



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:57 AM GMT

PDB ID : 3CMV
Title : Mechanism of homologous recombination from the RecA-ssDNA/dsDNA structures
Authors : Pavletich, N.P.
Deposited on : 2008-03-24
Resolution : 4.30 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

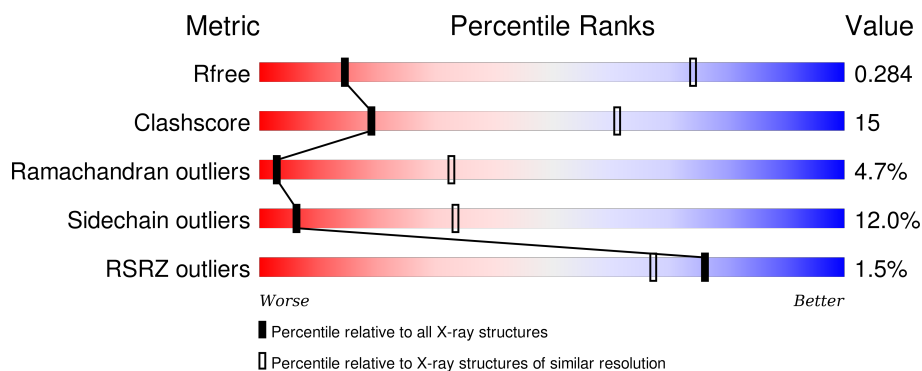
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	1357	<div> <div>2%</div> <div>55%</div> <div>27%</div> <div>6%</div> <div>12%</div> </div>
1	B	1357	<div> <div>54%</div> <div>27%</div> <div>5%</div> <div>14%</div> </div>
1	C	1357	<div> <div>54%</div> <div>27%</div> <div>5%</div> <div>13%</div> </div>
1	D	1357	<div> <div>2%</div> <div>55%</div> <div>27%</div> <div>5%</div> <div>13%</div> </div>
1	E	1357	<div> <div>2%</div> <div>53%</div> <div>27%</div> <div>5%</div> <div>14%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	1357	
1	G	1357	
1	H	1357	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	D	2701	-	-	-	X
2	MG	E	701	-	-	-	X
2	MG	F	701	-	-	-	X
2	MG	G	2701	-	-	-	X
3	ANP	A	1400	X	-	-	-
3	ANP	A	2400	X	-	-	-
3	ANP	A	3400	X	-	-	-
3	ANP	A	400	X	-	-	-
3	ANP	B	1400	X	-	-	-
3	ANP	B	2400	X	-	-	-
3	ANP	B	3400	X	-	-	-
3	ANP	B	400	X	-	-	-
3	ANP	C	1400	X	-	-	-
3	ANP	C	2400	X	-	-	-
3	ANP	C	3400	X	-	-	-
3	ANP	C	400	X	-	-	-
3	ANP	D	1400	X	-	-	-
3	ANP	D	2400	X	-	-	-
3	ANP	D	3400	X	-	-	-
3	ANP	D	400	X	-	-	-
3	ANP	E	1400	X	-	-	-
3	ANP	E	2400	X	-	-	-
3	ANP	E	3400	X	-	-	-
3	ANP	E	400	X	-	-	-
3	ANP	F	1400	X	-	-	-
3	ANP	F	2400	X	-	-	X
3	ANP	F	3400	X	-	-	-
3	ANP	F	400	X	-	-	-
3	ANP	G	1400	X	-	-	-
3	ANP	G	2400	X	-	-	X
3	ANP	G	3400	X	-	-	-
3	ANP	G	400	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ANP	H	1400	X	-	-	-
3	ANP	H	2400	X	-	-	-
3	ANP	H	3400	X	-	-	-
3	ANP	H	400	X	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 71761 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 Protein recA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1190	Total	C	N	O	S	0	0	0
			8970	5660	1553	1719	38			
1	B	1163	Total	C	N	O	S	0	0	0
			8769	5538	1519	1677	35			
1	C	1175	Total	C	N	O	S	0	0	0
			8856	5587	1533	1700	36			
1	D	1175	Total	C	N	O	S	0	0	0
			8856	5587	1533	1700	36			
1	E	1165	Total	C	N	O	S	0	0	0
			8787	5548	1521	1683	35			
1	F	1175	Total	C	N	O	S	0	0	0
			8856	5587	1533	1700	36			
1	G	1167	Total	C	N	O	S	0	0	0
			8799	5554	1523	1687	35			
1	H	1173	Total	C	N	O	S	0	0	0
			8844	5581	1531	1696	36			

There are 400 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	linker	UNP P0A7G6
A	27	ALA	-	linker	UNP P0A7G6
A	28	MET	-	linker	UNP P0A7G6
A	29	HIS	-	linker	UNP P0A7G6
A	986	THR	-	linker	UNP P0A7G6
A	987	GLY	-	linker	UNP P0A7G6
A	988	SER	-	linker	UNP P0A7G6
A	989	THR	-	linker	UNP P0A7G6
A	990	GLY	-	linker	UNP P0A7G6
A	991	SER	-	linker	UNP P0A7G6
A	992	GLY	-	linker	UNP P0A7G6
A	993	THR	-	linker	UNP P0A7G6
A	994	THR	-	linker	UNP P0A7G6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	995	GLY	-	linker	UNP P0A7G6
A	996	SER	-	linker	UNP P0A7G6
A	997	THR	-	linker	UNP P0A7G6
A	998	GLY	-	linker	UNP P0A7G6
A	999	SER	-	linker	UNP P0A7G6
A	1000	MET	-	linker	UNP P0A7G6
A	1986	THR	-	linker	UNP P0A7G6
A	1987	GLY	-	linker	UNP P0A7G6
A	1988	SER	-	linker	UNP P0A7G6
A	1989	THR	-	linker	UNP P0A7G6
A	1990	GLY	-	linker	UNP P0A7G6
A	1991	SER	-	linker	UNP P0A7G6
A	1992	MET	-	linker	UNP P0A7G6
A	1993	GLY	-	linker	UNP P0A7G6
A	1994	HIS	-	linker	UNP P0A7G6
A	1995	THR	-	linker	UNP P0A7G6
A	1996	THR	-	linker	UNP P0A7G6
A	1997	GLY	-	linker	UNP P0A7G6
A	1998	SER	-	linker	UNP P0A7G6
A	1999	MET	-	linker	UNP P0A7G6
A	2000	SER	-	linker	UNP P0A7G6
A	2985	THR	-	linker	UNP P0A7G6
A	2986	GLY	-	linker	UNP P0A7G6
A	2987	SER	-	linker	UNP P0A7G6
A	2988	THR	-	linker	UNP P0A7G6
A	2989	GLY	-	linker	UNP P0A7G6
A	2990	SER	-	linker	UNP P0A7G6
A	2991	ALA	-	linker	UNP P0A7G6
A	2992	SER	-	linker	UNP P0A7G6
A	2993	GLY	-	linker	UNP P0A7G6
A	2994	SER	-	linker	UNP P0A7G6
A	2995	SER	-	linker	UNP P0A7G6
A	2996	THR	-	linker	UNP P0A7G6
A	2997	GLY	-	linker	UNP P0A7G6
A	2998	SER	-	linker	UNP P0A7G6
A	2999	MET	-	linker	UNP P0A7G6
A	3000	SER	-	linker	UNP P0A7G6
B	26	GLY	-	linker	UNP P0A7G6
B	27	ALA	-	linker	UNP P0A7G6
B	28	MET	-	linker	UNP P0A7G6
B	29	HIS	-	linker	UNP P0A7G6
B	986	THR	-	linker	UNP P0A7G6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	987	GLY	-	linker	UNP P0A7G6
B	988	SER	-	linker	UNP P0A7G6
B	989	THR	-	linker	UNP P0A7G6
B	990	GLY	-	linker	UNP P0A7G6
B	991	SER	-	linker	UNP P0A7G6
B	992	GLY	-	linker	UNP P0A7G6
B	993	THR	-	linker	UNP P0A7G6
B	994	THR	-	linker	UNP P0A7G6
B	995	GLY	-	linker	UNP P0A7G6
B	996	SER	-	linker	UNP P0A7G6
B	997	THR	-	linker	UNP P0A7G6
B	998	GLY	-	linker	UNP P0A7G6
B	999	SER	-	linker	UNP P0A7G6
B	1000	MET	-	linker	UNP P0A7G6
B	1986	THR	-	linker	UNP P0A7G6
B	1987	GLY	-	linker	UNP P0A7G6
B	1988	SER	-	linker	UNP P0A7G6
B	1989	THR	-	linker	UNP P0A7G6
B	1990	GLY	-	linker	UNP P0A7G6
B	1991	SER	-	linker	UNP P0A7G6
B	1992	MET	-	linker	UNP P0A7G6
B	1993	GLY	-	linker	UNP P0A7G6
B	1994	HIS	-	linker	UNP P0A7G6
B	1995	THR	-	linker	UNP P0A7G6
B	1996	THR	-	linker	UNP P0A7G6
B	1997	GLY	-	linker	UNP P0A7G6
B	1998	SER	-	linker	UNP P0A7G6
B	1999	MET	-	linker	UNP P0A7G6
B	2000	SER	-	linker	UNP P0A7G6
B	2985	THR	-	linker	UNP P0A7G6
B	2986	GLY	-	linker	UNP P0A7G6
B	2987	SER	-	linker	UNP P0A7G6
B	2988	THR	-	linker	UNP P0A7G6
B	2989	GLY	-	linker	UNP P0A7G6
B	2990	SER	-	linker	UNP P0A7G6
B	2991	ALA	-	linker	UNP P0A7G6
B	2992	SER	-	linker	UNP P0A7G6
B	2993	GLY	-	linker	UNP P0A7G6
B	2994	SER	-	linker	UNP P0A7G6
B	2995	SER	-	linker	UNP P0A7G6
B	2996	THR	-	linker	UNP P0A7G6
B	2997	GLY	-	linker	UNP P0A7G6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	2998	SER	-	linker	UNP P0A7G6
B	2999	MET	-	linker	UNP P0A7G6
B	3000	SER	-	linker	UNP P0A7G6
C	26	GLY	-	linker	UNP P0A7G6
C	27	ALA	-	linker	UNP P0A7G6
C	28	MET	-	linker	UNP P0A7G6
C	29	HIS	-	linker	UNP P0A7G6
C	986	THR	-	linker	UNP P0A7G6
C	987	GLY	-	linker	UNP P0A7G6
C	988	SER	-	linker	UNP P0A7G6
C	989	THR	-	linker	UNP P0A7G6
C	990	GLY	-	linker	UNP P0A7G6
C	991	SER	-	linker	UNP P0A7G6
C	992	GLY	-	linker	UNP P0A7G6
C	993	THR	-	linker	UNP P0A7G6
C	994	THR	-	linker	UNP P0A7G6
C	995	GLY	-	linker	UNP P0A7G6
C	996	SER	-	linker	UNP P0A7G6
C	997	THR	-	linker	UNP P0A7G6
C	998	GLY	-	linker	UNP P0A7G6
C	999	SER	-	linker	UNP P0A7G6
C	1000	MET	-	linker	UNP P0A7G6
C	1986	THR	-	linker	UNP P0A7G6
C	1987	GLY	-	linker	UNP P0A7G6
C	1988	SER	-	linker	UNP P0A7G6
C	1989	THR	-	linker	UNP P0A7G6
C	1990	GLY	-	linker	UNP P0A7G6
C	1991	SER	-	linker	UNP P0A7G6
C	1992	MET	-	linker	UNP P0A7G6
C	1993	GLY	-	linker	UNP P0A7G6
C	1994	HIS	-	linker	UNP P0A7G6
C	1995	THR	-	linker	UNP P0A7G6
C	1996	THR	-	linker	UNP P0A7G6
C	1997	GLY	-	linker	UNP P0A7G6
C	1998	SER	-	linker	UNP P0A7G6
C	1999	MET	-	linker	UNP P0A7G6
C	2000	SER	-	linker	UNP P0A7G6
C	2985	THR	-	linker	UNP P0A7G6
C	2986	GLY	-	linker	UNP P0A7G6
C	2987	SER	-	linker	UNP P0A7G6
C	2988	THR	-	linker	UNP P0A7G6
C	2989	GLY	-	linker	UNP P0A7G6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	2990	SER	-	linker	UNP P0A7G6
C	2991	ALA	-	linker	UNP P0A7G6
C	2992	SER	-	linker	UNP P0A7G6
C	2993	GLY	-	linker	UNP P0A7G6
C	2994	SER	-	linker	UNP P0A7G6
C	2995	SER	-	linker	UNP P0A7G6
C	2996	THR	-	linker	UNP P0A7G6
C	2997	GLY	-	linker	UNP P0A7G6
C	2998	SER	-	linker	UNP P0A7G6
C	2999	MET	-	linker	UNP P0A7G6
C	3000	SER	-	linker	UNP P0A7G6
D	26	GLY	-	linker	UNP P0A7G6
D	27	ALA	-	linker	UNP P0A7G6
D	28	MET	-	linker	UNP P0A7G6
D	29	HIS	-	linker	UNP P0A7G6
D	986	THR	-	linker	UNP P0A7G6
D	987	GLY	-	linker	UNP P0A7G6
D	988	SER	-	linker	UNP P0A7G6
D	989	THR	-	linker	UNP P0A7G6
D	990	GLY	-	linker	UNP P0A7G6
D	991	SER	-	linker	UNP P0A7G6
D	992	GLY	-	linker	UNP P0A7G6
D	993	THR	-	linker	UNP P0A7G6
D	994	THR	-	linker	UNP P0A7G6
D	995	GLY	-	linker	UNP P0A7G6
D	996	SER	-	linker	UNP P0A7G6
D	997	THR	-	linker	UNP P0A7G6
D	998	GLY	-	linker	UNP P0A7G6
D	999	SER	-	linker	UNP P0A7G6
D	1000	MET	-	linker	UNP P0A7G6
D	1986	THR	-	linker	UNP P0A7G6
D	1987	GLY	-	linker	UNP P0A7G6
D	1988	SER	-	linker	UNP P0A7G6
D	1989	THR	-	linker	UNP P0A7G6
D	1990	GLY	-	linker	UNP P0A7G6
D	1991	SER	-	linker	UNP P0A7G6
D	1992	MET	-	linker	UNP P0A7G6
D	1993	GLY	-	linker	UNP P0A7G6
D	1994	HIS	-	linker	UNP P0A7G6
D	1995	THR	-	linker	UNP P0A7G6
D	1996	THR	-	linker	UNP P0A7G6
D	1997	GLY	-	linker	UNP P0A7G6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1998	SER	-	linker	UNP P0A7G6
D	1999	MET	-	linker	UNP P0A7G6
D	2000	SER	-	linker	UNP P0A7G6
D	2985	THR	-	linker	UNP P0A7G6
D	2986	GLY	-	linker	UNP P0A7G6
D	2987	SER	-	linker	UNP P0A7G6
D	2988	THR	-	linker	UNP P0A7G6
D	2989	GLY	-	linker	UNP P0A7G6
D	2990	SER	-	linker	UNP P0A7G6
D	2991	ALA	-	linker	UNP P0A7G6
D	2992	SER	-	linker	UNP P0A7G6
D	2993	GLY	-	linker	UNP P0A7G6
D	2994	SER	-	linker	UNP P0A7G6
D	2995	SER	-	linker	UNP P0A7G6
D	2996	THR	-	linker	UNP P0A7G6
D	2997	GLY	-	linker	UNP P0A7G6
D	2998	SER	-	linker	UNP P0A7G6
D	2999	MET	-	linker	UNP P0A7G6
D	3000	SER	-	linker	UNP P0A7G6
E	26	GLY	-	linker	UNP P0A7G6
E	27	ALA	-	linker	UNP P0A7G6
E	28	MET	-	linker	UNP P0A7G6
E	29	HIS	-	linker	UNP P0A7G6
E	986	THR	-	linker	UNP P0A7G6
E	987	GLY	-	linker	UNP P0A7G6
E	988	SER	-	linker	UNP P0A7G6
E	989	THR	-	linker	UNP P0A7G6
E	990	GLY	-	linker	UNP P0A7G6
E	991	SER	-	linker	UNP P0A7G6
E	992	GLY	-	linker	UNP P0A7G6
E	993	THR	-	linker	UNP P0A7G6
E	994	THR	-	linker	UNP P0A7G6
E	995	GLY	-	linker	UNP P0A7G6
E	996	SER	-	linker	UNP P0A7G6
E	997	THR	-	linker	UNP P0A7G6
E	998	GLY	-	linker	UNP P0A7G6
E	999	SER	-	linker	UNP P0A7G6
E	1000	MET	-	linker	UNP P0A7G6
E	1986	THR	-	linker	UNP P0A7G6
E	1987	GLY	-	linker	UNP P0A7G6
E	1988	SER	-	linker	UNP P0A7G6
E	1989	THR	-	linker	UNP P0A7G6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	1990	GLY	-	linker	UNP P0A7G6
E	1991	SER	-	linker	UNP P0A7G6
E	1992	MET	-	linker	UNP P0A7G6
E	1993	GLY	-	linker	UNP P0A7G6
E	1994	HIS	-	linker	UNP P0A7G6
E	1995	THR	-	linker	UNP P0A7G6
E	1996	THR	-	linker	UNP P0A7G6
E	1997	GLY	-	linker	UNP P0A7G6
E	1998	SER	-	linker	UNP P0A7G6
E	1999	MET	-	linker	UNP P0A7G6
E	2000	SER	-	linker	UNP P0A7G6
E	2985	THR	-	linker	UNP P0A7G6
E	2986	GLY	-	linker	UNP P0A7G6
E	2987	SER	-	linker	UNP P0A7G6
E	2988	THR	-	linker	UNP P0A7G6
E	2989	GLY	-	linker	UNP P0A7G6
E	2990	SER	-	linker	UNP P0A7G6
E	2991	ALA	-	linker	UNP P0A7G6
E	2992	SER	-	linker	UNP P0A7G6
E	2993	GLY	-	linker	UNP P0A7G6
E	2994	SER	-	linker	UNP P0A7G6
E	2995	SER	-	linker	UNP P0A7G6
E	2996	THR	-	linker	UNP P0A7G6
E	2997	GLY	-	linker	UNP P0A7G6
E	2998	SER	-	linker	UNP P0A7G6
E	2999	MET	-	linker	UNP P0A7G6
E	3000	SER	-	linker	UNP P0A7G6
F	26	GLY	-	linker	UNP P0A7G6
F	27	ALA	-	linker	UNP P0A7G6
F	28	MET	-	linker	UNP P0A7G6
F	29	HIS	-	linker	UNP P0A7G6
F	986	THR	-	linker	UNP P0A7G6
F	987	GLY	-	linker	UNP P0A7G6
F	988	SER	-	linker	UNP P0A7G6
F	989	THR	-	linker	UNP P0A7G6
F	990	GLY	-	linker	UNP P0A7G6
F	991	SER	-	linker	UNP P0A7G6
F	992	GLY	-	linker	UNP P0A7G6
F	993	THR	-	linker	UNP P0A7G6
F	994	THR	-	linker	UNP P0A7G6
F	995	GLY	-	linker	UNP P0A7G6
F	996	SER	-	linker	UNP P0A7G6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	997	THR	-	linker	UNP P0A7G6
F	998	GLY	-	linker	UNP P0A7G6
F	999	SER	-	linker	UNP P0A7G6
F	1000	MET	-	linker	UNP P0A7G6
F	1986	THR	-	linker	UNP P0A7G6
F	1987	GLY	-	linker	UNP P0A7G6
F	1988	SER	-	linker	UNP P0A7G6
F	1989	THR	-	linker	UNP P0A7G6
F	1990	GLY	-	linker	UNP P0A7G6
F	1991	SER	-	linker	UNP P0A7G6
F	1992	MET	-	linker	UNP P0A7G6
F	1993	GLY	-	linker	UNP P0A7G6
F	1994	HIS	-	linker	UNP P0A7G6
F	1995	THR	-	linker	UNP P0A7G6
F	1996	THR	-	linker	UNP P0A7G6
F	1997	GLY	-	linker	UNP P0A7G6
F	1998	SER	-	linker	UNP P0A7G6
F	1999	MET	-	linker	UNP P0A7G6
F	2000	SER	-	linker	UNP P0A7G6
F	2985	THR	-	linker	UNP P0A7G6
F	2986	GLY	-	linker	UNP P0A7G6
F	2987	SER	-	linker	UNP P0A7G6
F	2988	THR	-	linker	UNP P0A7G6
F	2989	GLY	-	linker	UNP P0A7G6
F	2990	SER	-	linker	UNP P0A7G6
F	2991	ALA	-	linker	UNP P0A7G6
F	2992	SER	-	linker	UNP P0A7G6
F	2993	GLY	-	linker	UNP P0A7G6
F	2994	SER	-	linker	UNP P0A7G6
F	2995	SER	-	linker	UNP P0A7G6
F	2996	THR	-	linker	UNP P0A7G6
F	2997	GLY	-	linker	UNP P0A7G6
F	2998	SER	-	linker	UNP P0A7G6
F	2999	MET	-	linker	UNP P0A7G6
F	3000	SER	-	linker	UNP P0A7G6
G	26	GLY	-	linker	UNP P0A7G6
G	27	ALA	-	linker	UNP P0A7G6
G	28	MET	-	linker	UNP P0A7G6
G	29	HIS	-	linker	UNP P0A7G6
G	986	THR	-	linker	UNP P0A7G6
G	987	GLY	-	linker	UNP P0A7G6
G	988	SER	-	linker	UNP P0A7G6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	989	THR	-	linker	UNP P0A7G6
G	990	GLY	-	linker	UNP P0A7G6
G	991	SER	-	linker	UNP P0A7G6
G	992	GLY	-	linker	UNP P0A7G6
G	993	THR	-	linker	UNP P0A7G6
G	994	THR	-	linker	UNP P0A7G6
G	995	GLY	-	linker	UNP P0A7G6
G	996	SER	-	linker	UNP P0A7G6
G	997	THR	-	linker	UNP P0A7G6
G	998	GLY	-	linker	UNP P0A7G6
G	999	SER	-	linker	UNP P0A7G6
G	1000	MET	-	linker	UNP P0A7G6
G	1986	THR	-	linker	UNP P0A7G6
G	1987	GLY	-	linker	UNP P0A7G6
G	1988	SER	-	linker	UNP P0A7G6
G	1989	THR	-	linker	UNP P0A7G6
G	1990	GLY	-	linker	UNP P0A7G6
G	1991	SER	-	linker	UNP P0A7G6
G	1992	MET	-	linker	UNP P0A7G6
G	1993	GLY	-	linker	UNP P0A7G6
G	1994	HIS	-	linker	UNP P0A7G6
G	1995	THR	-	linker	UNP P0A7G6
G	1996	THR	-	linker	UNP P0A7G6
G	1997	GLY	-	linker	UNP P0A7G6
G	1998	SER	-	linker	UNP P0A7G6
G	1999	MET	-	linker	UNP P0A7G6
G	2000	SER	-	linker	UNP P0A7G6
G	2985	THR	-	linker	UNP P0A7G6
G	2986	GLY	-	linker	UNP P0A7G6
G	2987	SER	-	linker	UNP P0A7G6
G	2988	THR	-	linker	UNP P0A7G6
G	2989	GLY	-	linker	UNP P0A7G6
G	2990	SER	-	linker	UNP P0A7G6
G	2991	ALA	-	linker	UNP P0A7G6
G	2992	SER	-	linker	UNP P0A7G6
G	2993	GLY	-	linker	UNP P0A7G6
G	2994	SER	-	linker	UNP P0A7G6
G	2995	SER	-	linker	UNP P0A7G6
G	2996	THR	-	linker	UNP P0A7G6
G	2997	GLY	-	linker	UNP P0A7G6
G	2998	SER	-	linker	UNP P0A7G6
G	2999	MET	-	linker	UNP P0A7G6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	3000	SER	-	linker	UNP P0A7G6
H	26	GLY	-	linker	UNP P0A7G6
H	27	ALA	-	linker	UNP P0A7G6
H	28	MET	-	linker	UNP P0A7G6
H	29	HIS	-	linker	UNP P0A7G6
H	986	THR	-	linker	UNP P0A7G6
H	987	GLY	-	linker	UNP P0A7G6
H	988	SER	-	linker	UNP P0A7G6
H	989	THR	-	linker	UNP P0A7G6
H	990	GLY	-	linker	UNP P0A7G6
H	991	SER	-	linker	UNP P0A7G6
H	992	GLY	-	linker	UNP P0A7G6
H	993	THR	-	linker	UNP P0A7G6
H	994	THR	-	linker	UNP P0A7G6
H	995	GLY	-	linker	UNP P0A7G6
H	996	SER	-	linker	UNP P0A7G6
H	997	THR	-	linker	UNP P0A7G6
H	998	GLY	-	linker	UNP P0A7G6
H	999	SER	-	linker	UNP P0A7G6
H	1000	MET	-	linker	UNP P0A7G6
H	1986	THR	-	linker	UNP P0A7G6
H	1987	GLY	-	linker	UNP P0A7G6
H	1988	SER	-	linker	UNP P0A7G6
H	1989	THR	-	linker	UNP P0A7G6
H	1990	GLY	-	linker	UNP P0A7G6
H	1991	SER	-	linker	UNP P0A7G6
H	1992	MET	-	linker	UNP P0A7G6
H	1993	GLY	-	linker	UNP P0A7G6
H	1994	HIS	-	linker	UNP P0A7G6
H	1995	THR	-	linker	UNP P0A7G6
H	1996	THR	-	linker	UNP P0A7G6
H	1997	GLY	-	linker	UNP P0A7G6
H	1998	SER	-	linker	UNP P0A7G6
H	1999	MET	-	linker	UNP P0A7G6
H	2000	SER	-	linker	UNP P0A7G6
H	2985	THR	-	linker	UNP P0A7G6
H	2986	GLY	-	linker	UNP P0A7G6
H	2987	SER	-	linker	UNP P0A7G6
H	2988	THR	-	linker	UNP P0A7G6
H	2989	GLY	-	linker	UNP P0A7G6
H	2990	SER	-	linker	UNP P0A7G6
H	2991	ALA	-	linker	UNP P0A7G6

Continued on next page...

