214	0
3	BW	164/173 (94%)	0.02	1 (0%) 85 68	121, 146, 163, 187	0
3	BX	162/173 (93%)	-0.04	2 (1%) 76 54	118, 143, 179, 200	0
3	BY	163/173 (94%)	-0.13	1 (0%) 85 68	127, 154, 182, 202	0
3	BZ	163/173 (94%)	-0.11	4 (2%) 58 40	116, 151, 180, 209	0
3	Ba	162/173 (93%)	-0.11	1 (0%) 85 68	124, 148, 179, 196	0
3	Bb	163/173 (94%)	0.02	3 (1%) 67 46	144, 200, 239, 255	0
3	Bc	164/173 (94%)	0.00	4 (2%) 59 41	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%)	-0.04	2 (1%) 76 54	120, 187, 209, 215	0
3	Be	163/173 (94%)	0.23	5 (3%) 51 35	128, 282, 288, 291	0
3	Bf	164/173 (94%)	0.23	5 (3%) 52 36	107, 277, 289, 291	0
3	Bg	163/173 (94%)	0.06	4 (2%) 58 40	109, 273, 286, 288	0
3	Bh	161/173 (93%)	0.24	12 (7%) 20 18	194, 259, 275, 278	0
3	Bi	162/173 (93%)	0.25	4 (2%) 58 40	164, 256, 274, 276	0
3	Bj	162/173 (93%)	0.32	7 (4%) 40 28	181, 259, 276, 278	0
3	Bk	163/173 (94%)	0.07	3 (1%) 67 46	160, 187, 214, 231	0
3	Bl	163/173 (94%)	-0.11	4 (2%) 58 40	161, 184, 203, 232	0
3	Bm	162/173 (93%)	0.17	3 (1%) 66 45	156, 181, 202, 213	0
3	Bn	162/173 (93%)	0.07	6 (3%) 45 31	146, 208, 256, 274	0
3	Bo	162/173 (93%)	0.08	2 (1%) 76 54	142, 203, 230, 238	0
3	Bp	164/173 (94%)	0.21	7 (4%) 40 28	133, 210, 240, 252	0
3	Bq	163/173 (94%)	0.01	2 (1%) 76 54	108, 192, 220, 232	0
3	Br	163/173 (94%)	-0.04	2 (1%) 76 54	100, 172, 207, 237	0
3	Bs	163/173 (94%)	-0.01	4 (2%) 58 40	99, 168, 208, 227	0
3	Bt	162/173 (93%)	0.21	4 (2%) 58 40	146, 213, 232, 257	0
3	Bu	162/173 (93%)	0.11	3 (1%) 66 45	138, 239, 271, 275	0
3	Bv	164/173 (94%)	0.13	3 (1%) 67 46	128, 225, 251, 257	0
3	Bw	163/173 (94%)	0.12	5 (3%) 51 35	182, 216, 245, 253	0
3	Bx	162/173 (93%)	0.29	7 (4%) 40 28	203, 239, 274, 280	0
3	By	162/173 (93%)	0.13	5 (3%) 51 35	195, 252, 267, 272	0
3	Bz	163/173 (94%)	0.13	5 (3%) 51 35	130, 170, 232, 238	0
All	All	15597/16242 (96%)	0.03	315 (2%) 65 44	82, 163, 274, 295	0

All (315) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Be	122	VAL	9.0
3	BM	121	LEU	8.8
3	BM	122	VAL	8.2
3	BS	122	VAL	7.3
3	Bg	121	LEU	6.9
3	Bb	122	VAL	6.9

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Mol	Chain	Res	Type	RSRZ
3	BN	122	VAL	6.4
3	BO	77	LEU	6.2
3	Be	123	GLY	6.0
3	BO	134	ILE	6.0
3	Bo	122	VAL	5.8
3	BO	90	ILE	5.8
3	B1	122	VAL	5.8
3	BR	121	LEU	5.6
3	BK	122	VAL	5.6
3	Bp	122	VAL	5.6
3	Bh	122	VAL	5.3
3	Bm	122	VAL	5.2
3	BU	122	VAL	5.2
1	AF	16	ASN	5.1
3	Bg	122	VAL	4.9
1	AE	56	ALA	4.9
3	Bh	75	ILE	4.7
3	BO	156	GLY	4.7
3	BO	91	GLY	4.7
1	AE	34	ALA	4.6
3	Be	121	LEU	4.6
3	BQ	135	ASP	4.5
3	BM	123	GLY	4.4
3	BD	123	GLY	4.4
3	B1	123	GLY	4.3
3	Bh	134	ILE	4.3
3	BK	121	LEU	4.2
3	BB	73	GLY	4.2
1	AJ	27	VAL	4.2