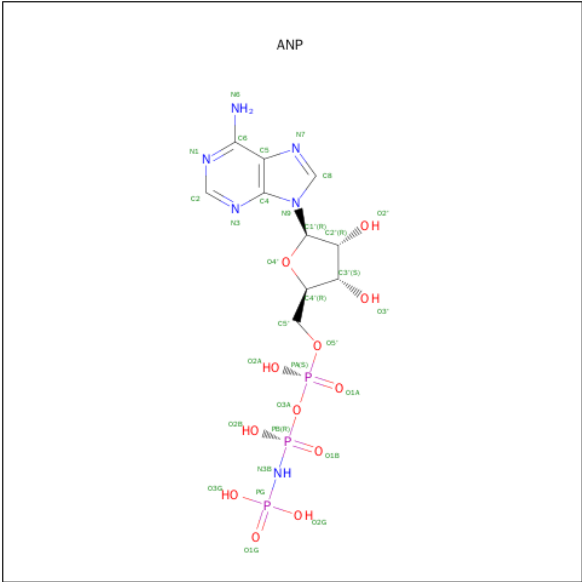
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	2992	SER	-	linker	UNP P0A7G6
H	2993	GLY	-	linker	UNP P0A7G6
H	2994	SER	-	linker	UNP P0A7G6
H	2995	SER	-	linker	UNP P0A7G6
H	2996	THR	-	linker	UNP P0A7G6
H	2997	GLY	-	linker	UNP P0A7G6
H	2998	SER	-	linker	UNP P0A7G6
H	2999	MET	-	linker	UNP P0A7G6
H	3000	SER	-	linker	UNP P0A7G6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	4	Total Mg 4 4	0	0
2	D	4	Total Mg 4 4	0	0
2	E	4	Total Mg 4 4	0	0
2	H	4	Total Mg 4 4	0	0
2	B	4	Total Mg 4 4	0	0
2	C	4	Total Mg 4 4	0	0
2	A	4	Total Mg 4 4	0	0
2	F	4	Total Mg 4 4	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

Continued on next page...

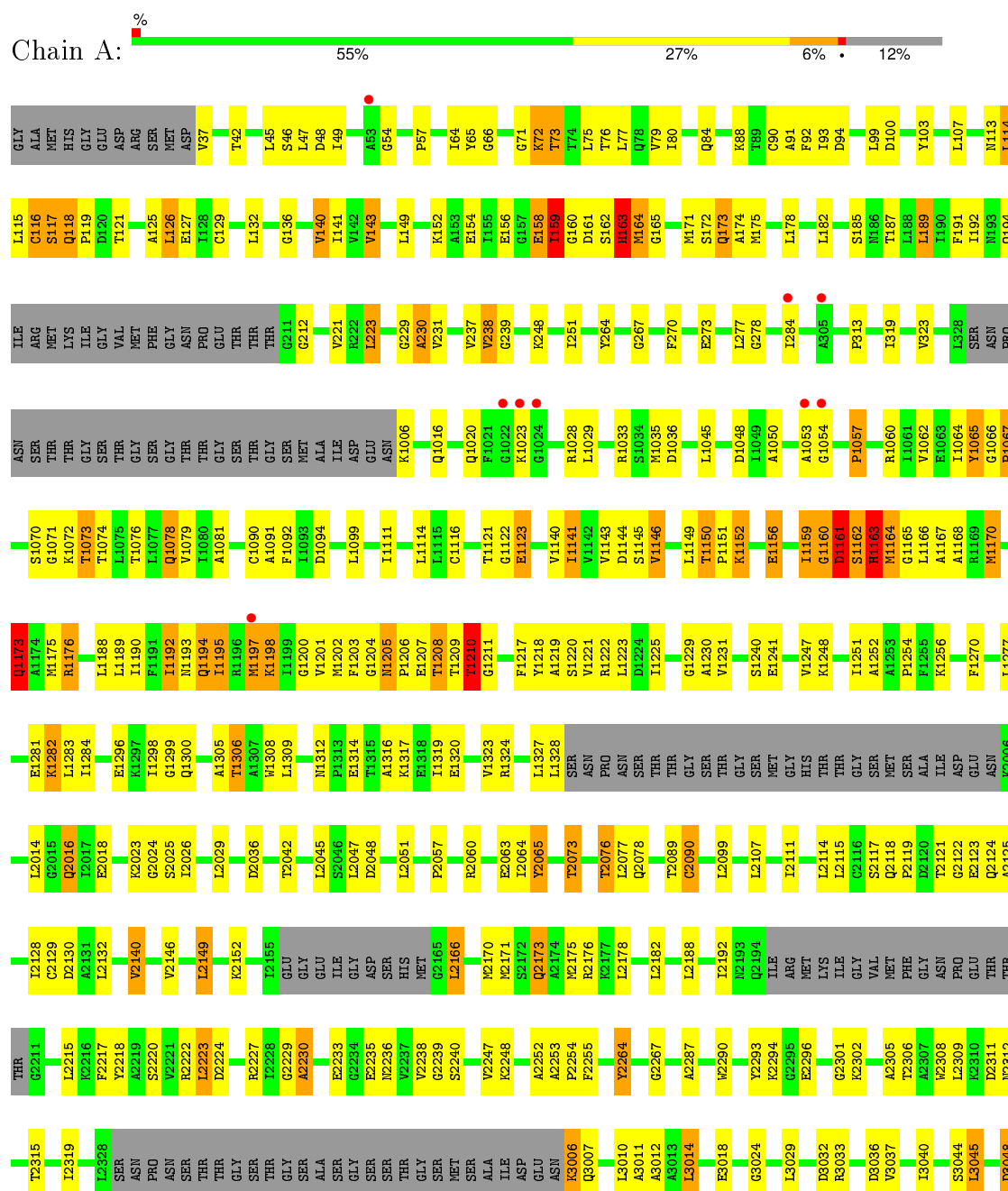
Continued from previous page...

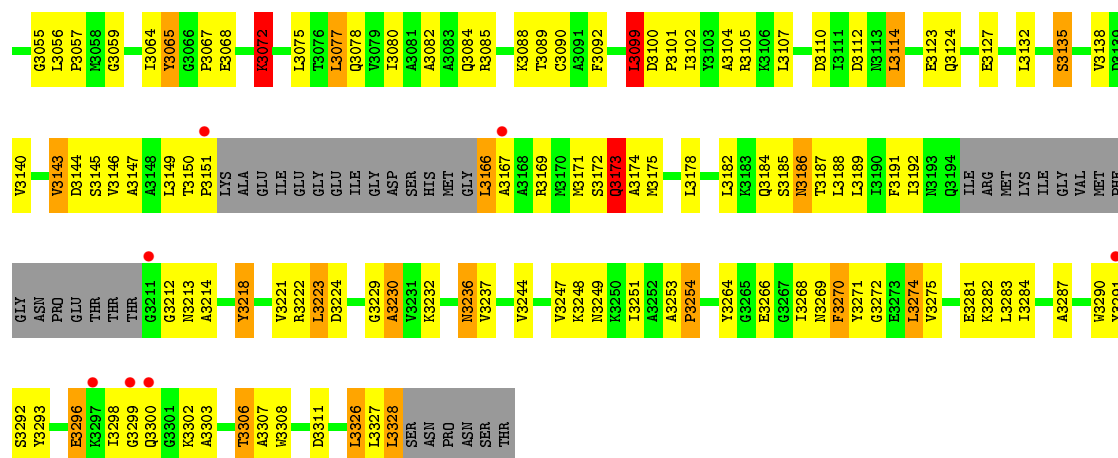
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	H	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

3 Residue-property plots

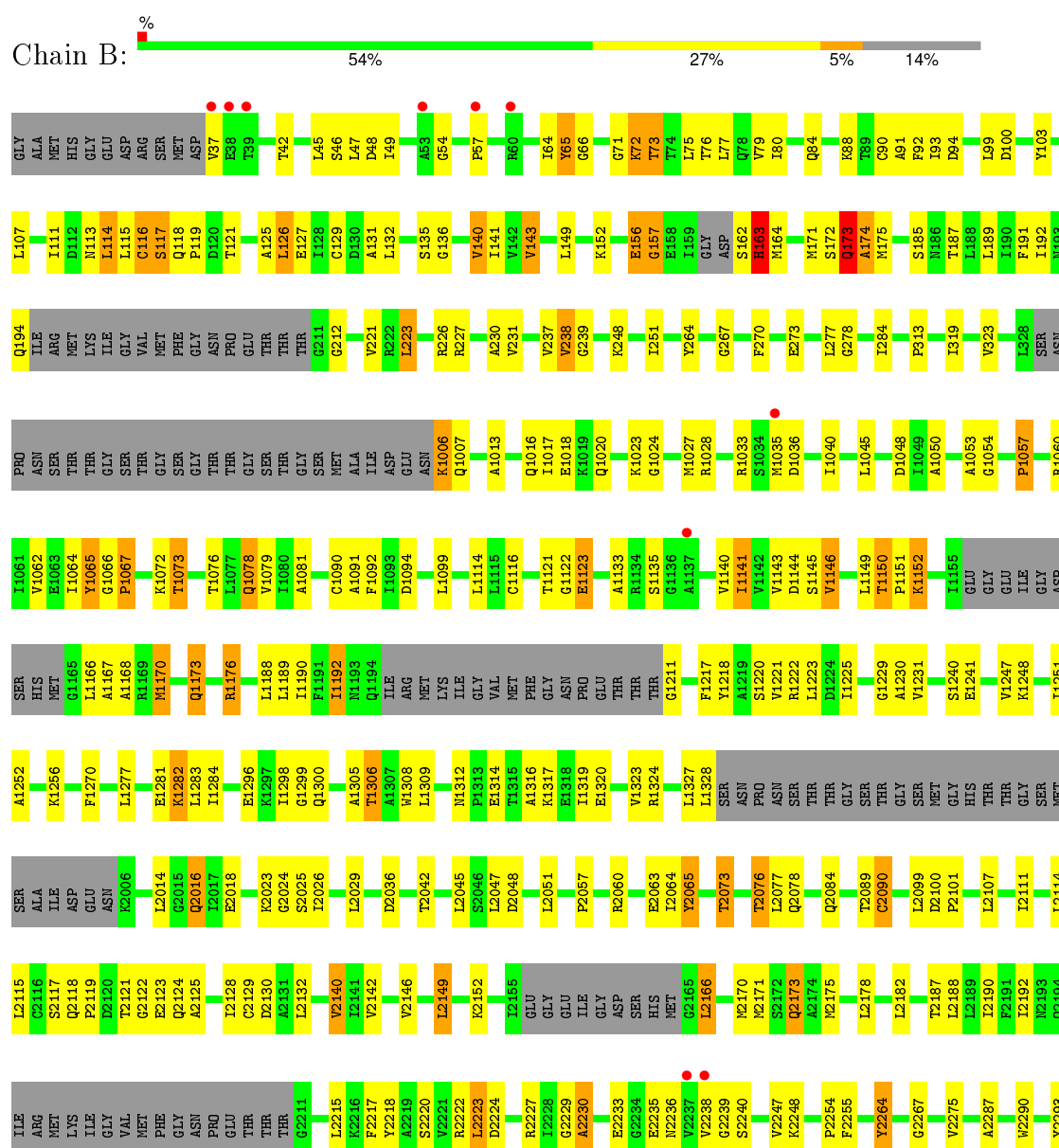
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: Protein recA





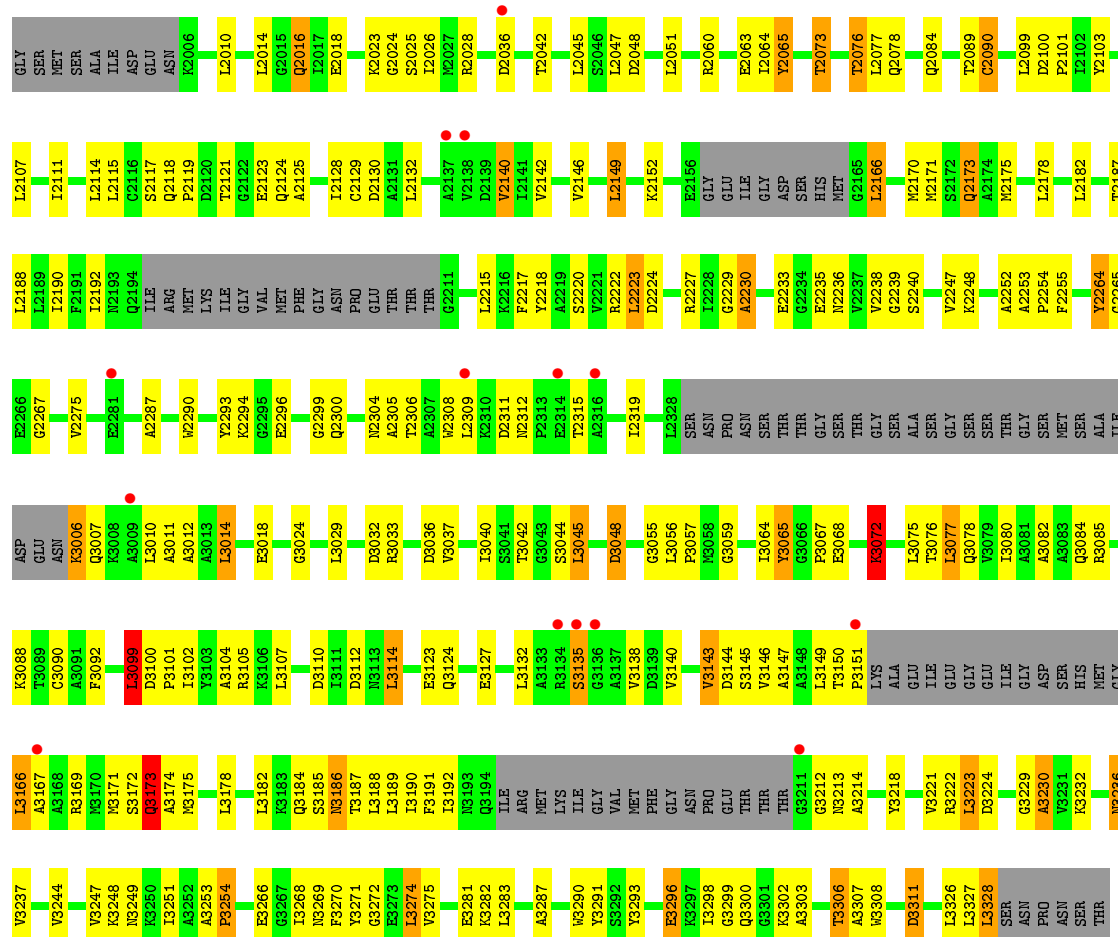
- Molecule 1: Protein recA



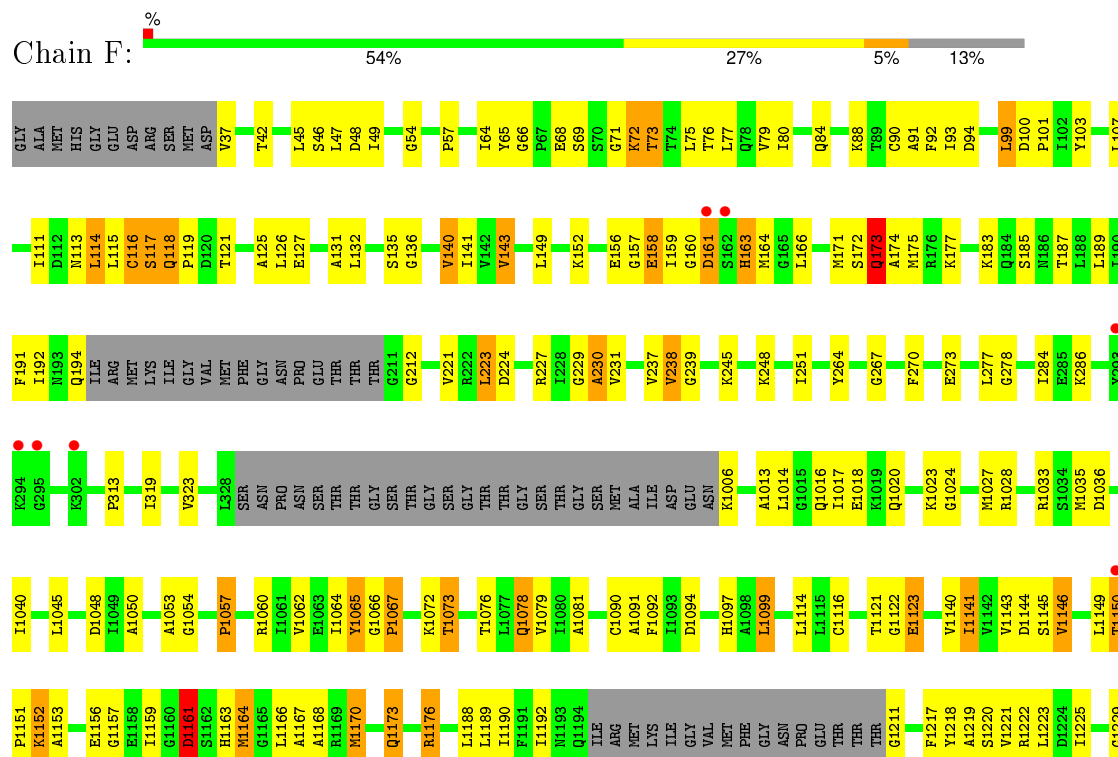


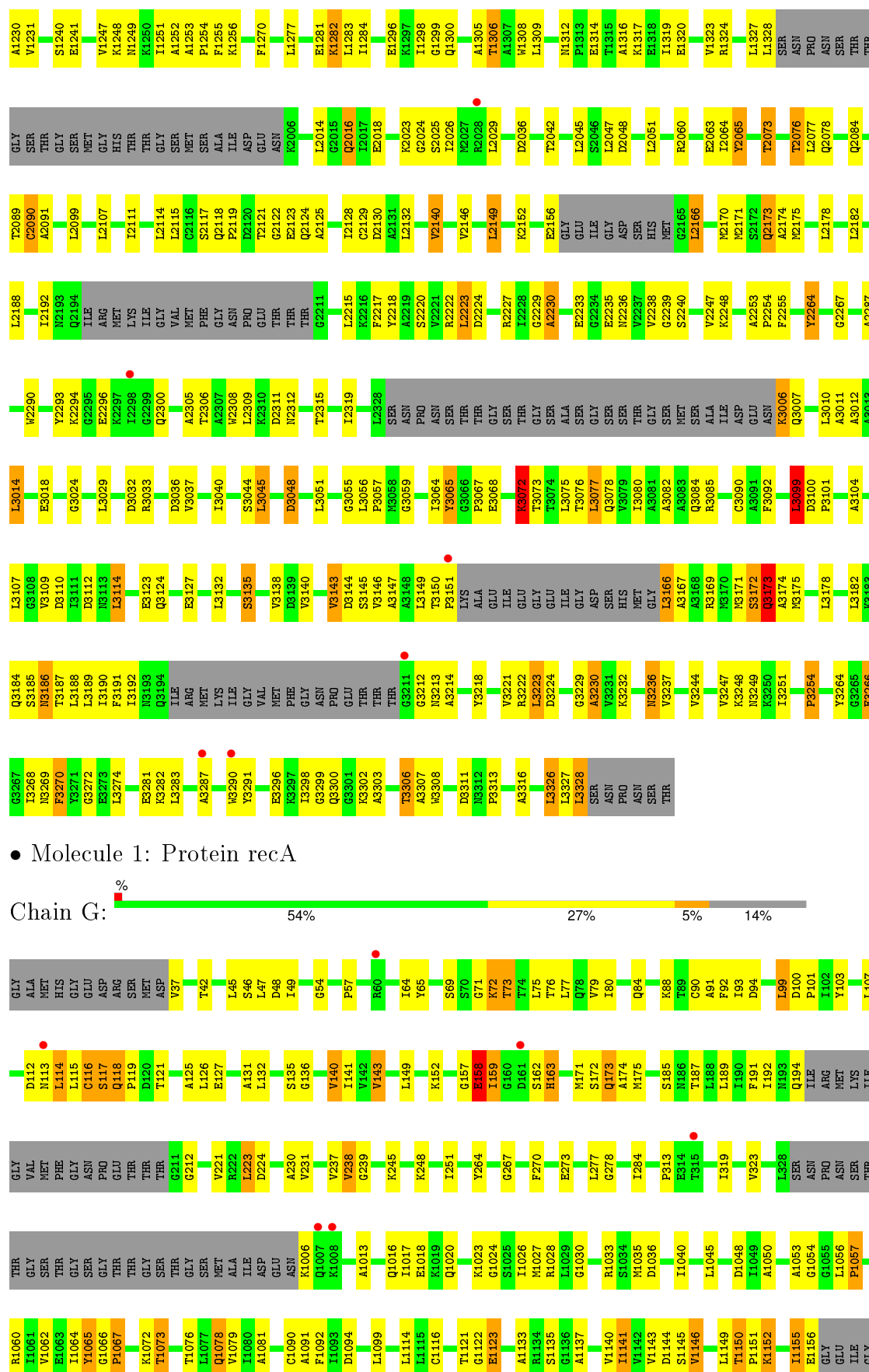






- Molecule 1: Protein recA









4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	176.60 Å 189.80 Å 424.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 4.30 39.93 – 4.30	Depositor EDS
% Data completeness (in resolution range)	92.7 (20.00-4.30) 92.7 (39.93-4.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 4.28 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.243 , 0.261 0.271 , 0.284	Depositor DCC
R_{free} test set	1841 reflections (2.02%)	DCC
Wilson B-factor (Å ²)	170.2	Xtriage
Anisotropy	0.220	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 116.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 96833 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	71761	wwPDB-VP
Average B, all atoms (Å ²)	220.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	A	0.81	6/9068 (0.1%)	0.80	10/12192 (0.1%)
1	B	0.76	4/8861 (0.0%)	0.76	1/11910 (0.0%)
1	C	0.77	0/8951	0.77	4/12033 (0.0%)
1	D	0.74	3/8951 (0.0%)	0.75	4/12033 (0.0%)
1	E	0.72	1/8879 (0.0%)	0.75	2/11934 (0.0%)
1	F	0.77	4/8951 (0.0%)	0.77	2/12033 (0.0%)
1	G	0.77	2/8892 (0.0%)	0.76	3/11953 (0.0%)
1	H	0.72	2/8938 (0.0%)	0.75	3/12014 (0.0%)
All	All	0.76	22/71491 (0.0%)	0.77	29/96102 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
1	B	0	3
1	C	0	4
1	D	0	7
1	E	0	6
1	F	0	6
1	G	0	5
1	H	0	4
All	All	0	46

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	HIS	N-CA	7.46	1.61	1.46
1	B	3266	GLU	CG-CD	6.68	1.61	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1164	MET	CB-CG	6.66	1.72	1.51
1	D	156	GLU	CG-CD	5.97	1.60	1.51
1	F	3270	PHE	CE1-CZ	5.74	1.48	1.37
1	D	3266	GLU	CG-CD	5.71	1.60	1.51
1	G	3270	PHE	CE1-CZ	5.63	1.48	1.37
1	F	3266	GLU	CG-CD	5.57	1.60	1.51
1	G	3266	GLU	CG-CD	5.55	1.60	1.51
1	B	3266	GLU	CB-CG	5.53	1.62	1.52
1	F	3270	PHE	CG-CD2	5.49	1.47	1.38
1	B	3270	PHE	CE1-CZ	5.49	1.47	1.37
1	A	3266	GLU	CG-CD	5.48	1.60	1.51
1	B	3270	PHE	CG-CD2	5.39	1.46	1.38
1	H	90	CYS	CB-SG	-5.38	1.73	1.81
1	E	3266	GLU	CG-CD	5.33	1.59	1.51
1	A	3270	PHE	CE1-CZ	5.29	1.47	1.37
1	F	1156	GLU	CG-CD	5.22	1.59	1.51
1	A	159	ILE	CA-C	5.19	1.66	1.52
1	D	3270	PHE	CE1-CZ	5.16	1.47	1.37
1	H	3266	GLU	CG-CD	5.15	1.59	1.51
1	A	1208	THR	CA-CB	5.04	1.66	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	MET	C-N-CA	-8.01	105.48	122.30
1	D	2166	LEU	CA-CB-CG	7.24	131.94	115.30
1	G	2166	LEU	CA-CB-CG	7.23	131.93	115.30
1	H	2166	LEU	CA-CB-CG	7.23	131.93	115.30
1	E	2166	LEU	CA-CB-CG	7.21	131.89	115.30
1	C	2166	LEU	CA-CB-CG	7.20	131.85	115.30
1	A	2166	LEU	CA-CB-CG	7.17	131.78	115.30
1	B	2166	LEU	CA-CB-CG	7.17	131.78	115.30
1	F	2166	LEU	CA-CB-CG	7.16	131.76	115.30
1	A	1164	MET	CB-CG-SD	6.70	132.50	112.40
1	G	158	GLU	N-CA-C	6.58	128.76	111.00
1	A	163	HIS	N-CA-C	6.40	128.28	111.00
1	H	2036	ASP	C-N-CA	5.59	135.68	121.70
1	D	1163	HIS	N-CA-C	5.55	126.00	111.00
1	C	1164	MET	N-CA-C	5.38	125.52	111.00
1	A	3072	LYS	CD-CE-NZ	5.36	124.04	111.70
1	D	3328	LEU	CA-CB-CG	5.34	127.57	115.30
1	G	3328	LEU	CA-CB-CG	5.32	127.52	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1210	THR	C-N-CA	5.22	133.26	122.30
1	H	3328	LEU	CA-CB-CG	5.18	127.22	115.30
1	A	1194	GLN	O-C-N	-5.18	114.41	122.70
1	A	1210	THR	CA-C-N	-5.14	105.91	116.20
1	F	3328	LEU	CA-CB-CG	5.13	127.09	115.30
1	A	3328	LEU	CA-CB-CG	5.08	126.98	115.30
1	D	1164	MET	CB-CG-SD	5.07	127.61	112.40
1	C	1036	ASP	O-C-N	5.06	130.79	122.70
1	A	1210	THR	CA-C-O	5.04	130.68	120.10
1	C	3328	LEU	CA-CB-CG	5.02	126.84	115.30
1	E	3328	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (46) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1161	ASP	Peptide
1	A	1163	HIS	Peptide
1	A	1197	MET	Peptide
1	A	1198	LYS	Peptide
1	A	1210	THR	Peptide
1	A	158	GLU	Peptide
1	A	161	ASP	Peptide
1	A	163	HIS	Peptide
1	A	3138	VAL	Peptide
1	A	3149	LEU	Peptide
1	A	3150	THR	Peptide
1	B	3138	VAL	Peptide
1	B	3149	LEU	Peptide
1	B	3150	THR	Peptide
1	C	1164	MET	Peptide
1	C	3138	VAL	Peptide
1	C	3149	LEU	Peptide
1	C	3150	THR	Peptide
1	D	1161	ASP	Peptide
1	D	1162	SER	Peptide
1	D	1164	MET	Peptide
1	D	164	MET	Peptide
1	D	3138	VAL	Peptide
1	D	3149	LEU	Peptide
1	D	3150	THR	Peptide
1	E	1155	ILE	Mainchain,Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	E	163	HIS	Peptide
1	E	3138	VAL	Peptide
1	E	3149	LEU	Peptide
1	E	3150	THR	Peptide
1	F	1164	MET	Peptide
1	F	161	ASP	Peptide
1	F	164	MET	Peptide
1	F	3138	VAL	Peptide
1	F	3149	LEU	Peptide
1	F	3150	THR	Peptide
1	G	1155	ILE	Mainchain
1	G	158	GLU	Peptide
1	G	3138	VAL	Peptide
1	G	3149	LEU	Peptide
1	G	3150	THR	Peptide
1	H	1163	HIS	Peptide
1	H	3138	VAL	Peptide
1	H	3149	LEU	Peptide
1	H	3150	THR	Peptide

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	A	8970	0	9264	308	1
1	B	8769	0	9070	275	0
1	C	8856	0	9139	294	1
1	D	8856	0	9139	268	0
1	E	8787	0	9082	304	0
1	F	8856	0	9139	314	0
1	G	8799	0	9090	269	0
1	H	8844	0	9131	304	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	4	0	0	0	0
2	H	4	0	0	0	0
3	A	124	0	52	7	0
3	B	124	0	52	2	0
3	C	124	0	52	3	0
3	D	124	0	52	2	0
3	E	124	0	52	3	0
3	F	124	0	52	9	0
3	G	124	0	52	4	0
3	H	124	0	52	4	0
All	All	71761	0	73470	2200	1

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 15.