2	AX	201	GLU	4.2
3	Bc	90	ILE	4.2
3	BD	122	VAL	4.1
3	Bq	122	VAL	4.1
3	BR	75	ILE	4.1
3	B2	122	VAL	4.0
3	BC	122	VAL	4.0
3	Be	75	ILE	3.8
3	Bv	136	ILE	3.8
3	BR	122	VAL	3.8
3	B1	120	SER	3.8
3	BM	134	ILE	3.8
1	AC	15	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	AM	299	ALA	3.7
3	BN	121	LEU	3.7
1	AB	36	ILE	3.6
1	AP	233	GLY	3.6
3	Bn	78	SER	3.6
3	BP	84	THR	3.6
3	BZ	10	GLY	3.6
3	Bx	75	ILE	3.6
3	BC	54	VAL	3.6
3	Be	134	ILE	3.6
3	Bm	123	GLY	3.5
3	Bl	121	LEU	3.5
1	AL	233	GLY	3.5
3	BN	120	SER	3.5
3	BO	75	ILE	3.5
1	AN	98	PHE	3.5
3	BO	89	SER	3.4
3	BR	134	ILE	3.4
3	Bu	75	ILE	3.4
3	Bc	121	LEU	3.4
3	BO	121	LEU	3.4
3	Bu	123	GLY	3.4
1	AG	237	ILE	3.4
3	BR	69	GLY	3.3
3	BS	123	GLY	3.3
3	BO	122	VAL	3.3
3	Bd	122	VAL	3.3
3	Bb	123	GLY	3.3
3	BO	136	ILE	3.2
1	AL	15	ASN	3.2
1	AP	299	ALA	3.2
1	AC	63	GLY	3.2
3	Bf	165	ALA	3.2
3	Bw	15	ALA	3.2
1	AB	56	ALA	3.1
3	BB	75	ILE	3.1
3	Bh	90	ILE	3.1
3	Bh	121	LEU	3.1
3	Bz	122	VAL	3.1
3	Bt	90	ILE	3.1
2	AW	33	GLU	3.0
3	Bp	121	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
3	Bs	122	VAL	3.0
1	AF	17	ILE	3.0
1	AH	233	GLY	3.0
3	Bj	120	SER	3.0
3	Bj	18	ILE	3.0
3	By	123	GLY	3.0
3	BB	76	ILE	2.9
2	AS	253	LEU	2.9
3	Bx	134	ILE	2.9
3	Bt	154	PRO	2.9
3	B2	10	GLY	2.9
1	AB	8	LEU	2.9
3	BS	36	VAL	2.8
3	Bu	54	VAL	2.8
3	BN	44	ILE	2.8
3	BP	136	ILE	2.8
1	AH	136	TRP	2.8
3	BG	121	LEU	2.8
3	BR	71	LEU	2.8
3	Br	156	GLY	2.8
1	AA	299	ALA	2.8
1	AO	139	PHE	2.8
3	BH	122	VAL	2.8
3	Bn	122	VAL	2.8
3	Bt	69	GLY	2.8
3	BW	119	CYS	2.8
3	Bv	119	CYS	2.8
3	Bx	76	ILE	2.8
2	AS	201	GLU	2.8
3	By	122	VAL	2.8
1	AQ	5	PHE	2.8
3	BP	123	GLY	2.8
3	Bn	91	GLY	2.8
3	B1	159	THR	2.8
1	AQ	233	GLY	2.7
3	BP	156	GLY	2.7
3	Bi	121	LEU	2.7
2	AS	221	ASP	2.7
3	BO	144	TRP	2.7
1	AP	34	ALA	2.7
3	Bk	156	GLY	2.7
3	Bk	157	THR	2.7

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Mol	Chain	Res	Type	RSRZ
3	Bx	122	VAL	2.7
2	AT	74	LEU	2.7
1	AC	19	ILE	2.7
3	Bo	134	ILE	2.7
3	Br	90	ILE	2.7
1	AL	63	GLY	2.7
3	BP	144	TRP	2.6
3	BQ	134	ILE	2.6
3	BT	165	ALA	2.6
3	BZ	14	GLY	2.6
3	Bn	92	GLY	2.6
3	Bz	121	LEU	2.6
1	AC	17	ILE	2.6
3	BM	75	ILE	2.6
1	AF	63	GLY	2.6
3	Bj	91	GLY	2.6
3	Bv	135	ASP	2.6
3	BG	165	ALA	2.6
1	AH	284	PHE	2.6
3	Bs	13	ASN	2.6
1	AO	63	GLY	2.6
3	Bk	22	LEU	2.6
2	AU	218	ASN	2.6
3	BA	134	ILE	2.6
3	Bj	77	LEU	2.6
3	Bi	83	GLY	2.6
1	AA	269	ASP	2.6
3	BQ	120	SER	2.6
1	AJ	299	ALA	2.6
3	Bs	10	GLY	2.6
3	Bz	119	CYS	2.5
3	BV	122	VAL	2.5
3	Bx	22	LEU	2.5
1	AB	34	ALA	2.5
3	Bp	165	ALA	2.5
3	Bw	134	ILE	2.5
3	Bx	88	TYR	2.5
3	BO	157	THR	2.5
3	BT	79	LEU	2.5
3	BY	122	VAL	2.5
3	Bh	77	LEU	2.5
3	BR	123	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	AT	231	LEU	2.5
3	Bj	22	LEU	2.5