All (2200) 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:A:1204:GLY:HA2	1:B:3115:LEU:CD2	1.50	1.42
1:A:1194:GLN:O	1:A:1195:ILE:CG2	1.73	1.37
1:A:162:SER:O	1:A:165:GLY:CA	1.71	1.35
1:A:1194:GLN:O	1:A:1195:ILE:CB	1.81	1.27
1:A:1194:GLN:O	1:A:1195:ILE:HG22	1.25	1.22
1:C:3151:PRO:HG2	1:D:3151:PRO:HG2	1.24	1.15
1:E:3151:PRO:HG2	1:F:3151:PRO:HG2	1.25	1.15
1:A:1204:GLY:CA	1:B:3115:LEU:HD22	1.77	1.13
1:C:3177:LYS:HE2	1:F:173:GLN:CG	1.80	1.11
1:C:3177:LYS:CE	1:F:173:GLN:HG3	1.80	1.11
1:G:3151:PRO:HG2	1:H:3151:PRO:HG2	1.32	1.11
1:C:3177:LYS:HE2	1:F:173:GLN:HG3	1.21	1.10
1:A:162:SER:O	1:A:165:GLY:HA3	0.91	1.09
1:D:1161:ASP:HB2	1:F:183:LYS:NZ	1.68	1.08
1:D:1161:ASP:HB3	1:F:183:LYS:HE2	1.28	1.08
1:F:156:GLU:OE2	1:F:1176:ARG:HG3	1.52	1.07
1:F:1161:ASP:HB3	1:F:1166:LEU:CD1	1.85	1.05
1:F:1161:ASP:HB3	1:F:1166:LEU:HD13	1.34	1.04
1:D:1161:ASP:HB2	1:F:183:LYS:HZ1	1.21	1.03
1:A:1204:GLY:HA2	1:B:3115:LEU:HD22	1.03	1.02
1:E:3105:ARG:HD3	1:F:227:ARG:NH2	1.74	1.01
1:E:3105:ARG:HD3	1:F:227:ARG:HH22	1.20	0.99
1:A:1194:GLN:O	1:A:1195:ILE:HB	1.61	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1204:GLY:CA	1:B:3115:LEU:CD2	2.38	0.97
1:E:3300:GLN:H	1:H:1300:GLN:NE2	1.64	0.96
1:F:3166:LEU:HB2	1:F:3169:ARG:HB2	1.47	0.96
1:A:3166:LEU:HB2	1:A:3169:ARG:HB2	1.47	0.96
1:C:3166:LEU:HB2	1:C:3169:ARG:HB2	1.47	0.95
1:B:3166:LEU:HB2	1:B:3169:ARG:HB2	1.47	0.95
1:E:3166:LEU:HB2	1:E:3169:ARG:HB2	1.47	0.95
1:H:3166:LEU:HB2	1:H:3169:ARG:HB2	1.48	0.95
1:D:3166:LEU:HB2	1:D:3169:ARG:HB2	1.48	0.95
1:E:1300:GLN:NE2	1:H:3300:GLN:H	1.65	0.93
1:E:1300:GLN:H	1:H:3300:GLN:NE2	1.66	0.93
1:G:3166:LEU:HB2	1:G:3169:ARG:HB2	1.47	0.93
1:F:1163:HIS:HB2	1:F:1166:LEU:HG	1.49	0.93
1:D:1161:ASP:CB	1:F:183:LYS:NZ	2.31	0.93
1:D:1161:ASP:HB3	1:F:183:LYS:CE	1.98	0.93
1:A:1164:MET:O	1:A:1166:LEU:N	2.01	0.91
1:A:1204:GLY:HA2	1:B:3115:LEU:HD23	1.51	0.91
1:A:158:GLU:HA	1:A:159:ILE:HD13	1.51	0.90
1:H:3064:ILE:HG12	1:H:3223:LEU:HB2	1.54	0.89
1:F:3064:ILE:HG12	1:F:3223:LEU:HB2	1.53	0.89
1:A:3064:ILE:HG12	1:A:3223:LEU:HB2	1.55	0.89
1:D:3064:ILE:HG12	1:D:3223:LEU:HB2	1.54	0.88
1:H:3072:LYS:HE3	3:H:3400:ANP:O1B	1.74	0.88
1:D:1159:ILE:HG21	1:D:1163:HIS:HD1	1.37	0.88
1:B:3064:ILE:HG12	1:B:3223:LEU:HB2	1.55	0.88
1:A:1193:ASN:ND2	1:A:1209:THR:HG23	1.88	0.87
1:A:162:SER:C	1:A:165:GLY:HA3	1.93	0.87
1:G:3064:ILE:HG12	1:G:3223:LEU:HB2	1.55	0.87
1:C:3064:ILE:HG12	1:C:3223:LEU:HB2	1.53	0.87
1:E:3064:ILE:HG12	1:E:3223:LEU:HB2	1.55	0.87
1:F:1153:ALA:O	1:F:1157:GLY:HA2	1.75	0.86
1:C:164:MET:O	1:C:166:LEU:N	2.09	0.85
1:F:3072:LYS:HE3	3:F:3400:ANP:O1B	1.74	0.85
1:C:2156:GLU:HA	1:C:3172:SER:OG	1.77	0.85
1:F:3143:VAL:HG23	1:F:3191:PHE:HA	1.59	0.84
1:C:1164:MET:HG3	1:C:1165:GLY:HA3	1.60	0.84
1:E:3300:GLN:H	1:H:1300:GLN:HE22	1.27	0.83
1:E:3072:LYS:HE3	3:E:3400:ANP:O1B	1.79	0.83
1:E:3300:GLN:NE2	1:H:1300:GLN:H	1.76	0.83
1:G:3143:VAL:HG23	1:G:3191:PHE:HA	1.61	0.82
1:D:3072:LYS:HE3	3:D:3400:ANP:O1B	1.78	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:SER:O	1:C:119:PRO:HD3	1.81	0.81
1:D:90:CYS:SG	1:D:140:VAL:HG13	2.21	0.81
1:G:3151:PRO:HG2	1:H:3151:PRO:CG	2.10	0.81
1:D:1158:GLU:O	1:D:1159:ILE:HB	1.81	0.81
1:E:117:SER:O	1:E:119:PRO:HD3	1.81	0.81
1:H:117:SER:O	1:H:119:PRO:HD3	1.81	0.81
1:A:90:CYS:SG	1:A:140:VAL:HG13	2.21	0.81
1:B:90:CYS:SG	1:B:140:VAL:HG13	2.20	0.81
1:A:163:HIS:C	1:A:165:GLY:H	1.80	0.81
1:B:117:SER:O	1:B:119:PRO:HD3	1.81	0.81
1:E:2300:GLN:HE22	1:H:2299:GLY:HA2	1.45	0.81
1:E:2300:GLN:H	1:H:2300:GLN:NE2	1.79	0.80
1:G:117:SER:O	1:G:119:PRO:HD3	1.81	0.80
1:D:117:SER:O	1:D:119:PRO:HD3	1.80	0.80
1:F:1123:GLU:HB2	1:F:1152:LYS:HE3	1.63	0.80
1:F:117:SER:O	1:F:119:PRO:HD3	1.81	0.80
1:E:90:CYS:SG	1:E:140:VAL:HG13	2.21	0.80
1:G:90:CYS:SG	1:G:140:VAL:HG13	2.21	0.80
1:D:3143:VAL:HG23	1:D:3191:PHE:HA	1.63	0.80
1:D:1222:ARG:HB2	1:D:1248:LYS:HB3	1.64	0.80
1:E:1123:GLU:HB2	1:E:1152:LYS:HE3	1.64	0.80
1:C:3143:VAL:HG23	1:C:3191:PHE:HA	1.64	0.80
1:A:162:SER:O	1:A:165:GLY:C	2.20	0.80
1:H:1123:GLU:HB2	1:H:1152:LYS:HE3	1.65	0.80
1:G:3151:PRO:CG	1:H:3151:PRO:HG2	2.11	0.79
1:E:3175:MET:HG3	1:E:3218:TYR:HD1	1.47	0.79
1:D:3077:LEU:HA	1:D:3080:ILE:HD12	1.64	0.79
1:A:1123:GLU:HB2	1:A:1152:LYS:HE3	1.64	0.79
1:A:117:SER:O	1:A:119:PRO:HD3	1.82	0.79
1:B:1222:ARG:HB2	1:B:1248:LYS:HB3	1.64	0.79
1:H:80:ILE:O	1:H:84:GLN:HB2	1.82	0.79
1:C:1123:GLU:HB2	1:C:1152:LYS:HE3	1.65	0.79
1:E:1222:ARG:HB2	1:E:1248:LYS:HB3	1.65	0.79
1:B:3175:MET:HG3	1:B:3218:TYR:HD1	1.47	0.78
1:B:80:ILE:O	1:B:84:GLN:HB2	1.83	0.78
1:B:1123:GLU:HB2	1:B:1152:LYS:HE3	1.66	0.78
1:C:90:CYS:SG	1:C:140:VAL:HG13	2.23	0.78
1:B:3143:VAL:HG23	1:B:3191:PHE:HA	1.64	0.78
1:D:80:ILE:O	1:D:84:GLN:HB2	1.82	0.78
1:H:3143:VAL:HG23	1:H:3191:PHE:HA	1.62	0.78
1:G:80:ILE:O	1:G:84:GLN:HB2	1.83	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:80:ILE:O	1:F:84:GLN:HB2	1.83	0.78
1:E:3143:VAL:HG23	1:E:3191:PHE:HA	1.64	0.78
1:F:3175:MET:HG3	1:F:3218:TYR:HD1	1.48	0.78
1:F:90:CYS:SG	1:F:140:VAL:HG13	2.23	0.78
1:A:1300:GLN:NE2	1:D:3300:GLN:H	1.81	0.78
1:C:80:ILE:O	1:C:84:GLN:HB2	1.84	0.78
1:A:3175:MET:HG3	1:A:3218:TYR:HD1	1.48	0.78
1:A:3072:LYS:HE3	3:A:3400:ANP:O1B	1.84	0.78
1:A:80:ILE:O	1:A:84:GLN:HB2	1.83	0.78
1:A:3143:VAL:HG23	1:A:3191:PHE:HA	1.64	0.78
1:H:90:CYS:SG	1:H:140:VAL:HG13	2.24	0.78
1:G:3175:MET:HG3	1:G:3218:TYR:HD1	1.49	0.78
1:C:1222:ARG:HB2	1:C:1248:LYS:HB3	1.65	0.77
1:H:1222:ARG:HB2	1:H:1248:LYS:HB3	1.65	0.77
1:D:3175:MET:HG3	1:D:3218:TYR:HD1	1.48	0.77
1:D:1123:GLU:HB2	1:D:1152:LYS:HE3	1.65	0.77
1:E:1300:GLN:HE22	1:H:3299:GLY:HA2	1.49	0.77
1:G:1123:GLU:HB2	1:G:1152:LYS:HE3	1.65	0.77
1:H:3077:LEU:HA	1:H:3080:ILE:HD12	1.67	0.77
1:H:3175:MET:HG3	1:H:3218:TYR:HD1	1.48	0.77
1:A:1197:MET:H	1:A:1198:LYS:HG3	1.47	0.77
1:E:80:ILE:O	1:E:84:GLN:HB2	1.84	0.77
1:F:1222:ARG:HB2	1:F:1248:LYS:HB3	1.65	0.77
1:G:1222:ARG:HB2	1:G:1248:LYS:HB3	1.66	0.76
1:F:71:GLY:HA2	3:F:400:ANP:H5'1	1.68	0.76
1:E:93:ILE:HA	1:E:117:SER:OG	1.86	0.75
1:A:1156:GLU:OE2	1:A:2176:ARG:HB2	1.85	0.75
1:C:3177:LYS:HE2	1:F:173:GLN:CD	2.06	0.75
1:A:1222:ARG:HB2	1:A:1248:LYS:HB3	1.66	0.75
1:C:3175:MET:HG3	1:C:3218:TYR:HD1	1.49	0.75
1:A:1195:ILE:HD11	1:A:1206:PRO:HB3	1.69	0.75
1:D:1161:ASP:CB	1:F:183:LYS:CE	2.66	0.74
1:B:2300:GLN:NE2	1:C:2300:GLN:H	1.86	0.74
1:B:3077:LEU:HA	1:B:3080:ILE:HD12	1.69	0.74
1:F:143:VAL:HG23	1:F:191:PHE:HA	1.70	0.74
1:D:2156:GLU:HA	1:D:3172:SER:OG	1.88	0.74
1:B:143:VAL:HG23	1:B:191:PHE:HA	1.70	0.74
1:A:156:GLU:OE1	1:A:1176:ARG:HG3	1.89	0.73
1:G:2121:THR:HG23	1:G:2124:GLN:H	1.54	0.73
1:C:3077:LEU:HA	1:C:3080:ILE:HD12	1.70	0.73
1:A:143:VAL:HG23	1:A:191:PHE:HA	1.68	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3077:LEU:HA	1:G:3080:ILE:HD12	1.68	0.73
1:A:2121:THR:HG23	1:A:2124:GLN:H	1.53	0.73
1:D:1159:ILE:HG21	1:D:1163:HIS:ND1	2.04	0.73
1:H:2121:THR:HG23	1:H:2124:GLN:H	1.53	0.73
1:H:93:ILE:HA	1:H:117:SER:OG	1.89	0.73
1:A:3151:PRO:HG2	1:B:3151:PRO:HG2	1.71	0.73
1:C:3072:LYS:HE3	3:C:3400:ANP:O1B	1.88	0.73
1:C:143:VAL:HG23	1:C:191:PHE:HA	1.70	0.72
1:E:143:VAL:HG23	1:E:191:PHE:HA	1.70	0.72
1:E:2121:THR:HG23	1:E:2124:GLN:H	1.54	0.72
1:A:93:ILE:HA	1:A:117:SER:OG	1.89	0.72
1:B:91:ALA:HB3	1:B:141:ILE:HG12	1.72	0.72
1:B:2121:THR:HG23	1:B:2124:GLN:H	1.54	0.72
1:B:2300:GLN:H	1:C:2300:GLN:NE2	1.88	0.72
1:A:91:ALA:HB3	1:A:141:ILE:HG12	1.72	0.72
1:E:3151:PRO:HG2	1:F:3151:PRO:CG	2.13	0.72
1:G:143:VAL:HG23	1:G:191:PHE:HA	1.71	0.72
1:H:143:VAL:HG23	1:H:191:PHE:HA	1.70	0.72
1:C:3151:PRO:HG2	1:D:3151:PRO:CG	2.12	0.72
1:G:3044:SER:OG	1:G:3045:LEU:N	2.23	0.72
1:D:157:GLY:CA	1:D:1172:SER:HB3	2.20	0.72
1:D:143:VAL:HG23	1:D:191:PHE:HA	1.71	0.72
1:A:1071:GLY:HA2	3:A:1400:ANP:H5'1	1.72	0.72
1:F:3044:SER:OG	1:F:3045:LEU:N	2.20	0.72
1:F:3077:LEU:HA	1:F:3080:ILE:HD12	1.70	0.72
1:A:1163:HIS:HB2	1:A:1166:LEU:HD12	1.71	0.71
1:C:2121:THR:HG23	1:C:2124:GLN:H	1.54	0.71
1:F:2121:THR:HG23	1:F:2124:GLN:H	1.55	0.71
1:A:1300:GLN:HE22	1:D:3300:GLN:H	1.36	0.71
1:E:3077:LEU:HA	1:E:3080:ILE:HD12	1.70	0.71
1:E:115:LEU:HA	1:E:1027:MET:O	1.91	0.71
1:B:2118:GLN:HE22	1:B:3249:ASN:H	1.39	0.71
1:E:2300:GLN:NE2	1:H:2300:GLN:H	1.87	0.71
1:D:2118:GLN:HE22	1:D:3249:ASN:H	1.39	0.71
1:D:1161:ASP:CB	1:F:183:LYS:HE2	2.16	0.71
1:A:156:GLU:OE2	1:A:1176:ARG:CG	2.38	0.71
1:F:91:ALA:HB3	1:F:141:ILE:HG12	1.73	0.71
1:D:2121:THR:HG23	1:D:2124:GLN:H	1.55	0.71
1:E:114:LEU:O	1:E:1028:ARG:HA	1.90	0.71
1:A:3077:LEU:HA	1:A:3080:ILE:HD12	1.72	0.71
1:D:93:ILE:HA	1:D:117:SER:OG	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1146:VAL:HG11	1:A:1211:GLY:HA3	1.73	0.71
1:E:3044:SER:OG	1:E:3045:LEU:N	2.24	0.71
1:F:1163:HIS:CG	1:F:1166:LEU:HD21	2.26	0.70
1:A:156:GLU:CD	1:A:1176:ARG:HG3	2.11	0.70
1:B:3072:LYS:HE3	3:B:3400:ANP:O1B	1.91	0.70
1:E:91:ALA:HB3	1:E:141:ILE:HG12	1.73	0.70
1:D:157:GLY:HA2	1:D:1172:SER:HB3	1.73	0.70
1:H:91:ALA:HB3	1:H:141:ILE:HG12	1.73	0.70
1:D:91:ALA:HB3	1:D:141:ILE:HG12	1.73	0.70
1:F:1163:HIS:CD2	1:F:1166:LEU:HD21	2.27	0.70
1:E:2304:ASN:HB3	1:H:2300:GLN:OE1	1.91	0.70
1:B:93:ILE:HA	1:B:117:SER:OG	1.91	0.70
1:F:2118:GLN:HE22	1:F:3249:ASN:H	1.37	0.70
1:G:91:ALA:HB3	1:G:141:ILE:HG12	1.73	0.70
1:H:2118:GLN:HE22	1:H:3249:ASN:H	1.39	0.70
1:D:3044:SER:OG	1:D:3045:LEU:N	2.23	0.70
1:F:93:ILE:HA	1:F:117:SER:OG	1.91	0.70
1:E:1300:GLN:H	1:H:3300:GLN:HE22	1.37	0.69
1:A:1161:ASP:N	1:A:1161:ASP:OD1	2.25	0.69
1:E:2304:ASN:HB3	1:H:2300:GLN:CD	2.12	0.69
1:C:2118:GLN:HE22	1:C:3249:ASN:H	1.40	0.69
1:G:93:ILE:HA	1:G:117:SER:OG	1.91	0.69
1:C:93:ILE:HA	1:C:117:SER:OG	1.92	0.69
1:C:91:ALA:HB3	1:C:141:ILE:HG12	1.74	0.68
1:E:1146:VAL:HG11	1:E:1211:GLY:HA3	1.76	0.68
1:H:131:ALA:HB1	1:H:1017:ILE:HD12	1.76	0.68
1:F:1217:PHE:HA	1:F:1248:LYS:HE3	1.76	0.68
1:A:163:HIS:C	1:A:165:GLY:N	2.47	0.68
1:B:2300:GLN:N	1:C:2300:GLN:NE2	2.42	0.68
1:G:157:GLY:HA2	1:G:1172:SER:CB	2.23	0.68
1:H:1146:VAL:HG11	1:H:1211:GLY:HA3	1.76	0.68
1:A:2117:SER:O	1:A:2119:PRO:HD3	1.94	0.68
1:A:2118:GLN:HE22	1:A:3249:ASN:H	1.41	0.68
1:A:1300:GLN:H	1:D:3300:GLN:NE2	1.92	0.67
1:E:2118:GLN:HE22	1:E:3249:ASN:H	1.43	0.67
1:G:2118:GLN:HE22	1:G:3249:ASN:H	1.42	0.67
1:H:1217:PHE:HA	1:H:1248:LYS:HE3	1.77	0.67
1:A:156:GLU:OE2	1:A:1176:ARG:HG2	1.95	0.67
1:H:3044:SER:OG	1:H:3045:LEU:N	2.26	0.67
1:C:2063:GLU:OE1	1:C:2222:ARG:HD2	1.95	0.67
1:C:1217:PHE:HA	1:C:1248:LYS:HE3	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2300:GLN:HE22	1:C:2300:GLN:H	1.40	0.67
1:C:1146:VAL:HG11	1:C:1211:GLY:HA3	1.76	0.67
1:G:1146:VAL:HG11	1:G:1211:GLY:HA3	1.76	0.67
1:D:1146:VAL:HG11	1:D:1211:GLY:HA3	1.77	0.67
1:E:3300:GLN:HE22	1:H:1300:GLN:H	1.43	0.67
1:A:3044:SER:OG	1:A:3045:LEU:N	2.27	0.67
1:B:3044:SER:OG	1:B:3045:LEU:N	2.25	0.67
1:C:3044:SER:OG	1:C:3045:LEU:N	2.27	0.67
1:C:2117:SER:O	1:C:2119:PRO:HD3	1.95	0.66
1:D:2117:SER:O	1:D:2119:PRO:HD3	1.95	0.66
1:F:1123:GLU:HB2	1:F:1152:LYS:CE	2.25	0.66
1:B:1217:PHE:HA	1:B:1248:LYS:HE3	1.77	0.66
1:F:1146:VAL:HG11	1:F:1211:GLY:HA3	1.77	0.66
1:G:1217:PHE:HA	1:G:1248:LYS:HE3	1.77	0.66
1:A:1160:GLY:C	1:A:1161:ASP:OD1	2.34	0.66
1:E:2117:SER:O	1:E:2119:PRO:HD3	1.95	0.66
1:H:156:GLU:CG	1:H:1176:ARG:HG3	2.26	0.66
1:H:2117:SER:O	1:H:2119:PRO:HD3	1.95	0.66
1:D:1217:PHE:HA	1:D:1248:LYS:HE3	1.77	0.66
1:G:114:LEU:O	1:G:1028:ARG:HA	1.96	0.65
1:D:3018:GLU:HG2	1:D:3024:GLY:H	1.61	0.65
1:C:3151:PRO:CG	1:D:3151:PRO:HG2	2.15	0.65
1:G:2117:SER:O	1:G:2119:PRO:HD3	1.95	0.65
1:E:1217:PHE:HA	1:E:1248:LYS:HE3	1.77	0.65
1:E:114:LEU:HB3	1:E:1029:LEU:HD12	1.78	0.65
1:A:1123:GLU:HB2	1:A:1152:LYS:CE	2.26	0.65
1:A:1217:PHE:HA	1:A:1248:LYS:HE3	1.79	0.65
1:E:1123:GLU:HB2	1:E:1152:LYS:CE	2.26	0.65
1:H:1123:GLU:HB2	1:H:1152:LYS:CE	2.27	0.65
1:D:1123:GLU:HB2	1:D:1152:LYS:CE	2.27	0.65
1:C:1123:GLU:HB2	1:C:1152:LYS:HZ1	1.61	0.65
1:C:1123:GLU:HB2	1:C:1152:LYS:CE	2.27	0.65
1:D:2063:GLU:OE1	1:D:2222:ARG:HD2	1.96	0.65
1:E:3300:GLN:N	1:H:1300:GLN:NE2	2.43	0.64
1:G:1123:GLU:HB2	1:G:1152:LYS:CE	2.27	0.64
1:G:1123:GLU:HB2	1:G:1152:LYS:HZ1	1.62	0.64
1:B:1146:VAL:HG11	1:B:1211:GLY:HA3	1.78	0.64
1:E:1308:TRP:HE3	1:E:1309:LEU:HD23	1.62	0.64
1:B:2117:SER:O	1:B:2119:PRO:HD3	1.97	0.64
1:H:2063:GLU:OE1	1:H:2222:ARG:HD2	1.97	0.64
1:A:1209:THR:O	1:A:1209:THR:HG22	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1123:GLU:HB2	1:B:1152:LYS:HZ1	1.63	0.64
1:A:2063:GLU:OE1	1:A:2222:ARG:HD2	1.97	0.64
1:C:3177:LYS:CE	1:F:173:GLN:CG	2.58	0.64
1:E:1300:GLN:NE2	1:H:3300:GLN:N	2.41	0.64
1:A:1300:GLN:H	1:D:3300:GLN:HE22	1.46	0.64
1:B:2063:GLU:OE1	1:B:2222:ARG:HD2	1.98	0.64
1:G:1156:GLU:OE2	1:G:1156:GLU:N	2.31	0.64
1:F:143:VAL:O	1:F:192:ILE:HG12	1.97	0.64
1:G:157:GLY:HA2	1:G:1172:SER:HB3	1.79	0.64
1:H:3029:LEU:HD23	1:H:3254:PRO:HD2	1.80	0.64
1:G:2076:THR:HG22	1:G:2077:LEU:HD12	1.80	0.64
1:F:160:GLY:HA2	1:F:166:LEU:HD11	1.79	0.64
1:E:3018:GLU:HG2	1:E:3024:GLY:H	1.63	0.64
1:H:156:GLU:HG2	1:H:1176:ARG:HG3	1.80	0.64
1:G:2063:GLU:OE1	1:G:2222:ARG:HD2	1.98	0.64
1:B:1123:GLU:HB2	1:B:1152:LYS:CE	2.28	0.63
1:C:1308:TRP:HE3	1:C:1309:LEU:HD23	1.63	0.63
1:B:1300:GLN:H	1:C:3300:GLN:NE2	1.97	0.63
1:F:1308:TRP:HE3	1:F:1309:LEU:HD23	1.61	0.63
1:F:68:GLU:HB2	3:F:400:ANP:O2G	1.98	0.63
1:D:1308:TRP:HE3	1:D:1309:LEU:HD23	1.62	0.63
1:D:143:VAL:O	1:D:192:ILE:HG12	1.98	0.63
1:F:3029:LEU:HD23	1:F:3254:PRO:HD2	1.80	0.63
1:C:1164:MET:HG3	1:C:1165:GLY:CA	2.28	0.63
1:C:143:VAL:O	1:C:192:ILE:HG12	1.98	0.63
1:B:2076:THR:HG22	1:B:2077:LEU:HD12	1.81	0.63
1:A:1308:TRP:HE3	1:A:1309:LEU:HD23	1.62	0.63
1:D:1123:GLU:HB2	1:D:1152:LYS:HZ1	1.63	0.63
1:H:143:VAL:O	1:H:192:ILE:HG12	1.97	0.63
1:E:2063:GLU:OE1	1:E:2222:ARG:HD2	1.98	0.63
1:H:118:GLN:HE21	1:H:1254:PRO:HB3	1.64	0.63
1:H:1308:TRP:HE3	1:H:1309:LEU:HD23	1.62	0.63
1:G:3018:GLU:HG2	1:G:3024:GLY:H	1.64	0.63
1:C:3029:LEU:HD23	1:C:3254:PRO:HD2	1.80	0.63
1:E:1300:GLN:HE22	1:H:3300:GLN:H	1.45	0.63
1:A:1123:GLU:HB2	1:A:1152:LYS:HZ1	1.63	0.63
1:H:1140:VAL:HG12	1:H:1188:LEU:HB3	1.81	0.63
1:B:2300:GLN:NE2	1:C:2300:GLN:N	2.46	0.62
1:G:1305:ALA:O	1:G:1306:THR:C	2.38	0.62
1:G:1308:TRP:HE3	1:G:1309:LEU:HD23	1.64	0.62
1:D:1140:VAL:HG12	1:D:1188:LEU:HB3	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:VAL:O	1:B:239:GLY:N	2.29	0.62
1:F:1300:GLN:H	1:G:3300:GLN:NE2	1.97	0.62
1:G:3029:LEU:HD23	1:G:3254:PRO:HD2	1.81	0.62
1:F:3018:GLU:HG2	1:F:3024:GLY:H	1.63	0.62
1:F:2117:SER:O	1:F:2119:PRO:HD3	1.98	0.62
1:B:3029:LEU:HD23	1:B:3254:PRO:HD2	1.81	0.62
1:F:3185:SER:C	1:F:3187:THR:H	2.03	0.62
1:F:2063:GLU:OE1	1:F:2222:ARG:HD2	1.98	0.62
1:D:3029:LEU:HD23	1:D:3254:PRO:HD2	1.80	0.62
1:B:1308:TRP:HE3	1:B:1309:LEU:HD23	1.63	0.62
1:F:1140:VAL:HG12	1:F:1188:LEU:HB3	1.81	0.62
1:A:1156:GLU:OE2	1:A:2176:ARG:CB	2.47	0.62
1:B:3185:SER:C	1:B:3187:THR:H	2.02	0.62
1:B:3018:GLU:HG2	1:B:3024:GLY:H	1.64	0.62
1:E:1123:GLU:HB2	1:E:1152:LYS:HZ1	1.64	0.62
1:F:1123:GLU:HB2	1:F:1152:LYS:HZ1	1.64	0.62
1:E:3029:LEU:HD23	1:E:3254:PRO:HD2	1.80	0.62
1:F:1153:ALA:O	1:F:1157:GLY:CA	2.47	0.62
1:C:3018:GLU:HG2	1:C:3024:GLY:H	1.64	0.62
1:C:3177:LYS:NZ	1:F:173:GLN:HG3	2.15	0.61
1:C:1305:ALA:O	1:C:1306:THR:C	2.37	0.61
1:F:1305:ALA:O	1:F:1306:THR:C	2.39	0.61
1:A:3018:GLU:HG2	1:A:3024:GLY:H	1.64	0.61
1:G:3229:GLY:O	1:G:3230:ALA:CB	2.48	0.61
1:E:2076:THR:HG22	1:E:2077:LEU:HD12	1.82	0.61
1:A:1159:ILE:HG22	1:A:1160:GLY:H	1.64	0.61
1:C:2076:THR:HG22	1:C:2077:LEU:HD12	1.82	0.61
1:D:1053:ALA:HB2	1:D:1251:ILE:HG21	1.83	0.61
1:B:1300:GLN:NE2	1:C:3300:GLN:H	1.98	0.61
1:D:3185:SER:C	1:D:3187:THR:H	2.04	0.61
1:H:3018:GLU:HG2	1:H:3024:GLY:H	1.64	0.61
1:A:3029:LEU:HD23	1:A:3254:PRO:HD2	1.81	0.61
1:E:143:VAL:O	1:E:192:ILE:HG12	2.01	0.61
1:A:2076:THR:HG22	1:A:2077:LEU:HD12	1.83	0.61
1:G:237:VAL:O	1:G:239:GLY:N	2.30	0.61
1:G:3185:SER:C	1:G:3187:THR:H	2.04	0.61
1:G:143:VAL:O	1:G:192:ILE:HG12	2.00	0.61
1:B:2300:GLN:HE21	1:C:2300:GLN:HB3	1.66	0.61
1:H:143:VAL:HG21	1:H:191:PHE:CD1	2.36	0.61
1:C:1140:VAL:HG12	1:C:1188:LEU:HB3	1.83	0.61
1:B:3229:GLY:O	1:B:3230:ALA:CB	2.49	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:HG21	1:A:191:PHE:CD1	2.36	0.60
1:G:1281:GLU:O	1:G:1283:LEU:N	2.33	0.60
1:E:3105:ARG:CD	1:F:227:ARG:HH22	2.04	0.60
1:F:143:VAL:HG21	1:F:191:PHE:CD1	2.36	0.60
1:D:3229:GLY:O	1:D:3230:ALA:CB	2.49	0.60
1:E:1140:VAL:HG12	1:E:1188:LEU:HB3	1.83	0.60
1:E:3229:GLY:O	1:E:3230:ALA:CB	2.49	0.60
1:A:1121:THR:OG1	1:A:1122:GLY:N	2.33	0.60
1:D:2076:THR:HG22	1:D:2077:LEU:HD12	1.82	0.60
1:E:3185:SER:C	1:E:3187:THR:H	2.05	0.60
1:A:1193:ASN:HD22	1:A:1209:THR:HG23	1.61	0.60
1:A:1071:GLY:HA2	3:A:1400:ANP:C5'	2.31	0.60
1:D:1230:ALA:H	1:D:1241:GLU:H	1.50	0.60
1:B:42:THR:HG21	1:B:47:LEU:HD22	1.84	0.60
1:D:1161:ASP:CB	1:F:183:LYS:HZ3	2.14	0.60
1:B:143:VAL:HG21	1:B:191:PHE:CD1	2.37	0.60
1:E:2090:CYS:HB3	1:E:2140:VAL:HG13	1.84	0.60
1:C:3185:SER:C	1:C:3187:THR:H	2.05	0.60
1:C:1121:THR:OG1	1:C:1122:GLY:N	2.35	0.60
1:A:3185:SER:C	1:A:3187:THR:H	2.05	0.60
1:C:2090:CYS:HB3	1:C:2140:VAL:HG13	1.84	0.60
1:A:1193:ASN:HD21	1:A:1211:GLY:H	1.47	0.60
1:G:143:VAL:HG21	1:G:191:PHE:CD1	2.36	0.60
1:A:1305:ALA:O	1:A:1306:THR:C	2.40	0.60
1:G:2090:CYS:HB3	1:G:2140:VAL:HG13	1.83	0.60
1:C:2155:ILE:O	1:C:2156:GLU:HG3	2.02	0.60
1:E:2300:GLN:NE2	1:H:2300:GLN:N	2.49	0.60
1:C:2229:GLY:O	1:C:2230:ALA:HB2	2.01	0.60
1:G:1121:THR:OG1	1:G:1122:GLY:N	2.34	0.60
1:D:1305:ALA:O	1:D:1306:THR:C	2.40	0.60
1:B:1140:VAL:HG12	1:B:1188:LEU:HB3	1.83	0.60
1:D:1161:ASP:HB2	1:F:183:LYS:HZ3	1.61	0.60
1:B:2229:GLY:O	1:B:2230:ALA:HB2	2.02	0.60
1:A:1053:ALA:HB2	1:A:1251:ILE:HG21	1.83	0.60
1:G:3082:ALA:HA	1:G:3085:ARG:HB2	1.83	0.60
1:A:114:LEU:HB3	1:A:1029:LEU:HD12	1.84	0.60
1:H:2229:GLY:O	1:H:2230:ALA:HB2	2.02	0.60
1:C:71:GLY:HA2	3:C:400:ANP:H5'1	1.84	0.60
1:F:2229:GLY:O	1:F:2230:ALA:HB2	2.02	0.60
1:C:3229:GLY:O	1:C:3230:ALA:CB	2.49	0.60
1:E:1053:ALA:HB2	1:E:1251:ILE:HG21	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2090:CYS:HB3	1:F:2140:VAL:HG13	1.84	0.59
1:F:42:THR:HG21	1:F:47:LEU:HD22	1.84	0.59
1:A:1161:ASP:HB3	1:A:1166:LEU:HD13	1.83	0.59
1:A:2090:CYS:HB3	1:A:2140:VAL:HG13	1.84	0.59
1:F:1053:ALA:HB2	1:F:1251:ILE:HG21	1.84	0.59
1:H:2076:THR:HG22	1:H:2077:LEU:HD12	1.82	0.59
1:B:2090:CYS:HB3	1:B:2140:VAL:HG13	1.82	0.59
1:A:3229:GLY:O	1:A:3230:ALA:CB	2.50	0.59
1:A:2229:GLY:O	1:A:2230:ALA:HB2	2.02	0.59
1:E:143:VAL:HG21	1:E:191:PHE:CD1	2.37	0.59
1:C:2018:GLU:HG2	1:C:2024:GLY:H	1.67	0.59
1:C:1281:GLU:O	1:C:1283:LEU:N	2.35	0.59
1:E:2229:GLY:O	1:E:2230:ALA:HB2	2.03	0.59
1:G:3057:PRO:O	1:G:3188:LEU:HD13	2.02	0.59
1:E:237:VAL:O	1:E:239:GLY:N	2.30	0.59
1:B:143:VAL:O	1:B:192:ILE:HG12	2.01	0.59
1:D:270:PHE:HA	1:D:273:GLU:HG2	1.84	0.59
1:D:2229:GLY:O	1:D:2230:ALA:HB2	2.02	0.59
1:G:1053:ALA:HB2	1:G:1251:ILE:HG21	1.84	0.59
1:C:3057:PRO:O	1:C:3188:LEU:HD13	2.02	0.59
1:D:2090:CYS:HB3	1:D:2140:VAL:HG13	1.84	0.59
1:C:237:VAL:O	1:C:239:GLY:N	2.31	0.59
1:B:156:GLU:CD	1:B:1176:ARG:HG3	2.23	0.59
1:H:3229:GLY:O	1:H:3230:ALA:CB	2.50	0.59
1:H:1281:GLU:O	1:H:1283:LEU:N	2.36	0.59
1:H:1123:GLU:HB2	1:H:1152:LYS:HZ1	1.66	0.59
1:E:3082:ALA:HA	1:E:3085:ARG:HB2	1.84	0.59
1:A:42:THR:HG21	1:A:47:LEU:HD22	1.84	0.59
1:D:3082:ALA:HA	1:D:3085:ARG:HB2	1.84	0.59
1:D:42:THR:HG21	1:D:47:LEU:HD22	1.85	0.59
1:B:1053:ALA:HB2	1:B:1251:ILE:HG21	1.84	0.59
1:H:3185:SER:C	1:H:3187:THR:H	2.05	0.59
1:A:1163:HIS:O	1:A:1164:MET:C	2.41	0.59
1:F:3064:ILE:HG12	1:F:3223:LEU:CB	2.31	0.59
1:B:2300:GLN:H	1:C:2300:GLN:HE22	1.49	0.59
1:E:1092:PHE:CE2	1:E:1094:ASP:HB2	2.38	0.59
1:F:3229:GLY:O	1:F:3230:ALA:CB	2.50	0.59
1:G:270:PHE:HA	1:G:273:GLU:HG2	1.84	0.59
1:E:3300:GLN:NE2	1:H:1300:GLN:N	2.49	0.58
1:D:3175:MET:HG3	1:D:3218:TYR:CD1	2.36	0.58
1:F:3057:PRO:O	1:F:3188:LEU:HD13	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1230:ALA:H	1:E:1241:GLU:H	1.51	0.58
1:C:1053:ALA:HB2	1:C:1251:ILE:HG21	1.84	0.58
1:D:237:VAL:O	1:D:239:GLY:N	2.30	0.58
1:H:3057:PRO:O	1:H:3188:LEU:HD13	2.03	0.58
1:C:143:VAL:HG21	1:C:191:PHE:CD1	2.38	0.58
1:D:143:VAL:HG21	1:D:191:PHE:CD1	2.38	0.58
1:A:143:VAL:O	1:A:192:ILE:HG12	2.03	0.58
1:A:3082:ALA:HA	1:A:3085:ARG:HB2	1.84	0.58
1:F:2076:THR:HG22	1:F:2077:LEU:HD12	1.82	0.58
1:H:1230:ALA:H	1:H:1241:GLU:H	1.51	0.58
1:F:3006:LYS:HG3	1:F:3007:GLN:H	1.68	0.58
1:D:3057:PRO:O	1:D:3188:LEU:HD13	2.03	0.58
1:A:2018:GLU:HG2	1:A:2024:GLY:H	1.67	0.58
1:H:237:VAL:O	1:H:239:GLY:N	2.31	0.58
1:B:2018:GLU:HG2	1:B:2024:GLY:H	1.69	0.58
1:E:1145:SER:HB2	1:E:1192:ILE:O	2.02	0.58
1:G:3006:LYS:HG3	1:G:3007:GLN:H	1.69	0.58
1:D:1281:GLU:O	1:D:1283:LEU:N	2.37	0.58
1:B:1121:THR:OG1	1:B:1122:GLY:N	2.36	0.58
1:H:1053:ALA:HB2	1:H:1251:ILE:HG21	1.84	0.58
1:D:1141:ILE:HG21	1:D:1189:LEU:HD12	1.85	0.58
1:F:1121:THR:OG1	1:F:1122:GLY:N	2.36	0.58
1:G:1140:VAL:HG12	1:G:1188:LEU:HB3	1.85	0.58
1:B:1092:PHE:CE2	1:B:1094:ASP:HB2	2.39	0.58
1:A:1230:ALA:H	1:A:1241:GLU:H	1.52	0.58
1:B:3057:PRO:O	1:B:3188:LEU:HD13	2.03	0.58
1:D:1092:PHE:CE2	1:D:1094:ASP:HB2	2.38	0.58
1:F:1114:LEU:HB3	1:F:2029:LEU:HD12	1.86	0.58
1:C:1092:PHE:CE2	1:C:1094:ASP:HB2	2.39	0.58
1:A:1141:ILE:HG21	1:A:1189:LEU:HD12	1.85	0.58
1:E:270:PHE:HA	1:E:273:GLU:HG2	1.85	0.58
1:E:3057:PRO:O	1:E:3188:LEU:HD13	2.04	0.58
1:B:2217:PHE:O	1:B:2248:LYS:NZ	2.37	0.58
1:B:1299:GLY:HA2	1:C:3300:GLN:HE22	1.68	0.58
1:E:42:THR:HG21	1:E:47:LEU:HD22	1.85	0.58
1:F:3082:ALA:HA	1:F:3085:ARG:HB2	1.86	0.58
1:F:1161:ASP:CB	1:F:1166:LEU:HD13	2.23	0.58
1:A:1145:SER:HB2	1:A:1192:ILE:O	2.03	0.58
1:G:3072:LYS:HE3	3:G:3400:ANP:O1B	2.03	0.58
1:G:42:THR:HG21	1:G:47:LEU:HD22	1.86	0.58
1:D:2018:GLU:HG2	1:D:2024:GLY:H	1.69	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3006:LYS:HG3	1:C:3007:GLN:H	1.68	0.58
1:C:1230:ALA:HA	1:C:1240:SER:HA	1.86	0.58
1:A:1140:VAL:HG12	1:A:1188:LEU:HB3	1.85	0.58
1:F:3300:GLN:NE2	1:G:1300:GLN:H	2.02	0.58
1:G:2229:GLY:O	1:G:2230:ALA:HB2	2.03	0.58
1:E:1300:GLN:N	1:H:3300:GLN:NE2	2.46	0.57
1:A:1161:ASP:CB	1:A:1166:LEU:HD13	2.34	0.57
1:E:2300:GLN:N	1:H:2300:GLN:NE2	2.50	0.57
1:D:1145:SER:HB2	1:D:1192:ILE:O	2.04	0.57
1:E:1230:ALA:HA	1:E:1240:SER:HA	1.86	0.57
1:F:3300:GLN:H	1:G:1300:GLN:NE2	2.02	0.57
1:E:2018:GLU:HG2	1:E:2024:GLY:H	1.69	0.57
1:G:1141:ILE:HG21	1:G:1189:LEU:HD12	1.86	0.57
1:A:1281:GLU:O	1:A:1283:LEU:N	2.37	0.57
1:C:1230:ALA:H	1:C:1241:GLU:H	1.52	0.57
1:C:2217:PHE:O	1:C:2248:LYS:NZ	2.36	0.57
1:H:2090:CYS:HB3	1:H:2140:VAL:HG13	1.85	0.57
1:E:1141:ILE:HG21	1:E:1189:LEU:HD12	1.86	0.57
1:F:3175:MET:HG3	1:F:3218:TYR:CD1	2.37	0.57
1:B:1230:ALA:H	1:B:1241:GLU:H	1.52	0.57
1:F:2018:GLU:HG2	1:F:2024:GLY:H	1.68	0.57
1:H:3082:ALA:HA	1:H:3085:ARG:HB2	1.87	0.57
1:A:1230:ALA:HA	1:A:1240:SER:HA	1.87	0.57
1:D:92:PHE:N	1:D:115:LEU:O	2.37	0.57
1:H:153:ALA:O	1:H:157:GLY:N	2.37	0.57
1:C:42:THR:HG21	1:C:47:LEU:HD22	1.86	0.57
1:H:270:PHE:HA	1:H:273:GLU:HG2	1.85	0.57
1:F:92:PHE:N	1:F:115:LEU:O	2.37	0.57
1:H:2018:GLU:HG2	1:H:2024:GLY:H	1.69	0.57
1:H:1092:PHE:CE2	1:H:1094:ASP:HB2	2.39	0.57
1:H:1305:ALA:O	1:H:1306:THR:C	2.43	0.57
1:A:237:VAL:O	1:A:239:GLY:N	2.31	0.57
1:C:3082:ALA:HA	1:C:3085:ARG:HB2	1.85	0.57
1:H:3006:LYS:HG3	1:H:3007:GLN:H	1.70	0.57
1:C:270:PHE:HA	1:C:273:GLU:HG2	1.84	0.57
1:F:1230:ALA:HA	1:F:1240:SER:HA	1.86	0.57
1:B:1305:ALA:O	1:B:1306:THR:C	2.41	0.57
1:A:2217:PHE:O	1:A:2248:LYS:NZ	2.37	0.57
1:E:3006:LYS:HG3	1:E:3007:GLN:H	1.70	0.57
1:C:1091:ALA:HB3	1:C:1141:ILE:HG12	1.87	0.57
1:D:2217:PHE:O	1:D:2248:LYS:NZ	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3306:THR:O	1:A:3308:TRP:N	2.38	0.57
1:G:2018:GLU:HG2	1:G:2024:GLY:H	1.69	0.57
1:E:1300:GLN:HE21	1:H:3300:GLN:H	1.53	0.57
1:G:1230:ALA:H	1:G:1241:GLU:H	1.52	0.57
1:B:3006:LYS:HG3	1:B:3007:GLN:H	1.70	0.57
1:E:1121:THR:OG1	1:E:1122:GLY:N	2.37	0.57
1:F:2217:PHE:O	1:F:2248:LYS:NZ	2.37	0.57
1:B:2300:GLN:N	1:C:2300:GLN:HE22	2.02	0.57
1:G:42:THR:HA	1:G:79:VAL:HG12	1.87	0.57
1:D:3006:LYS:HG3	1:D:3007:GLN:H	1.69	0.57
1:E:2217:PHE:O	1:E:2248:LYS:NZ	2.38	0.57
1:F:1145:SER:HB2	1:F:1192:ILE:O	2.04	0.56
1:F:1092:PHE:CE2	1:F:1094:ASP:HB2	2.39	0.56
1:H:1230:ALA:HA	1:H:1240:SER:HA	1.86	0.56
1:D:3064:ILE:HG12	1:D:3223:LEU:CB	2.31	0.56
1:A:270:PHE:HA	1:A:273:GLU:HG2	1.85	0.56
1:G:1155:ILE:C	1:G:1156:GLU:OE2	2.44	0.56
1:D:1230:ALA:HA	1:D:1240:SER:HA	1.86	0.56
1:H:92:PHE:N	1:H:115:LEU:O	2.37	0.56
1:G:2217:PHE:O	1:G:2248:LYS:NZ	2.38	0.56
1:C:1060:ARG:HB3	1:C:1220:SER:OG	2.06	0.56
1:F:131:ALA:HB1	1:F:1017:ILE:HD12	1.87	0.56
1:B:3082:ALA:HA	1:B:3085:ARG:HB2	1.86	0.56
1:C:92:PHE:N	1:C:115:LEU:O	2.36	0.56
1:G:1092:PHE:CE2	1:G:1094:ASP:HB2	2.40	0.56
1:A:1092:PHE:CE2	1:A:1094:ASP:HB2	2.40	0.56
1:E:1091:ALA:HB3	1:E:1141:ILE:HG12	1.88	0.56
1:G:1230:ALA:HA	1:G:1240:SER:HA	1.87	0.56
1:A:3006:LYS:HG3	1:A:3007:GLN:H	1.70	0.56
1:F:270:PHE:HA	1:F:273:GLU:HG2	1.86	0.56
1:C:3306:THR:O	1:C:3308:TRP:N	2.39	0.56
1:F:1163:HIS:HB2	1:F:1166:LEU:CG	2.29	0.56
1:E:92:PHE:N	1:E:115:LEU:O	2.39	0.56
1:F:1230:ALA:H	1:F:1241:GLU:H	1.53	0.56
1:H:2217:PHE:O	1:H:2248:LYS:NZ	2.39	0.56
1:H:1091:ALA:HB3	1:H:1141:ILE:HG12	1.88	0.56
1:H:1145:SER:HB2	1:H:1192:ILE:O	2.05	0.56
1:F:1281:GLU:O	1:F:1283:LEU:N	2.39	0.56
1:B:1281:GLU:O	1:B:1283:LEU:N	2.38	0.56
1:C:1145:SER:HB2	1:C:1192:ILE:O	2.06	0.56
1:G:1145:SER:HB2	1:G:1192:ILE:O	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1145:SER:HB2	1:B:1192:ILE:O	2.05	0.56
1:H:42:THR:HG21	1:H:47:LEU:HD22	1.87	0.56
1:B:1091:ALA:HB3	1:B:1141:ILE:HG12	1.88	0.56
1:E:3311:ASP:HB3	1:F:286:LYS:NZ	2.20	0.56
1:B:1141:ILE:HG21	1:B:1189:LEU:HD12	1.87	0.56
1:A:1060:ARG:HB3	1:A:1220:SER:OG	2.06	0.56
1:E:1305:ALA:O	1:E:1306:THR:C	2.43	0.56
1:F:237:VAL:O	1:F:239:GLY:N	2.33	0.56
1:E:3151:PRO:CG	1:F:3151:PRO:HG2	2.18	0.56
1:D:1091:ALA:HB3	1:D:1141:ILE:HG12	1.88	0.56
1:H:1141:ILE:HG21	1:H:1189:LEU:HD12	1.87	0.56
1:C:1298:ILE:HG13	1:C:1299:GLY:N	2.20	0.56
1:H:3064:ILE:HG12	1:H:3223:LEU:CB	2.32	0.55
1:E:3175:MET:HG3	1:E:3218:TYR:CD1	2.35	0.55
1:A:154:GLU:O	1:A:156:GLU:O	2.23	0.55
1:F:3065:TYR:C	1:F:3065:TYR:CD2	2.80	0.55
1:A:3064:ILE:HG12	1:A:3223:LEU:CB	2.32	0.55
1:G:3175:MET:HG3	1:G:3218:TYR:CD1	2.37	0.55
1:F:3300:GLN:HE22	1:G:1300:GLN:H	1.54	0.55
1:G:1060:ARG:HB3	1:G:1220:SER:OG	2.06	0.55
1:F:1141:ILE:HG21	1:F:1189:LEU:HD12	1.87	0.55
1:F:3072:LYS:CE	3:F:3400:ANP:O1B	2.50	0.55
1:B:1230:ALA:HA	1:B:1240:SER:HA	1.88	0.55
1:B:3175:MET:HG3	1:B:3218:TYR:CD1	2.35	0.55
1:B:3306:THR:O	1:B:3308:TRP:N	2.39	0.55
1:C:1153:ALA:O	1:C:1158:GLU:HA	2.06	0.55
1:C:1078:GLN:O	1:C:1081:ALA:HB3	2.06	0.55
1:B:270:PHE:HA	1:B:273:GLU:HG2	1.87	0.55
1:E:3065:TYR:HD2	1:E:3065:TYR:C	2.10	0.55
1:F:3306:THR:O	1:F:3308:TRP:N	2.39	0.55
1:B:42:THR:HA	1:B:79:VAL:HG12	1.89	0.55