2	AX	156	ASN	2.5
3	Bf	142	CYS	2.5
3	Bj	76	ILE	2.5
2	AV	69	TYR	2.5
3	BC	25	ILE	2.5
3	BR	156	GLY	2.5
3	Bh	104	LEU	2.5
3	BC	18	ILE	2.4
1	AG	299	ALA	2.4
3	BV	164	SER	2.4
3	Bp	13	ASN	2.4
3	Bd	25	ILE	2.4
3	By	134	ILE	2.4
3	Bl	9	ARG	2.4
1	AL	16	ASN	2.4
2	AV	153	SER	2.4
3	BF	122	VAL	2.4
1	AR	119	TYR	2.4
2	AX	33	GLU	2.4
3	BD	165	ALA	2.4
3	BM	131	ALA	2.4
3	BN	75	ILE	2.4
3	Bn	88	TYR	2.4
1	AD	161	VAL	2.4
2	AT	253	LEU	2.4
1	AC	65	SER	2.3
3	Bm	120	SER	2.3
3	BS	22	LEU	2.3
1	AB	32	ILE	2.3
1	AF	233	GLY	2.3
3	B1	60	LEU	2.3
3	Bp	109	VAL	2.3
3	BK	88	TYR	2.3
3	Bt	75	ILE	2.3
1	AF	15	ASN	2.3
3	BG	122	VAL	2.3
3	Bq	88	TYR	2.3
1	AR	177	LEU	2.3
2	AX	253	LEU	2.3
1	AB	6	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
3	BC	132	PHE	2.3
3	By	121	LEU	2.3
3	BN	109	VAL	2.3
3	BF	159	THR	2.3
3	BA	22	LEU	2.3
3	BJ	165	ALA	2.3
3	BP	134	ILE	2.3
3	Bp	134	ILE	2.3
1	AG	233	GLY	2.3
3	BQ	159	THR	2.3
3	BV	159	THR	2.3
3	BA	165	ALA	2.3
3	B1	119	CYS	2.3
1	AF	129	PRO	2.3
3	Bc	122	VAL	2.3
1	AL	177	LEU	2.2
3	Bz	22	LEU	2.2
1	AN	52	PHE	2.2
3	BN	134	ILE	2.2
3	Bp	75	ILE	2.2
3	BN	54	VAL	2.2
3	BT	159	THR	2.2
3	Bf	77	LEU	2.2
3	BM	133	HIS	2.2
1	AH	184	ILE	2.2
3	BU	113	PHE	2.2
3	Bc	15	ALA	2.2
3	BO	160	TYR	2.2
3	Bw	122	VAL	2.2
2	AU	253	LEU	2.2
3	Bi	48	LYS	2.2
3	BI	22	LEU	2.2
3	Bg	54	VAL	2.2
1	AM	171	ILE	2.2
2	AV	159	ILE	2.2
3	BO	142	CYS	2.2
3	BC	9	ARG	2.2
3	BE	156	GLY	2.2
3	Bh	156	GLY	2.2
3	Bj	92	GLY	2.2
3	B2	156	GLY	2.2
1	AP	219	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
3	BR	25	ILE	2.2
3	Bh	120	SER	2.2
3	BK	36	VAL	2.2
3	Bl	88	TYR	2.2
2	AU	201	GLU	2.2
3	Bi	157	THR	2.2
3	BI	122	VAL	2.1
1	AC	284	PHE	2.1
3	BR	77	LEU	2.1
1	AC	64	VAL	2.1
3	BM	90	ILE	2.1
3	Bx	18	ILE	2.1
3	BX	113	PHE	2.1
3	BP	85	THR	2.1
3	B2	90	ILE	2.1
3	Bn	36	VAL	2.1
1	AG	269	ASP	2.1
3	Bl	21	ASP	2.1
3	Bb	88	TYR	2.1
3	Bw	160	TYR	2.1
1	AI	233	GLY	2.1
3	BI	159	THR	2.1
1	AD	299	ALA	2.1
1	AL	64	VAL	2.1
3	Bg	60	LEU	2.1
1	AO	17	ILE	2.1
1	AF	113	SER	2.1
3	BL	122	VAL	2.1
3	BP	56	VAL	2.1
3	BB	22	LEU	2.1
3	By	77	LEU	2.1
3	BO	123	GLY	2.1
3	Bz	142	CYS	2.1
1	AC	273	LEU	2.1
3	BD	121	LEU	2.1
3	Bf	122	VAL	2.1
3	Bh	144	TRP	2.0
3	Bh	9	ARG	2.0
1	AK	36	ILE	2.0
3	Bw	164	SER	2.0
3	BR	60	LEU	2.0
3	Bf	79	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	Bs	119	CYS	2.0
3	BT	36	VAL	2.0
1	AR	233	GLY	2.0
3	BQ	136	ILE	2.0
3	Bh	162	ILE	2.0
3	BM	120	SER	2.0
3	BO	78	SER	2.0
1	AR	15	ASN	2.0
3	BX	111	ASN	2.0
1	AE	233	GLY	2.0
1	AE	219	ILE	2.0
3	BZ	157	THR	2.0
3	Ba	121	LEU	2.0
1	AB	20	VAL	2.0
3	BZ	36	VAL	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 oligosaccharides 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.