1:A:42:THR:HA	1:A:79:VAL:HG12	1.88	0.55
1:C:42:THR:HA	1:C:79:VAL:HG12	1.89	0.55
1:B:92:PHE:N	1:B:115:LEU:O	2.38	0.55
1:H:1121:THR:OG1	1:H:1122:GLY:N	2.37	0.55
1:D:3065:TYR:HD2	1:D:3065:TYR:C	2.10	0.55
1:E:1281:GLU:O	1:E:1283:LEU:N	2.38	0.55
1:F:1123:GLU:HB2	1:F:1152:LYS:NZ	2.21	0.55
1:F:42:THR:HA	1:F:79:VAL:HG12	1.88	0.55
1:C:1141:ILE:HG21	1:C:1189:LEU:HD12	1.88	0.55
1:E:42:THR:HA	1:E:79:VAL:HG12	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3065:TYR:C	1:H:3065:TYR:HD2	2.10	0.55
1:F:118:GLN:NE2	1:F:1249:ASN:H	2.04	0.55
1:A:1204:GLY:HA3	1:B:3115:LEU:HD22	1.84	0.55
1:D:42:THR:HA	1:D:79:VAL:HG12	1.88	0.55
1:E:3065:TYR:CD2	1:E:3065:TYR:C	2.80	0.55
1:G:3306:THR:O	1:G:3308:TRP:N	2.40	0.55
1:F:3065:TYR:C	1:F:3065:TYR:HD2	2.10	0.54
1:E:3306:THR:O	1:E:3308:TRP:N	2.40	0.54
1:A:3057:PRO:O	1:A:3188:LEU:HD13	2.07	0.54
1:D:1121:THR:OG1	1:D:1122:GLY:N	2.37	0.54
1:F:1057:PRO:HB2	1:F:1060:ARG:HG3	1.89	0.54
1:H:3072:LYS:CE	3:H:3400:ANP:O1B	2.53	0.54
1:D:3065:TYR:CD2	1:D:3065:TYR:C	2.81	0.54
1:H:3065:TYR:CD2	1:H:3065:TYR:C	2.81	0.54
1:B:1060:ARG:HB3	1:B:1220:SER:OG	2.08	0.54
1:D:1060:ARG:HB3	1:D:1220:SER:OG	2.08	0.54
1:E:1123:GLU:HB2	1:E:1152:LYS:NZ	2.22	0.54
1:F:3268:ILE:HG22	1:F:3269:ASN:N	2.23	0.54
1:B:2300:GLN:HE22	1:C:2300:GLN:N	2.03	0.54
1:B:1057:PRO:HB2	1:B:1060:ARG:HG3	1.90	0.54
1:E:1060:ARG:HB3	1:E:1220:SER:OG	2.08	0.54
1:C:1123:GLU:HB2	1:C:1152:LYS:NZ	2.22	0.54
1:C:1229:GLY:O	1:C:1230:ALA:HB3	2.08	0.54
1:A:1057:PRO:HB2	1:A:1060:ARG:HG3	1.90	0.54
1:C:3064:ILE:HG12	1:C:3223:LEU:CB	2.30	0.54
1:A:156:GLU:OE2	1:A:1176:ARG:HG3	2.07	0.54
1:H:1114:LEU:HB3	1:H:2029:LEU:HD12	1.89	0.54
1:G:131:ALA:HB1	1:G:1017:ILE:HD12	1.88	0.54
1:G:1078:GLN:O	1:G:1081:ALA:HB3	2.08	0.54
1:G:3065:TYR:C	1:G:3065:TYR:HD2	2.12	0.54
1:C:156:GLU:HG2	1:C:1176:ARG:HG2	1.89	0.54
1:D:1123:GLU:HB2	1:D:1152:LYS:NZ	2.22	0.54
1:F:1060:ARG:HB3	1:F:1220:SER:OG	2.08	0.54
1:H:1057:PRO:HB2	1:H:1060:ARG:HG3	1.90	0.54
1:D:155:ILE:C	1:D:157:GLY:N	2.60	0.54
1:A:1229:GLY:O	1:A:1230:ALA:HB3	2.07	0.54
1:D:1143:VAL:O	1:D:1192:ILE:HG13	2.08	0.54
1:C:1057:PRO:HB2	1:C:1060:ARG:HG3	1.90	0.54
1:G:1057:PRO:HB2	1:G:1060:ARG:HG3	1.89	0.54
1:A:1123:GLU:HB2	1:A:1152:LYS:NZ	2.22	0.53
1:B:1143:VAL:O	1:B:1192:ILE:HG13	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1091:ALA:HB3	1:G:1141:ILE:HG12	1.89	0.53
1:C:227:ARG:NH2	1:D:3105:ARG:HD3	2.24	0.53
1:G:3065:TYR:C	1:G:3065:TYR:CD2	2.82	0.53
1:G:2029:LEU:HD23	1:G:2254:PRO:HD2	1.89	0.53
1:A:1161:ASP:CG	1:A:1166:LEU:HD13	2.29	0.53
1:D:157:GLY:HA3	1:D:1172:SER:HB3	1.90	0.53
1:B:1092:PHE:HB2	1:B:1114:LEU:HD11	1.90	0.53
1:F:1091:ALA:HB3	1:F:1141:ILE:HG12	1.90	0.53
1:C:3084:GLN:HG2	1:C:3110:ASP:H	1.74	0.53
1:A:3065:TYR:HD2	1:A:3065:TYR:C	2.12	0.53
1:F:2156:GLU:HA	1:F:3172:SER:OG	2.08	0.53
1:G:3143:VAL:HG21	1:G:3191:PHE:CD1	2.44	0.53
1:G:92:PHE:N	1:G:115:LEU:O	2.39	0.53
1:C:3065:TYR:C	1:C:3065:TYR:HD2	2.12	0.53
1:E:3064:ILE:HG12	1:E:3223:LEU:CB	2.33	0.53
1:H:1123:GLU:HB2	1:H:1152:LYS:NZ	2.23	0.53
1:G:1123:GLU:HB2	1:G:1152:LYS:NZ	2.23	0.53
1:B:1078:GLN:O	1:B:1081:ALA:HB3	2.09	0.53
1:F:3100:ASP:O	1:F:3101:PRO:C	2.46	0.53
1:E:1229:GLY:O	1:E:1230:ALA:HB3	2.08	0.53
1:H:1060:ARG:HB3	1:H:1220:SER:OG	2.09	0.53
1:H:3084:GLN:HG2	1:H:3110:ASP:H	1.74	0.53
1:B:131:ALA:HB1	1:B:1017:ILE:HD12	1.90	0.53
1:H:3306:THR:O	1:H:3308:TRP:N	2.41	0.53
1:G:1298:ILE:HG13	1:G:1299:GLY:N	2.23	0.53
1:A:1298:ILE:HG13	1:A:1299:GLY:N	2.23	0.53
1:G:3059:GLY:HA2	1:G:3187:THR:O	2.08	0.53
1:E:3300:GLN:HE22	1:H:1299:GLY:HA2	1.73	0.53
1:B:1123:GLU:HB2	1:B:1152:LYS:NZ	2.23	0.53
1:C:3175:MET:HG3	1:C:3218:TYR:CD1	2.37	0.53
1:G:1229:GLY:O	1:G:1230:ALA:HB3	2.09	0.53
1:A:3105:ARG:HD3	1:B:227:ARG:NH2	2.24	0.53
1:E:2300:GLN:H	1:H:2300:GLN:HE22	1.55	0.53
1:A:1091:ALA:HB3	1:A:1141:ILE:HG12	1.89	0.53
1:C:3065:TYR:C	1:C:3065:TYR:CD2	2.82	0.53
1:D:3100:ASP:O	1:D:3101:PRO:C	2.46	0.53
1:C:1073:THR:HA	1:C:1076:THR:HB	1.91	0.53
1:F:3143:VAL:HG21	1:F:3191:PHE:CD1	2.44	0.53
1:D:1222:ARG:HB2	1:D:1248:LYS:CB	2.37	0.53
1:A:1176:ARG:HA	1:A:1218:TYR:HE1	1.74	0.53
1:G:1143:VAL:O	1:G:1192:ILE:HG13	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:42:THR:HA	1:H:79:VAL:HG12	1.90	0.53
1:D:1057:PRO:HB2	1:D:1060:ARG:HG3	1.90	0.53
1:E:1057:PRO:HB2	1:E:1060:ARG:HG3	1.90	0.53
1:C:1065:TYR:C	1:C:1065:TYR:CD1	2.82	0.53
1:A:46:SER:HA	1:A:49:ILE:HD12	1.91	0.53
1:F:1308:TRP:CE3	1:F:1309:LEU:HD23	2.44	0.52
1:D:1229:GLY:O	1:D:1230:ALA:HB3	2.09	0.52
1:G:1176:ARG:HA	1:G:1218:TYR:HE1	1.74	0.52
1:C:153:ALA:O	1:C:158:GLU:HB2	2.09	0.52
1:H:1112:ASP:HA	1:H:2030:GLY:HA3	1.91	0.52
1:G:3064:ILE:HG12	1:G:3223:LEU:CB	2.33	0.52
1:B:1176:ARG:HA	1:B:1218:TYR:HE1	1.73	0.52
1:A:1092:PHE:HB2	1:A:1114:LEU:HD11	1.91	0.52
1:B:1229:GLY:O	1:B:1230:ALA:HB3	2.08	0.52
1:D:3306:THR:O	1:D:3308:TRP:N	2.42	0.52
1:A:3084:GLN:HG2	1:A:3110:ASP:H	1.73	0.52
1:E:1222:ARG:HB2	1:E:1248:LYS:CB	2.37	0.52
1:B:156:GLU:O	1:B:157:GLY:O	2.28	0.52
1:H:1065:TYR:CD1	1:H:1065:TYR:C	2.83	0.52
1:D:2178:LEU:O	1:D:2182:LEU:HG	2.09	0.52
1:F:1176:ARG:HA	1:F:1218:TYR:HE1	1.74	0.52
1:A:1208:THR:HG21	1:A:1222:ARG:HH22	1.75	0.52
1:C:1143:VAL:O	1:C:1192:ILE:HG13	2.10	0.52
1:C:1114:LEU:HB3	1:C:2029:LEU:HD12	1.90	0.52
1:A:1078:GLN:O	1:A:1081:ALA:HB3	2.09	0.52
1:B:121:THR:HG21	1:B:152:LYS:HG3	1.92	0.52
1:D:1176:ARG:HA	1:D:1218:TYR:HE1	1.75	0.52
1:C:2178:LEU:O	1:C:2182:LEU:HG	2.10	0.52
1:A:1143:VAL:O	1:A:1192:ILE:HG13	2.09	0.52
1:H:1092:PHE:HB2	1:H:1114:LEU:HD11	1.91	0.52
1:H:3059:GLY:HA2	1:H:3187:THR:O	2.10	0.52
1:A:3221:VAL:HA	1:A:3248:LYS:O	2.10	0.52
1:D:1159:ILE:HG22	1:D:1161:ASP:H	1.74	0.52
1:E:3300:GLN:N	1:H:1300:GLN:HE22	2.02	0.52
1:C:1222:ARG:HB2	1:C:1248:LYS:CB	2.37	0.52
1:H:118:GLN:NE2	1:H:1254:PRO:HB3	2.25	0.52
1:G:2178:LEU:O	1:G:2182:LEU:HG	2.10	0.52
1:C:1316:ALA:O	1:C:1319:ILE:N	2.43	0.52
1:C:3177:LYS:CE	1:F:173:GLN:CD	2.76	0.52
1:A:114:LEU:O	1:A:1028:ARG:HA	2.10	0.52
1:E:1065:TYR:CD1	1:E:1065:TYR:C	2.83	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:GLY:HA2	1:D:1172:SER:CB	2.39	0.52
1:C:1176:ARG:HA	1:C:1218:TYR:HE1	1.74	0.52
1:D:1065:TYR:C	1:D:1065:TYR:CD1	2.83	0.52
1:D:1298:ILE:HG13	1:D:1299:GLY:N	2.24	0.52
1:B:2178:LEU:O	1:B:2182:LEU:HG	2.10	0.52
1:E:3105:ARG:HH11	1:F:227:ARG:NH2	2.09	0.52
1:C:2155:ILE:C	1:C:2156:GLU:HG3	2.30	0.52
1:F:1222:ARG:HB2	1:F:1248:LYS:CB	2.37	0.52
1:F:71:GLY:CA	3:F:400:ANP:H5'1	2.38	0.52
1:C:3072:LYS:CE	3:C:3400:ANP:O1B	2.57	0.52
1:F:1229:GLY:O	1:F:1230:ALA:HB3	2.10	0.52
1:G:1065:TYR:C	1:G:1065:TYR:CD1	2.84	0.52
1:B:1065:TYR:CD1	1:B:1065:TYR:C	2.84	0.52
1:D:3268:ILE:HG22	1:D:3269:ASN:N	2.25	0.52
1:D:1078:GLN:O	1:D:1081:ALA:HB3	2.10	0.52
1:H:3175:MET:HG3	1:H:3218:TYR:CD1	2.36	0.51
1:B:1298:ILE:HG13	1:B:1299:GLY:N	2.23	0.51
1:E:1092:PHE:HB2	1:E:1114:LEU:HD11	1.91	0.51
1:A:92:PHE:N	1:A:115:LEU:O	2.38	0.51
1:F:2178:LEU:O	1:F:2182:LEU:HG	2.10	0.51
1:F:2146:VAL:HA	1:F:2149:LEU:HD23	1.92	0.51
1:H:3143:VAL:HG21	1:H:3191:PHE:CD1	2.45	0.51
1:A:1222:ARG:HB2	1:A:1248:LYS:CB	2.38	0.51
1:H:1229:GLY:O	1:H:1230:ALA:HB3	2.09	0.51
1:F:46:SER:HA	1:F:49:ILE:HD12	1.92	0.51
1:F:107:LEU:CD2	1:F:267:GLY:HA3	2.40	0.51
1:B:3249:ASN:OD1	1:B:3251:ILE:HG22	2.10	0.51
1:F:2118:GLN:NE2	1:F:3249:ASN:H	2.08	0.51
1:E:1143:VAL:O	1:E:1192:ILE:HG13	2.10	0.51
1:A:1091:ALA:HB3	1:A:1141:ILE:HA	1.93	0.51
1:G:3100:ASP:O	1:G:3101:PRO:C	2.49	0.51
1:G:121:THR:HG21	1:G:152:LYS:HG3	1.92	0.51
1:B:3065:TYR:C	1:B:3065:TYR:CD2	2.84	0.51
1:A:132:LEU:HB2	1:A:141:ILE:HD11	1.92	0.51
1:D:1092:PHE:HB2	1:D:1114:LEU:HD11	1.92	0.51
1:A:3065:TYR:CD2	1:A:3065:TYR:C	2.82	0.51
1:C:2123:GLU:HG3	1:C:2170:MET:HG3	1.92	0.51
1:C:121:THR:HG21	1:C:152:LYS:HG3	1.93	0.51
1:F:3298:ILE:HG13	1:F:3299:GLY:N	2.26	0.51
1:F:118:GLN:HE21	1:F:1249:ASN:H	1.57	0.51
1:E:1078:GLN:O	1:E:1081:ALA:HB3	2.09	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2178:LEU:O	1:A:2182:LEU:HG	2.10	0.51
1:D:3084:GLN:HG2	1:D:3110:ASP:H	1.75	0.51
1:F:99:LEU:HD23	1:F:1255:PHE:CZ	2.46	0.51
1:D:3059:GLY:HA2	1:D:3187:THR:O	2.10	0.51
1:A:1065:TYR:CD1	1:A:1065:TYR:C	2.84	0.51
1:D:46:SER:HA	1:D:49:ILE:HD12	1.93	0.51
1:D:2308:TRP:HE3	1:D:2309:LEU:HD23	1.75	0.51
1:F:3221:VAL:HA	1:F:3248:LYS:O	2.11	0.51
1:H:2178:LEU:O	1:H:2182:LEU:HG	2.10	0.51
1:C:131:ALA:HB1	1:C:1017:ILE:HD12	1.93	0.51
1:A:2042:THR:HG21	1:A:2047:LEU:HD22	1.93	0.51
1:A:3175:MET:HG3	1:A:3218:TYR:CD1	2.37	0.51
1:H:1222:ARG:HB2	1:H:1248:LYS:CB	2.38	0.51
1:B:2299:GLY:HA2	1:C:2300:GLN:HE22	1.76	0.51
1:A:3249:ASN:OD1	1:A:3251:ILE:HG22	2.10	0.51
1:H:114:LEU:O	1:H:1028:ARG:HA	2.10	0.51
1:F:1065:TYR:CD1	1:F:1065:TYR:C	2.83	0.51
1:E:1176:ARG:HA	1:E:1218:TYR:HE1	1.75	0.51
1:E:2300:GLN:NE2	1:H:2299:GLY:HA2	2.21	0.51
1:H:1176:ARG:HA	1:H:1218:TYR:HE1	1.75	0.51
1:F:1092:PHE:HB2	1:F:1114:LEU:HD11	1.91	0.51
1:E:1053:ALA:HB2	1:E:1251:ILE:CG2	2.41	0.51
1:F:3300:GLN:H	1:G:1300:GLN:HE22	1.59	0.51
1:H:115:LEU:CD2	1:H:1028:ARG:HG2	2.41	0.51
1:F:121:THR:HG21	1:F:152:LYS:HG3	1.93	0.51
1:B:3100:ASP:O	1:B:3101:PRO:C	2.47	0.51
1:E:3084:GLN:HG2	1:E:3110:ASP:H	1.75	0.51
1:C:164:MET:C	1:C:166:LEU:H	2.14	0.51
1:G:132:LEU:HB2	1:G:141:ILE:HD11	1.92	0.51
1:C:3059:GLY:HA2	1:C:3187:THR:O	2.10	0.51
1:H:135:SER:OG	1:H:1013:ALA:HB1	2.11	0.51
1:H:3221:VAL:HA	1:H:3248:LYS:O	2.11	0.51
1:B:3221:VAL:HA	1:B:3248:LYS:O	2.11	0.51
1:A:3143:VAL:HG21	1:A:3191:PHE:CD1	2.46	0.51
1:A:2123:GLU:HG3	1:A:2170:MET:HG3	1.93	0.51
1:F:1143:VAL:O	1:F:1192:ILE:HG13	2.11	0.51
1:B:3059:GLY:HA2	1:B:3187:THR:O	2.11	0.51
1:D:107:LEU:CD2	1:D:267:GLY:HA3	2.42	0.51
1:B:107:LEU:CD2	1:B:267:GLY:HA3	2.41	0.51
1:G:3221:VAL:HA	1:G:3248:LYS:O	2.10	0.51
1:A:107:LEU:CD2	1:A:267:GLY:HA3	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3078:GLN:HG3	1:H:3268:ILE:HG13	1.93	0.51
1:D:3249:ASN:OD1	1:D:3251:ILE:HG22	2.11	0.50
1:D:132:LEU:HB2	1:D:141:ILE:HD11	1.93	0.50
1:C:185:SER:HB2	1:C:187:THR:OG1	2.10	0.50
1:H:1078:GLN:O	1:H:1081:ALA:HB3	2.11	0.50
1:G:185:SER:HB2	1:G:187:THR:OG1	2.11	0.50
1:D:2107:LEU:CD2	1:D:2267:GLY:HA3	2.41	0.50
1:E:232:LYS:NZ	1:F:3266:GLU:HG3	2.26	0.50
1:A:1145:SER:O	1:A:1146:VAL:C	2.50	0.50
1:C:3143:VAL:HG21	1:C:3191:PHE:CD1	2.47	0.50
1:D:1091:ALA:HB3	1:D:1141:ILE:HA	1.94	0.50
1:G:1092:PHE:HB2	1:G:1114:LEU:HD11	1.93	0.50
1:H:2042:THR:HG21	1:H:2047:LEU:HD22	1.94	0.50
1:D:3221:VAL:HA	1:D:3248:LYS:O	2.11	0.50
1:F:1078:GLN:O	1:F:1081:ALA:HB3	2.11	0.50
1:F:2308:TRP:HE3	1:F:2309:LEU:HD23	1.76	0.50
1:A:2107:LEU:CD2	1:A:2267:GLY:HA3	2.42	0.50
1:B:1073:THR:HA	1:B:1076:THR:HB	1.93	0.50
1:D:3298:ILE:HG13	1:D:3299:GLY:N	2.27	0.50
1:G:107:LEU:CD2	1:G:267:GLY:HA3	2.42	0.50
1:C:3221:VAL:HA	1:C:3248:LYS:O	2.10	0.50
1:A:1197:MET:O	1:A:1202:MET:HB2	2.11	0.50
1:F:1300:GLN:NE2	1:G:3300:GLN:H	2.10	0.50
1:B:1308:TRP:CE3	1:B:1309:LEU:HD23	2.46	0.50
1:C:1092:PHE:HB2	1:C:1114:LEU:HD11	1.92	0.50
1:E:1091:ALA:HB3	1:E:1141:ILE:HA	1.93	0.50
1:B:3065:TYR:C	1:B:3065:TYR:HD2	2.15	0.50
1:B:3065:TYR:HE2	1:B:3224:ASP:CG	2.15	0.50
1:D:185:SER:HB2	1:D:187:THR:OG1	2.12	0.50
1:E:121:THR:HG21	1:E:152:LYS:HG3	1.92	0.50
1:H:46:SER:HA	1:H:49:ILE:HD12	1.92	0.50
1:E:1298:ILE:HG13	1:E:1299:GLY:N	2.25	0.50
1:A:3064:ILE:O	1:A:3192:ILE:HA	2.11	0.50
1:B:1222:ARG:HB2	1:B:1248:LYS:CB	2.37	0.50
1:G:1222:ARG:HB2	1:G:1248:LYS:CB	2.38	0.50
1:H:152:LYS:O	1:H:156:GLU:OE2	2.29	0.50
1:G:1308:TRP:CE3	1:G:1309:LEU:HD23	2.46	0.50
1:F:2073:THR:HG23	1:F:2077:LEU:HD13	1.93	0.50
1:F:3078:GLN:HG3	1:F:3268:ILE:HG13	1.93	0.50
1:E:185:SER:HB2	1:E:187:THR:OG1	2.12	0.50
1:B:162:SER:O	1:B:163:HIS:HB2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1298:ILE:HG13	1:F:1299:GLY:N	2.26	0.50
1:F:2300:GLN:HB3	1:G:2300:GLN:HE21	1.76	0.50
1:H:1143:VAL:O	1:H:1192:ILE:HG13	2.11	0.50
1:E:1308:TRP:CE3	1:E:1309:LEU:HD23	2.45	0.50
1:C:2073:THR:HG23	1:C:2077:LEU:HD13	1.94	0.50
1:C:3222:ARG:HG3	1:C:3248:LYS:HB3	1.93	0.50
1:E:1153:ALA:O	1:E:1156:GLU:C	2.50	0.50
1:F:3084:GLN:HG2	1:F:3110:ASP:H	1.76	0.50
1:G:1316:ALA:O	1:G:1319:ILE:N	2.44	0.50
1:H:2107:LEU:CD2	1:H:2267:GLY:HA3	2.41	0.50
1:E:3143:VAL:HG21	1:E:3191:PHE:CD1	2.46	0.50
1:F:132:LEU:HB2	1:F:141:ILE:HD11	1.93	0.50
1:H:121:THR:HG21	1:H:152:LYS:HG3	1.92	0.50
1:G:2073:THR:HG23	1:G:2077:LEU:HD13	1.94	0.50
1:H:1308:TRP:CE3	1:H:1309:LEU:HD23	2.44	0.50
1:F:3059:GLY:HA2	1:F:3187:THR:O	2.11	0.50
1:E:3059:GLY:HA2	1:E:3187:THR:O	2.11	0.50
1:C:1091:ALA:HB3	1:C:1141:ILE:HA	1.92	0.50
1:D:3222:ARG:HG3	1:D:3248:LYS:HB3	1.93	0.50
1:C:107:LEU:CD2	1:C:267:GLY:HA3	2.41	0.50
1:E:2107:LEU:CD2	1:E:2267:GLY:HA3	2.42	0.50
1:E:3145:SER:O	1:E:3147:ALA:N	2.44	0.50
1:E:3222:ARG:HG3	1:E:3248:LYS:HB3	1.93	0.50
1:D:2173:GLN:C	1:D:2175:MET:H	2.15	0.50
1:G:2042:THR:HG21	1:G:2047:LEU:HD22	1.92	0.50
1:D:3143:VAL:HG21	1:D:3191:PHE:CD1	2.47	0.50
1:H:132:LEU:HB2	1:H:141:ILE:HD11	1.93	0.50
1:H:3249:ASN:OD1	1:H:3251:ILE:HG22	2.11	0.50
1:C:132:LEU:HB2	1:C:141:ILE:HD11	1.94	0.50
1:G:3249:ASN:OD1	1:G:3251:ILE:HG22	2.12	0.50
1:B:2073:THR:HG23	1:B:2077:LEU:HD13	1.94	0.50
1:D:2073:THR:HG23	1:D:2077:LEU:HD13	1.94	0.50
1:A:185:SER:HB2	1:A:187:THR:OG1	2.11	0.50
1:G:2308:TRP:HE3	1:G:2309:LEU:HD23	1.77	0.50
1:H:278:GLY:HA3	1:H:284:ILE:HD12	1.94	0.50
1:E:1299:GLY:HA2	1:H:3300:GLN:HE22	1.76	0.50
1:A:1193:ASN:ND2	1:A:1209:THR:CG2	2.68	0.50
1:E:2300:GLN:HB3	1:H:2300:GLN:HB3	1.93	0.50
1:A:1300:GLN:NE2	1:D:3300:GLN:N	2.57	0.50
1:B:132:LEU:HB2	1:B:141:ILE:HD11	1.93	0.50
1:C:1308:TRP:CE3	1:C:1309:LEU:HD23	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1319:ILE:O	1:A:1323:VAL:HG23	2.12	0.50
1:E:1016:GLN:O	1:E:1020:GLN:HB2	2.12	0.50
1:C:319:ILE:O	1:C:323:VAL:HG23	2.11	0.50
1:B:2300:GLN:HB3	1:C:2300:GLN:HB3	1.94	0.50
1:D:157:GLY:CA	1:D:1172:SER:CB	2.88	0.50
1:H:45:LEU:HD23	1:H:270:PHE:CD1	2.47	0.50
1:A:3222:ARG:HG3	1:A:3248:LYS:HB3	1.93	0.50
1:G:2123:GLU:HG3	1:G:2170:MET:HG3	1.93	0.50
1:F:1073:THR:HA	1:F:1076:THR:HB	1.93	0.50
1:E:46:SER:HA	1:E:49:ILE:HD12	1.93	0.50
1:B:2123:GLU:HG3	1:B:2170:MET:HG3	1.94	0.50
1:D:1319:ILE:O	1:D:1323:VAL:HG23	2.12	0.50
1:E:3249:ASN:OD1	1:E:3251:ILE:HG22	2.12	0.49
1:D:1053:ALA:HB2	1:D:1251:ILE:CG2	2.42	0.49
1:E:3221:VAL:HA	1:E:3248:LYS:O	2.12	0.49
1:C:2264:TYR:H	1:C:2264:TYR:HD2	1.60	0.49
1:D:121:THR:HG21	1:D:152:LYS:HG3	1.93	0.49
1:F:2173:GLN:C	1:F:2175:MET:H	2.15	0.49
1:F:2042:THR:HG21	1:F:2047:LEU:HD22	1.94	0.49
1:E:112:ASP:HA	1:E:1030:GLY:H	1.77	0.49
1:F:3171:MET:O	1:F:3173:GLN:N	2.45	0.49
1:E:2178:LEU:O	1:E:2182:LEU:HG	2.10	0.49
1:B:2308:TRP:HE3	1:B:2309:LEU:HD23	1.77	0.49
1:G:3084:GLN:HG2	1:G:3110:ASP:H	1.77	0.49
1:B:2264:TYR:HD2	1:B:2264:TYR:H	1.60	0.49
1:D:2264:TYR:H	1:D:2264:TYR:HD2	1.60	0.49
1:H:2173:GLN:C	1:H:2175:MET:H	2.15	0.49
1:C:2107:LEU:CD2	1:C:2267:GLY:HA3	2.41	0.49
1:G:3145:SER:O	1:G:3147:ALA:N	2.45	0.49
1:C:46:SER:HA	1:C:49:ILE:HD12	1.93	0.49
1:E:132:LEU:HB2	1:E:141:ILE:HD11	1.93	0.49
1:E:2073:THR:HG23	1:E:2077:LEU:HD13	1.94	0.49
1:H:1091:ALA:HB3	1:H:1141:ILE:HA	1.92	0.49
1:F:3222:ARG:HG3	1:F:3248:LYS:HB3	1.94	0.49
1:F:185:SER:HB2	1:F:187:THR:OG1	2.12	0.49
1:E:2123:GLU:HG3	1:E:2170:MET:HG3	1.94	0.49
1:H:156:GLU:HG3	1:H:1176:ARG:HG3	1.93	0.49
1:A:3059:GLY:HA2	1:A:3187:THR:O	2.11	0.49
1:B:1176:ARG:HA	1:B:1218:TYR:CE1	2.47	0.49
1:C:1065:TYR:C	1:C:1065:TYR:HD1	2.16	0.49
1:G:3222:ARG:HG3	1:G:3248:LYS:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:GLY:HA2	3:B:400:ANP:H5'1	1.94	0.49
1:G:319:ILE:O	1:G:323:VAL:HG23	2.12	0.49
1:B:2042:THR:HG21	1:B:2047:LEU:HD22	1.94	0.49
1:A:2173:GLN:C	1:A:2175:MET:H	2.16	0.49
1:H:1316:ALA:O	1:H:1319:ILE:N	2.46	0.49
1:G:1073:THR:HA	1:G:1076:THR:HB	1.94	0.49
1:D:2123:GLU:HG3	1:D:2170:MET:HG3	1.93	0.49
1:E:2173:GLN:C	1:E:2175:MET:H	2.15	0.49
1:B:2118:GLN:NE2	1:B:3249:ASN:H	2.10	0.49
1:B:3222:ARG:HG3	1:B:3248:LYS:HB3	1.94	0.49
1:E:107:LEU:CD2	1:E:267:GLY:HA3	2.43	0.49
1:B:2107:LEU:CD2	1:B:2267:GLY:HA3	2.43	0.49
1:E:2042:THR:HG21	1:E:2047:LEU:HD22	1.93	0.49
1:C:3100:ASP:O	1:C:3101:PRO:C	2.50	0.49
1:E:1073:THR:HA	1:E:1076:THR:HB	1.94	0.49
1:F:1176:ARG:HA	1:F:1218:TYR:CE1	2.48	0.49
1:H:1298:ILE:HG13	1:H:1299:GLY:N	2.26	0.49
1:A:1053:ALA:HB2	1:A:1251:ILE:CG2	2.42	0.49
1:H:2107:LEU:HD21	1:H:2267:GLY:HA3	1.95	0.49
1:B:3178:LEU:O	1:B:3182:LEU:HG	2.13	0.49
1:G:2107:LEU:CD2	1:G:2267:GLY:HA3	2.43	0.49
1:G:2175:MET:HG3	1:G:2218:TYR:HD1	1.78	0.49
1:C:3078:GLN:HG3	1:C:3268:ILE:HG13	1.95	0.49
1:B:319:ILE:O	1:B:323:VAL:HG23	2.13	0.49
1:H:2123:GLU:HG3	1:H:2170:MET:HG3	1.94	0.49
1:F:2107:LEU:CD2	1:F:2267:GLY:HA3	2.43	0.49
1:C:48:ASP:HB3	1:C:54:GLY:HA2	1.95	0.49
1:C:1166:LEU:O	1:C:1168:ALA:N	2.46	0.49
1:H:2308:TRP:HE3	1:H:2309:LEU:HD23	1.77	0.49
1:B:2300:GLN:HB3	1:C:2300:GLN:HE21	1.78	0.49
1:F:3249:ASN:OD1	1:F:3251:ILE:HG22	2.13	0.49
1:G:1091:ALA:HB3	1:G:1141:ILE:HA	1.93	0.49
1:C:1176:ARG:HA	1:C:1218:TYR:CE1	2.48	0.49
1:H:1065:TYR:HD1	1:H:1065:TYR:C	2.16	0.49
1:D:2107:LEU:HD21	1:D:2267:GLY:HA3	1.94	0.49
1:B:2107:LEU:HD21	1:B:2267:GLY:HA3	1.95	0.49
1:A:2146:VAL:HA	1:A:2149:LEU:HD23	1.95	0.49
1:B:1319:ILE:O	1:B:1323:VAL:HG23	2.13	0.49
1:B:3298:ILE:HG13	1:B:3299:GLY:N	2.27	0.49
1:F:319:ILE:O	1:F:323:VAL:HG23	2.12	0.49
1:A:2308:TRP:HE3	1:A:2309:LEU:HD23	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3078:GLN:HG3	1:D:3268:ILE:HG13	1.95	0.49
1:H:3222:ARG:HG3	1:H:3248:LYS:HB3	1.93	0.49
1:F:2175:MET:HG3	1:F:2218:TYR:HD1	1.78	0.49
1:C:3145:SER:O	1:C:3147:ALA:N	2.46	0.49
1:E:2264:TYR:H	1:E:2264:TYR:HD2	1.61	0.49
1:C:2042:THR:HG21	1:C:2047:LEU:HD22	1.93	0.49
1:E:48:ASP:HB3	1:E:54:GLY:HA2	1.95	0.49
1:E:2308:TRP:HE3	1:E:2309:LEU:HD23	1.78	0.49
1:H:3100:ASP:O	1:H:3101:PRO:C	2.51	0.49
1:D:2146:VAL:HA	1:D:2149:LEU:HD23	1.94	0.49
1:F:156:GLU:OE2	1:F:1176:ARG:CG	2.42	0.49
1:H:1053:ALA:HB2	1:H:1251:ILE:CG2	2.43	0.49
1:B:1091:ALA:HB3	1:B:1141:ILE:HA	1.93	0.49
1:A:2107:LEU:HD21	1:A:2267:GLY:HA3	1.94	0.49
1:G:1319:ILE:O	1:G:1323:VAL:HG23	2.13	0.49
1:E:2175:MET:HG3	1:E:2218:TYR:HD1	1.78	0.49
1:F:2264:TYR:H	1:F:2264:TYR:HD2	1.60	0.49
1:G:3298:ILE:HG13	1:G:3299:GLY:N	2.28	0.49
1:B:2173:GLN:C	1:B:2175:MET:H	2.16	0.49
1:G:46:SER:HA	1:G:49:ILE:HD12	1.94	0.49
1:E:1319:ILE:O	1:E:1323:VAL:HG23	2.12	0.49
1:H:3145:SER:O	1:H:3147:ALA:N	2.46	0.49
1:A:118:GLN:HE21	1:A:1254:PRO:HB3	1.78	0.49
1:A:2264:TYR:H	1:A:2264:TYR:HD2	1.61	0.49
1:E:2146:VAL:HA	1:E:2149:LEU:HD23	1.95	0.49
1:C:2308:TRP:HE3	1:C:2309:LEU:HD23	1.78	0.49
1:B:46:SER:HA	1:B:49:ILE:HD12	1.93	0.49
1:D:1073:THR:HA	1:D:1076:THR:HB	1.93	0.49
1:A:1166:LEU:C	1:A:1168:ALA:H	2.16	0.48
1:A:1166:LEU:O	1:A:1168:ALA:N	2.46	0.48
1:E:2299:GLY:HA2	1:H:2300:GLN:HE22	1.77	0.48
1:A:1308:TRP:CE3	1:A:1309:LEU:HD23	2.45	0.48
1:B:1053:ALA:HB2	1:B:1251:ILE:CG2	2.43	0.48
1:F:1091:ALA:HB3	1:F:1141:ILE:HA	1.94	0.48
1:E:2107:LEU:HD21	1:E:2267:GLY:HA3	1.95	0.48
1:D:3048:ASP:OD1	1:D:3048:ASP:N	2.46	0.48
1:F:2114:LEU:HD22	1:F:2115:LEU:H	1.78	0.48
1:A:3298:ILE:HG13	1:A:3299:GLY:N	2.27	0.48
1:D:2042:THR:HG21	1:D:2047:LEU:HD22	1.94	0.48
1:A:1073:THR:HA	1:A:1076:THR:HB	1.94	0.48
1:C:2173:GLN:C	1:C:2175:MET:H	2.16	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2175:MET:HG3	1:C:2218:TYR:HD1	1.78	0.48
1:F:2123:GLU:HG3	1:F:2170:MET:HG3	1.94	0.48
1:A:121:THR:HG21	1:A:152:LYS:HG3	1.93	0.48
1:D:319:ILE:O	1:D:323:VAL:HG23	2.13	0.48
1:H:107:LEU:CD2	1:H:267:GLY:HA3	2.43	0.48
1:H:3171:MET:C	1:H:3173:GLN:N	2.67	0.48
1:F:3064:ILE:O	1:F:3192:ILE:HA	2.13	0.48
1:B:3064:ILE:HG12	1:B:3223:LEU:CB	2.33	0.48
1:E:3064:ILE:O	1:E:3192:ILE:HA	2.13	0.48
1:D:1308:TRP:CE3	1:D:1309:LEU:HD23	2.45	0.48
1:G:1053:ALA:HB2	1:G:1251:ILE:CG2	2.43	0.48
1:F:2178:LEU:HD23	1:F:2182:LEU:HD11	1.95	0.48
1:C:1166:LEU:C	1:C:1168:ALA:H	2.16	0.48
1:B:3269:ASN:O	1:B:3272:GLY:N	2.46	0.48
1:G:1166:LEU:C	1:G:1168:ALA:H	2.17	0.48
1:H:1073:THR:HA	1:H:1076:THR:HB	1.94	0.48
1:A:3105:ARG:HD3	1:B:227:ARG:HH22	1.78	0.48
1:D:3101:PRO:O	1:D:3104:ALA:HB3	2.13	0.48
1:E:1176:ARG:HA	1:E:1218:TYR:CE1	2.48	0.48
1:C:2107:LEU:HD21	1:C:2267:GLY:HA3	1.94	0.48
1:A:2175:MET:HG3	1:A:2218:TYR:HD1	1.78	0.48
1:E:1073:THR:HG22	3:E:1400:ANP:PA	2.54	0.48
1:G:2173:GLN:C	1:G:2175:MET:H	2.15	0.48
1:F:2107:LEU:HD21	1:F:2267:GLY:HA3	1.95	0.48
1:G:2264:TYR:H	1:G:2264:TYR:HD2	1.61	0.48
1:E:1166:LEU:C	1:E:1168:ALA:H	2.16	0.48
1:B:3281:GLU:O	1:B:3283:LEU:N	2.47	0.48
1:D:3171:MET:C	1:D:3173:GLN:N	2.66	0.48
1:G:278:GLY:HA3	1:G:284:ILE:HD12	1.95	0.48
1:G:3326:LEU:O	1:G:3327:LEU:HG	2.13	0.48
1:A:48:ASP:HB3	1:A:54:GLY:HA2	1.95	0.48
1:E:3100:ASP:O	1:E:3101:PRO:C	2.52	0.48
1:D:1166:LEU:C	1:D:1168:ALA:H	2.17	0.48
1:B:3143:VAL:HG21	1:B:3191:PHE:CD1	2.49	0.48
1:A:2073:THR:HG23	1:A:2077:LEU:HD13	1.95	0.48
1:D:2175:MET:HG3	1:D:2218:TYR:HD1	1.79	0.48
1:E:112:ASP:HA	1:E:1030:GLY:N	2.28	0.48
1:B:2175:MET:HG3	1:B:2218:TYR:HD1	1.78	0.48
1:H:2146:VAL:HA	1:H:2149:LEU:HD23	1.96	0.48
1:H:2264:TYR:HD2	1:H:2264:TYR:H	1.61	0.48
1:G:2114:LEU:HD22	1:G:2115:LEU:H	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2114:LEU:HD22	1:B:2115:LEU:H	1.78	0.48
1:E:319:ILE:O	1:E:323:VAL:HG23	2.13	0.48
1:C:3064:ILE:O	1:C:3192:ILE:HA	2.13	0.48
1:C:3249:ASN:OD1	1:C:3251:ILE:HG22	2.13	0.48
1:F:1053:ALA:HB2	1:F:1251:ILE:CG2	2.43	0.48
1:C:1319:ILE:O	1:C:1323:VAL:HG23	2.13	0.48
1:F:3171:MET:C	1:F:3173:GLN:N	2.65	0.48
1:H:73:THR:HG23	1:H:77:LEU:HD13	1.95	0.48
1:C:3178:LEU:O	1:C:3182:LEU:HG	2.14	0.48
1:B:1016:GLN:O	1:B:1020:GLN:HB2	2.13	0.48
1:F:278:GLY:HA3	1:F:284:ILE:HD12	1.96	0.48
1:G:48:ASP:HB3	1:G:54:GLY:HA2	1.95	0.48
1:H:2175:MET:HG3	1:H:2218:TYR:HD1	1.78	0.48
1:G:1166:LEU:O	1:G:1168:ALA:N	2.46	0.48
1:D:278:GLY:HA3	1:D:284:ILE:HD12	1.96	0.48
1:G:118:GLN:NE2	1:G:1249:ASN:H	2.11	0.48
1:C:221:VAL:HA	1:C:248:LYS:O	2.13	0.48
1:B:3145:SER:O	1:B:3147:ALA:N	2.46	0.48
1:A:1176:ARG:HA	1:A:1218:TYR:CE1	2.48	0.48
1:H:1176:ARG:HA	1:H:1218:TYR:CE1	2.49	0.48
1:E:3311:ASP:HB3	1:F:286:LYS:HZ2	1.78	0.48
1:C:3065:TYR:HE2	1:C:3224:ASP:CG	2.17	0.48
1:F:1065:TYR:C	1:F:1065:TYR:HD1	2.17	0.48
1:A:1316:ALA:O	1:A:1319:ILE:N	2.47	0.48
1:G:2107:LEU:HD21	1:G:2267:GLY:HA3	1.95	0.48
1:B:3171:MET:C	1:B:3173:GLN:N	2.66	0.48
1:A:3100:ASP:O	1:A:3101:PRO:C	2.52	0.48
1:B:1166:LEU:O	1:B:1168:ALA:N	2.47	0.48
1:E:3078:GLN:HG3	1:E:3268:ILE:HG13	1.96	0.48
1:H:185:SER:HB2	1:H:187:THR:OG1	2.12	0.48
1:F:1166:LEU:O	1:F:1168:ALA:N	2.46	0.48
1:D:1219:ALA:O	1:D:1248:LYS:NZ	2.46	0.48
1:B:2300:GLN:OE1	1:C:2304:ASN:HB3	2.13	0.48
1:B:1145:SER:O	1:B:1146:VAL:C	2.52	0.48
1:A:1114:LEU:HB3	1:A:2029:LEU:HD12	1.96	0.48
1:F:3101:PRO:O	1:F:3104:ALA:HB3	2.14	0.48
1:F:101:PRO:HG3	1:F:1255:PHE:O	2.13	0.48
1:B:1316:ALA:O	1:B:1319:ILE:N	2.46	0.48
1:D:3171:MET:O	1:D:3173:GLN:N	2.47	0.48
1:A:3178:LEU:O	1:A:3182:LEU:HG	2.13	0.48
1:F:1319:ILE:O	1:F:1323:VAL:HG23	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:3174:ALA:O	1:H:3178:LEU:HD12	2.14	0.48
1:C:1016:GLN:O	1:C:1020:GLN:HB2	2.14	0.48
1:E:3171:MET:O	1:E:3173:GLN:N	2.47	0.48
1:G:3171:MET:C	1:G:3173:GLN:N	2.66	0.48
1:A:3065:TYR:HE2	1:A:3224:ASP:CG	2.17	0.48
1:E:3171:MET:C	1:E:3173:GLN:N	2.66	0.48
1:B:2111:ILE:HA	1:B:2111:ILE:HD13	1.74	0.48
1:G:1137:ALA:O	1:G:2010:LEU:HD13	2.12	0.48
1:H:3291:TYR:HE1	1:H:3302:LYS:HA	1.78	0.48
1:C:101:PRO:HG3	1:C:1255:PHE:O	2.13	0.48
1:E:1065:TYR:HD1	1:E:1065:TYR:C	2.17	0.48
1:A:3171:MET:O	1:A:3173:GLN:N	2.47	0.48
1:G:71:GLY:HA2	3:G:400:ANP:H5'1	1.96	0.48
1:H:75:LEU:O	1:H:75:LEU:HD23	2.14	0.48
1:B:3084:GLN:HG2	1:B:3110:ASP:H	1.79	0.48
1:C:3073:THR:O	1:C:3076:THR:OG1	2.26	0.48
1:D:48:ASP:HB3	1:D:54:GLY:HA2	1.95	0.48
1:B:185:SER:HB2	1:B:187:THR:OG1	2.14	0.48
1:H:48:ASP:HB3	1:H:54:GLY:HA2	1.96	0.48
1:F:3281:GLU:O	1:F:3283:LEU:N	2.47	0.48
1:H:3064:ILE:O	1:H:3192:ILE:HA	2.14	0.47
1:D:1166:LEU:O	1:D:1168:ALA:N	2.46	0.47
1:B:1166:LEU:C	1:B:1168:ALA:H	2.17	0.47
1:G:3171:MET:O	1:G:3173:GLN:N	2.47	0.47
1:B:2065:TYR:HE1	1:B:2224:ASP:CG	2.17	0.47
1:C:1327:LEU:C	1:C:1328:LEU:HD12	2.34	0.47
1:E:3287:ALA:HB3	1:E:3290:TRP:HB2	1.96	0.47
1:H:3298:ILE:HG13	1:H:3299:GLY:N	2.29	0.47
1:F:72:LYS:HE3	3:F:400:ANP:O1B	2.14	0.47
1:D:2118:GLN:NE2	1:D:3249:ASN:H	2.08	0.47
1:E:1316:ALA:O	1:E:1319:ILE:N	2.48	0.47
1:C:2146:VAL:HA	1:C:2149:LEU:HD23	1.94	0.47
1:G:3291:TYR:HE1	1:G:3302:LYS:HA	1.79	0.47
1:G:1016:GLN:O	1:G:1020:GLN:HB2	2.13	0.47
1:A:3264:TYR:CE1	3:A:3400:ANP:H1'	2.49	0.47
1:F:1300:GLN:H	1:G:3300:GLN:HE22	1.59	0.47
1:B:3171:MET:O	1:B:3173:GLN:N	2.47	0.47
1:C:2114:LEU:HD22	1:C:2115:LEU:H	1.79	0.47
1:H:1166:LEU:C	1:H:1168:ALA:H	2.17	0.47
1:B:278:GLY:HA3	1:B:284:ILE:HD12	1.94	0.47
1:G:3178:LEU:O	1:G:3182:LEU:HG	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1300:GLN:HE22	1:D:3300:GLN:N	2.10	0.47
1:G:3037:VAL:HG21	1:G:3251:ILE:HD11	1.97	0.47
1:F:3065:TYR:HE2	1:F:3224:ASP:CG	2.18	0.47
1:D:3065:TYR:HE2	1:D:3224:ASP:CG	2.18	0.47
1:C:156:GLU:HG2	1:C:1176:ARG:CG	2.43	0.47
1:E:3048:ASP:N	1:E:3048:ASP:OD1	2.48	0.47
1:B:3287:ALA:HB3	1:B:3290:TRP:HB2	1.97	0.47
1:D:3178:LEU:O	1:D:3182:LEU:HG	2.14	0.47
1:B:1150:THR:HA	1:B:1151:PRO:HD3	1.59	0.47
1:A:2060:ARG:HB3	1:A:2220:SER:OG	2.15	0.47
1:A:3145:SER:O	1:A:3147:ALA:N	2.48	0.47
1:A:2114:LEU:HD22	1:A:2115:LEU:H	1.80	0.47
1:H:2114:LEU:HD22	1:H:2115:LEU:H	1.79	0.47
1:G:64:ILE:HG12	1:G:223:LEU:HB2	1.97	0.47
1:G:2146:VAL:HA	1:G:2149:LEU:HD23	1.96	0.47
1:F:1166:LEU:C	1:F:1168:ALA:H	2.17	0.47
1:G:157:GLY:O	1:G:158:GLU:HG3	2.15	0.47
1:H:1114:LEU:O	1:H:2028:ARG:HA	2.13	0.47
1:C:1053:ALA:HB2	1:C:1251:ILE:CG2	2.43	0.47
1:E:3065:TYR:HE2	1:E:3224:ASP:CG	2.17	0.47
1:C:227:ARG:HH22	1:D:3105:ARG:HD3	1.79	0.47
1:G:2178:LEU:HD23	1:G:2182:LEU:HD11	1.96	0.47
1:A:2178:LEU:HD23	1:A:2182:LEU:HD11	1.96	0.47
1:E:1166:LEU:O	1:E:1168:ALA:N	2.47	0.47
1:F:1316:ALA:O	1:F:1319:ILE:N	2.47	0.47
1:H:3178:LEU:O	1:H:3182:LEU:HG	2.14	0.47
1:H:3048:ASP:OD1	1:H:3048:ASP:N	2.47	0.47
1:G:1327:LEU:C	1:G:1328:LEU:HD12	2.34	0.47
1:A:319:ILE:O	1:A:323:VAL:HG23	2.14	0.47
1:B:2064:ILE:O	1:B:2192:ILE:HA	2.15	0.47
1:A:1146:VAL:CG1	1:A:1211:GLY:HA3	2.41	0.47
1:B:1144:ASP:HA	1:B:1145:SER:HB3	1.97	0.47
1:G:1176:ARG:HA	1:G:1218:TYR:CE1	2.48	0.47
1:H:2129:CYS:HB2	1:H:2178:LEU:HD11	1.96	0.47
1:F:2111:ILE:HD13	1:F:2111:ILE:HA	1.72	0.47
1:C:3287:ALA:HB3	1:C:3290:TRP:HB2	1.97	0.47
1:F:48:ASP:HB3	1:F:54:GLY:HA2	1.96	0.47
1:E:3300:GLN:HE22	1:H:1300:GLN:N	2.09	0.47
1:A:1162:SER:O	1:A:1164:MET:N	2.48	0.47
1:D:3064:ILE:O	1:D:3192:ILE:HA	2.14	0.47
1:F:1145:SER:O	1:F:1146:VAL:C	2.53	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1305:ALA:O	1:C:1306:THR:O	2.32	0.47
1:C:2178:LEU:HD23	1:C:2182:LEU:HD11	1.97	0.47
1:D:1176:ARG:HA	1:D:1218:TYR:CE1	2.48	0.47
1:H:1319:ILE:O	1:H:1323:VAL:HG23	2.14	0.47
1:H:1166:LEU:O	1:H:1168:ALA:N	2.47	0.47
1:G:3174:ALA:O	1:G:3178:LEU:HD12	2.14	0.47
1:A:3145:SER:C	1:A:3147:ALA:N	2.68	0.47
1:D:3174:ALA:O	1:D:3178:LEU:HD12	2.15	0.47
1:C:75:LEU:O	1:C:75:LEU:HD23	2.15	0.47
1:A:3114:LEU:O	1:A:3114:LEU:HD13	2.15	0.47
1:F:3048:ASP:OD1	1:F:3048:ASP:N	2.48	0.47
1:H:2156:GLU:HA	1:H:3172:SER:OG	2.14	0.47
1:G:3010:LEU:O	1:G:3014:LEU:HG	2.15	0.47
1:F:3145:SER:O	1:F:3147:ALA:N	2.48	0.47
1:F:2060:ARG:HB3	1:F:2220:SER:OG	2.14	0.47
1:F:75:LEU:O	1:F:75:LEU:HD23	2.14	0.47
1:B:114:LEU:O	1:B:1028:ARG:HA	2.15	0.47
1:F:1016:GLN:O	1:F:1020:GLN:HB2	2.15	0.47
1:G:3078:GLN:HG3	1:G:3268:ILE:HG13	1.97	0.47
1:B:1065:TYR:HD1	1:B:1065:TYR:C	2.17	0.47
1:D:75:LEU:O	1:D:75:LEU:HD23	2.15	0.47
1:B:2146:VAL:HA	1:B:2149:LEU:HD23	1.95	0.47
1:G:135:SER:OG	1:G:1013:ALA:HB1	2.14	0.47
1:H:319:ILE:O	1:H:323:VAL:HG23	2.14	0.47
1:H:3010:LEU:O	1:H:3014:LEU:HG	2.15	0.47
1:E:3178:LEU:O	1:E:3182:LEU:HG	2.15	0.47
1:A:278:GLY:HA3	1:A:284:ILE:HD12	1.95	0.47
1:C:160:GLY:O	1:C:162:SER:N	2.48	0.47
1:D:3073:THR:O	1:D:3076:THR:OG1	2.28	0.47
1:H:2118:GLN:NE2	1:H:3249:ASN:H	2.10	0.47
1:D:1316:ALA:O	1:D:1319:ILE:N	2.48	0.47
1:C:3174:ALA:O	1:C:3178:LEU:HD12	2.15	0.47
1:C:278:GLY:HA3	1:C:284:ILE:HD12	1.96	0.47
1:A:3291:TYR:HE1	1:A:3302:LYS:HA	1.78	0.47
1:C:3171:MET:C	1:C:3173:GLN:N	2.67	0.47
1:F:3174:ALA:O	1:F:3178:LEU:HD12	2.14	0.47
1:E:1137:ALA:O	1:E:2010:LEU:HD13	2.15	0.47
1:E:3298:ILE:HG13	1:E:3299:GLY:N	2.28	0.47
1:C:3037:VAL:HG21	1:C:3251:ILE:HD11	1.97	0.47
1:G:157:GLY:HA2	1:G:1172:SER:HB2	1.96	0.47
1:D:1145:SER:O	1:D:1146:VAL:C	2.53	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3056:LEU:HA	1:F:3057:PRO:HD3	1.65	0.47
1:F:115:LEU:HA	1:F:1027:MET:O	2.15	0.47
1:B:75:LEU:O	1:B:75:LEU:HD23	2.15	0.47
1:H:3114:LEU:HD13	1:H:3114:LEU:O	2.15	0.47
1:D:2114:LEU:HD22	1:D:2115:LEU:H	1.79	0.47
1:F:2065:TYR:HE1	1:F:2224:ASP:CG	2.18	0.47
1:A:1193:ASN:HD21	1:A:1209:THR:C	2.19	0.46
1:F:69:SER:N	3:F:400:ANP:O1B	2.48	0.46
1:D:1144:ASP:HA	1:D:1145:SER:HB3	1.97	0.46
1:D:92:PHE:O	1:D:116:CYS:HA	2.15	0.46
1:D:2178:LEU:HD23	1:D:2182:LEU:HD11	1.96	0.46
1:F:2129:CYS:HB2	1:F:2178:LEU:HD11	1.96	0.46
1:B:3174:ALA:O	1:B:3178:LEU:HD12	2.14	0.46
1:E:278:GLY:HA3	1:E:284:ILE:HD12	1.96	0.46
1:D:73:THR:HG23	1:D:77:LEU:HD13	1.95	0.46
1:C:3291:TYR:HE1	1:C:3302:LYS:HA	1.79	0.46
1:C:3298:ILE:HG13	1:C:3299:GLY:N	2.29	0.46
1:H:2073:THR:HG23	1:H:2077:LEU:HD13	1.96	0.46
1:H:3171:MET:O	1:H:3173:GLN:N	2.47	0.46
1:B:64:ILE:HG12	1:B:223:LEU:HB2	1.97	0.46
1:B:3075:LEU:O	1:B:3075:LEU:HD23	2.15	0.46
1:A:3287:ALA:HB3	1:A:3290:TRP:HB2	1.97	0.46
1:B:3326:LEU:O	1:B:3327:LEU:HG	2.15	0.46
1:F:125:ALA:C	1:F:127:GLU:H	2.17	0.46
1:E:2300:GLN:HE22	1:H:2299:GLY:CA	2.22	0.46
1:H:3037:VAL:HG21	1:H:3251:ILE:HD11	1.98	0.46
1:G:2118:GLN:NE2	1:G:3249:ASN:H	2.12	0.46
1:E:112:ASP:HA	1:E:1030:GLY:HA3	1.98	0.46
1:E:3174:ALA:O	1:E:3178:LEU:HD12	2.14	0.46
1:F:64:ILE:HG12	1:F:223:LEU:HB2	1.96	0.46
1:D:3114:LEU:O	1:D:3114:LEU:HD13	2.14	0.46
1:A:1050:ALA:HB1	1:A:1256:LYS:HB3	1.98	0.46
1:C:3134:ARG:HD2	1:F:177:LYS:HD2	1.97	0.46
1:B:2060:ARG:HB3	1:B:2220:SER:OG	2.15	0.46
1:B:90:CYS:HG	1:B:140:VAL:HG13	1.79	0.46
1:D:1170:MET:HG2	1:D:1170:MET:O	2.16	0.46
1:H:1144:ASP:HA	1:H:1145:SER:HB3	1.98	0.46
1:H:1145:SER:O	1:H:1146:VAL:C	2.53	0.46
1:E:3253:ALA:HA	1:E:3254:PRO:HD3	1.82	0.46
1:E:3065:TYR:O	1:E:3065:TYR:HD2	1.98	0.46
1:A:1065:TYR:C	1:A:1065:TYR:HD1	2.18	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3109:VAL:HG12	1:F:3110:ASP:N	2.31	0.46
1:E:2178:LEU:HD23	1:E:2182:LEU:HD11	1.97	0.46
1:A:3174:ALA:O	1:A:3178:LEU:HD12	2.16	0.46
1:F:3178:LEU:O	1:F:3182:LEU:HG	2.14	0.46
1:H:1111:ILE:HA	1:H:1111:ILE:HD13	1.80	0.46
1:F:3114:LEU:HD13	1:F:3114:LEU:O	2.15	0.46
1:E:75:LEU:HD23	1:E:75:LEU:O	2.16	0.46
1:D:3145:SER:O	1:D:3147:ALA:N	2.49	0.46
1:H:125:ALA:C	1:H:127:GLU:H	2.18	0.46
1:A:3010:LEU:O	1:A:3014:LEU:HG	2.15	0.46
1:A:1150:THR:HA	1:A:1151:PRO:HD3	1.60	0.46
1:D:2064:ILE:O	1:D:2192:ILE:HA	2.15	0.46
1:E:118:GLN:NE2	1:E:1249:ASN:H	2.13	0.46
1:D:64:ILE:HG12	1:D:223:LEU:HB2	1.96	0.46
1:E:3291:TYR:HE1	1:E:3302:LYS:HA	1.79	0.46
1:F:1170:MET:HG2	1:F:1170:MET:O	2.16	0.46
1:G:1170:MET:HG2	1:G:1170:MET:O	2.16	0.46
1:D:2129:CYS:HB2	1:D:2178:LEU:HD11	1.97	0.46
1:C:2111:ILE:HD13	1:C:2111:ILE:HA	1.75	0.46
1:G:75:LEU:HD23	1:G:75:LEU:O	2.16	0.46
1:C:2048:ASP:O	1:C:2051:LEU:HB2	2.16	0.46
1:E:3271:TYR:O	1:E:3275:VAL:HG23	2.16	0.46
1:D:1064:ILE:HG23	1:D:1223:LEU:HB3	1.98	0.46
1:D:3037:VAL:HG21	1:D:3251:ILE:HD11	1.98	0.46
1:F:1144:ASP:HA	1:F:1145:SER:HB3	1.98	0.46
1:D:1065:TYR:C	1:D:1065:TYR:HD1	2.17	0.46
1:B:3048:ASP:OD1	1:B:3048:ASP:N	2.47	0.46
1:B:3092:PHE:CE2	1:B:3099:LEU:HD22	2.50	0.46
1:C:3010:LEU:O	1:C:3014:LEU:HG	2.15	0.46
1:A:3326:LEU:O	1:A:3327:LEU:HG	2.15	0.46
1:E:73:THR:HG23	1:E:77:LEU:HD13	1.97	0.46
1:E:2064:ILE:O	1:E:2192:ILE:HA	2.16	0.46
1:D:3056:LEU:HA	1:D:3057:PRO:HD3	1.65	0.46
1:G:1114:LEU:O	1:G:2028:ARG:HA	2.15	0.46
1:H:3065:TYR:HE2	1:H:3224:ASP:CG	2.18	0.46
1:E:3145:SER:C	1:E:3147:ALA:N	2.68	0.46
1:C:3171:MET:O	1:C:3173:GLN:N	2.48	0.46
1:A:3078:GLN:HG3	1:A:3268:ILE:HG13	1.97	0.46
1:A:2048:ASP:O	1:A:2051:LEU:HB2	2.16	0.46
1:A:1016:GLN:O	1:A:1020:GLN:HB2	2.16	0.46
1:G:3048:ASP:N	1:G:3048:ASP:OD1	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3287:ALA:HB3	1:G:3290:TRP:HB2	1.97	0.46
1:D:1016:GLN:O	1:D:1020:GLN:HB2	2.15	0.46
1:C:1050:ALA:HB1	1:C:1256:LYS:HB3	1.97	0.46
1:E:64:ILE:HG12	1:E:223:LEU:HB2	1.98	0.46
1:F:1090:CYS:HB3	1:F:1140:VAL:HG23	1.98	0.46
1:H:2178:LEU:HD23	1:H:2182:LEU:HD11	1.97	0.46
1:G:3281:GLU:O	1:G:3283:LEU:N	2.49	0.46
1:F:2064:ILE:O	1:F:2192:ILE:HA	2.16	0.46
1:D:114:LEU:HB3	1:D:1029:LEU:HD12	1.96	0.46
1:E:2065:TYR:HE1	1:E:2224:ASP:CG	2.18	0.46
1:E:1050:ALA:HB1	1:E:1256:LYS:HB3	1.98	0.46
1:E:3010:LEU:O	1:E:3014:LEU:HG	2.16	0.46
1:E:1144:ASP:HA	1:E:1145:SER:HB3	1.98	0.46
1:A:3037:VAL:HG21	1:A:3251:ILE:HD11	1.97	0.46
1:G:1144:ASP:HA	1:G:1145:SER:HB3	1.98	0.46
1:E:3090:CYS:SG	1:E:3140:VAL:CG1	3.04	0.46
1:E:2129:CYS:HB2	1:E:2178:LEU:HD11	1.98	0.46
1:B:3145:SER:C	1:B:3147:ALA:N	2.69	0.46
1:A:3171:MET:C	1:A:3173:GLN:N	2.67	0.46
1:G:73:THR:HG23	1:G:77:LEU:HD13	1.98	0.46
1:C:3114:LEU:HD13	1:C:3114:LEU:O	2.16	0.46
1:A:221:VAL:HA	1:A:248:LYS:O	2.15	0.46
1:G:1050:ALA:HB1	1:G:1256:LYS:HB3	1.98	0.46
1:A:1327:LEU:C	1:A:1328:LEU:HD12	2.37	0.46
1:H:64:ILE:HG12	1:H:223:LEU:HB2	1.97	0.46
1:C:1062:VAL:HB	1:C:1190:ILE:HG12	1.98	0.46
1:A:3300:GLN:NE2	1:D:1300:GLN:H	2.14	0.46
1:F:2227:ARG:HG3	1:F:2240:SER:HB3	1.98	0.46
1:B:48:ASP:HB3	1:B:54:GLY:HA2	1.96	0.46
1:E:1170:MET:O	1:E:1170:MET:HG2	2.16	0.46
1:B:3037:VAL:HG21	1:B:3251:ILE:HD11	1.98	0.46
1:G:3065:TYR:HE2	1:G:3224:ASP:CG	2.19	0.46
1:G:1065:TYR:C	1:G:1065:TYR:HD1	2.18	0.46
1:C:1029:LEU:HD23	1:C:1254:PRO:HD2	1.98	0.46
1:G:3092:PHE:CE2	1:G:3099:LEU:HD22	2.51	0.46
1:F:1150:THR:HA	1:F:1151:PRO:HD3	1.62	0.46
1:B:2029:LEU:HD23	1:B:2254:PRO:HD2	1.97	0.46
1:C:3092:PHE:CE2	1:C:3099:LEU:HD22	2.51	0.46
1:C:2065:TYR:HE1	1:C:2224:ASP:CG	2.19	0.46
1:F:1099:LEU:HB3	1:F:2255:PHE:CE1	2.51	0.46
1:H:221:VAL:HA	1:H:248:LYS:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2293:TYR:CE1	1:F:2319:ILE:HD11	2.51	0.46
1:D:3010:LEU:O	1:D:3014:LEU:HG	2.16	0.46
1:D:1161:ASP:CB	1:F:183:LYS:HZ1	2.02	0.45
1:A:1161:ASP:OD2	1:A:1166:LEU:HD13	2.16	0.45
1:A:1144:ASP:HA	1:A:1145:SER:HB3	1.98	0.45
1:E:1145:SER:O	1:E:1146:VAL:C	2.54	0.45
1:C:1144:ASP:HA	1:C:1145:SER:HB3	1.99	0.45
1:D:3065:TYR:O	1:D:3065:TYR:HD2	1.99	0.45
1:G:69:SER:N	3:G:400:ANP:O1B	2.49	0.45
1:F:3145:SER:C	1:F:3147:ALA:N	2.70	0.45
1:D:3123:GLU:O	1:D:3124:GLN:C	2.55	0.45
1:E:1150:THR:HA	1:E:1151:PRO:HD3	1.61	0.45
1:B:221:VAL:HA	1:B:248:LYS:O	2.16	0.45
1:C:73:THR:HG23	1:C:77:LEU:HD13	1.97	0.45
1:G:125:ALA:C	1:G:127:GLU:H	2.20	0.45
1:B:1064:ILE:HG23	1:B:1223:LEU:HB3	1.99	0.45
1:G:3064:ILE:O	1:G:3192:ILE:HA	2.16	0.45
1:C:2129:CYS:HB2	1:C:2178:LEU:HD11	1.97	0.45
1:B:2178:LEU:HD23	1:B:2182:LEU:HD11	1.96	0.45
1:A:2129:CYS:HB2	1:A:2178:LEU:HD11	1.97	0.45
1:G:3145:SER:C	1:G:3147:ALA:N	2.67	0.45
1:H:2065:TYR:HE1	1:H:2224:ASP:CG	2.20	0.45
1:H:2293:TYR:CE1	1:H:2319:ILE:HD11	2.52	0.45
1:B:1170:MET:O	1:B:1170:MET:HG2	2.16	0.45
1:H:2064:ILE:O	1:H:2192:ILE:HA	2.16	0.45
1:C:118:GLN:NE2	1:C:1249:ASN:H	2.14	0.45
1:G:221:VAL:HA	1:G:248:LYS:O	2.16	0.45
1:E:221:VAL:HA	1:E:248:LYS:O	2.15	0.45
1:E:1327:LEU:C	1:E:1328:LEU:HD12	2.37	0.45
1:E:3037:VAL:HG21	1:E:3251:ILE:HD11	1.98	0.45
1:H:3090:CYS:SG	1:H:3140:VAL:CG1	3.04	0.45
1:C:92:PHE:O	1:C:116:CYS:HA	2.16	0.45
1:B:2129:CYS:HB2	1:B:2178:LEU:HD11	1.97	0.45
1:H:3145:SER:C	1:H:3147:ALA:N	2.69	0.45
1:D:171:MET:O	1:D:175:MET:HB2	2.17	0.45
1:C:2060:ARG:HB3	1:C:2220:SER:OG	2.17	0.45
1:E:2293:TYR:CE1	1:E:2319:ILE:HD11	2.51	0.45
1:F:1050:ALA:HB1	1:F:1256:LYS:HB3	1.98	0.45
1:E:125:ALA:C	1:E:127:GLU:H	2.20	0.45
1:F:2048:ASP:O	1:F:2051:LEU:HB2	2.16	0.45
1:A:2065:TYR:HE1	1:A:2224:ASP:CG	2.19	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3037:VAL:HG21	1:F:3251:ILE:HD11	1.99	0.45
1:F:1305:ALA:O	1:F:1306:THR:O	2.34	0.45
1:E:232:LYS:HZ3	1:F:3266:GLU:HG3	1.82	0.45
1:H:3075:LEU:O	1:H:3075:LEU:HD23	2.17	0.45
1:A:1062:VAL:HB	1:A:1190:ILE:HG12	1.98	0.45
1:B:3010:LEU:O	1:B:3014:LEU:HG	2.16	0.45
1:G:3123:GLU:O	1:G:3124:GLN:C	2.55	0.45
1:F:3327:LEU:O	1:F:3328:LEU:HD12	2.16	0.45
1:H:1062:VAL:HB	1:H:1190:ILE:HG12	1.98	0.45
1:H:3326:LEU:O	1:H:3327:LEU:HG	2.17	0.45
1:F:73:THR:HG23	1:F:77:LEU:HD13	1.97	0.45
1:A:2118:GLN:NE2	1:A:3249:ASN:H	2.12	0.45
1:F:161:ASP:H	1:F:163:HIS:H	1.65	0.45
1:H:2229:GLY:O	1:H:2230:ALA:CB	2.65	0.45
1:B:2090:CYS:CB	1:B:2140:VAL:HG13	2.47	0.45
1:B:3078:GLN:HG3	1:B:3268:ILE:HG13	1.98	0.45
1:F:171:MET:O	1:F:175:MET:HB2	2.17	0.45
1:G:2287:ALA:HB3	1:G:2290:TRP:HB2	1.98	0.45
1:B:1327:LEU:C	1:B:1328:LEU:HD12	2.37	0.45
1:D:3287:ALA:HB3	1:D:3290:TRP:HB2	1.99	0.45
1:G:2305:ALA:O	1:G:2306:THR:C	2.55	0.45
1:D:1062:VAL:HB	1:D:1190:ILE:HG12	1.98	0.45
1:F:221:VAL:HA	1:F:248:LYS:O	2.17	0.45
1:G:3271:TYR:O	1:G:3275:VAL:HG23	2.17	0.45
1:A:3092:PHE:CE2	1:A:3099:LEU:HD22	2.52	0.45
1:C:64:ILE:HG12	1:C:223:LEU:HB2	1.98	0.45
1:D:2227:ARG:HG3	1:D:2240:SER:HB3	1.99	0.45
1:D:2060:ARG:HB3	1:D:2220:SER:OG	2.16	0.45
1:E:3092:PHE:CE2	1:E:3099:LEU:HD22	2.52	0.45
1:G:3151:PRO:HG2	1:H:3151:PRO:CB	2.47	0.45
1:C:1170:MET:HG2	1:C:1170:MET:O	2.16	0.45
1:F:72:LYS:HB2	1:F:72:LYS:HE3	1.75	0.45
1:G:1145:SER:O	1:G:1146:VAL:C	2.55	0.45
1:H:1112:ASP:HA	1:H:2030:GLY:CA	2.47	0.45
1:E:2171:MET:O	1:E:2175:MET:HB2	2.16	0.45
1:A:75:LEU:O	1:A:75:LEU:HD23	2.16	0.45
1:B:2048:ASP:O	1:B:2051:LEU:HB2	2.17	0.45
1:F:2287:ALA:HB3	1:F:2290:TRP:HB2	1.99	0.45
1:D:72:LYS:HE3	1:D:72:LYS:HB2	1.74	0.45
1:H:1064:ILE:HG23	1:H:1223:LEU:HB3	1.98	0.45
1:H:1050:ALA:HB1	1:H:1256:LYS:HB3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ALA:C	1:A:127:GLU:H	2.20	0.45
1:C:1090:CYS:HB3	1:C:1140:VAL:HG23	1.99	0.45
1:D:2171:MET:O	1:D:2175:MET:HB2	2.17	0.45
1:G:2171:MET:O	1:G:2175:MET:HB2	2.16	0.45
1:B:2171:MET:O	1:B:2175:MET:HB2	2.17	0.45
1:B:2065:TYR:CD1	1:B:2065:TYR:C	2.90	0.45
1:G:1324:ARG:HA	1:G:1328:LEU:HD13	1.99	0.45
1:E:1324:ARG:HA	1:E:1328:LEU:HD13	1.99	0.45
1:F:3010:LEU:O	1:F:3014:LEU:HG	2.17	0.45
1:E:171:MET:O	1:E:175:MET:HB2	2.17	0.45
1:E:2114:LEU:HD22	1:E:2115:LEU:H	1.81	0.45
1:G:3132:LEU:HA	1:G:3135:SER:HB2	1.99	0.45
1:H:3029:LEU:CD2	1:H:3254:PRO:HD2	2.47	0.45
1:E:1090:CYS:HB3	1:E:1140:VAL:HG23	1.98	0.45
1:C:3065:TYR:HD2	1:C:3065:TYR:O	2.00	0.45
1:B:3114:LEU:O	1:B:3114:LEU:HD13	2.17	0.45
1:B:2227:ARG:HG3	1:B:2240:SER:HB3	1.97	0.45
1:H:3287:ALA:HB3	1:H:3290:TRP:HB2	1.98	0.45
1:C:2227:ARG:HG3	1:C:2240:SER:HB3	1.98	0.45
1:A:2287:ALA:HB3	1:A:2290:TRP:HB2	1.99	0.45
1:H:1150:THR:HA	1:H:1151:PRO:HD3	1.61	0.45
1:F:1062:VAL:HB	1:F:1190:ILE:HG12	1.98	0.45
1:D:3291:TYR:HE1	1:D:3302:LYS:HA	1.81	0.45
1:G:2227:ARG:HG3	1:G:2240:SER:HB3	1.99	0.45
1:C:3132:LEU:HA	1:C:3135:SER:HB2	1.99	0.45
1:D:2287:ALA:HB3	1:D:2290:TRP:HB2	1.99	0.45
1:G:158:GLU:HB3	1:G:159:ILE:H	1.59	0.45
1:D:2090:CYS:CB	1:D:2140:VAL:HG13	2.47	0.45
1:B:92:PHE:O	1:B:116:CYS:HA	2.17	0.45
1:G:2129:CYS:HB2	1:G:2178:LEU:HD11	1.99	0.45
1:D:2065:TYR:HE1	1:D:2224:ASP:CG	2.20	0.45
1:E:2060:ARG:HB3	1:E:2220:SER:OG	2.17	0.45
1:D:1327:LEU:C	1:D:1328:LEU:HD12	2.37	0.45
1:D:1150:THR:HA	1:D:1151:PRO:HD3	1.61	0.45
1:G:2065:TYR:HE1	1:G:2224:ASP:CG	2.20	0.45
1:D:1067:PRO:O	1:D:1070:SER:OG	2.23	0.45
1:E:132:LEU:HD11	1:E:1026:ILE:HD12	1.99	0.44
1:H:3253:ALA:HA	1:H:3254:PRO:HD3	1.80	0.44
1:F:2090:CYS:CB	1:F:2140:VAL:HG13	2.48	0.44
1:F:3065:TYR:O	1:F:3065:TYR:HD2	1.99	0.44
1:G:2253:ALA:HA	1:G:2254:PRO:HD3	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2171:MET:O	1:H:2175:MET:HB2	2.17	0.44
1:E:1282:LYS:HG2	1:E:1282:LYS:H	1.60	0.44
1:A:3281:GLU:O	1:A:3283:LEU:N	2.50	0.44
1:G:99:LEU:HD23	1:G:1255:PHE:CZ	2.52	0.44
1:F:3291:TYR:HE1	1:F:3302:LYS:HA	1.82	0.44
1:E:3040:ILE:O	1:E:3055:GLY:HA3	2.16	0.44
1:E:1062:VAL:HB	1:E:1190:ILE:HG12	1.98	0.44
1:H:1327:LEU:C	1:H:1328:LEU:HD12	2.37	0.44
1:H:3264:TYR:CE1	3:H:3400:ANP:HI'	2.52	0.44
1:F:160:GLY:HA3	1:F:163:HIS:HA	1.99	0.44
1:G:3075:LEU:HD23	1:G:3075:LEU:O	2.16	0.44
1:H:1018:GLU:OE2	1:H:1024:GLY:HA2	2.17	0.44
1:A:64:ILE:HG12	1:A:223:LEU:HB2	1.98	0.44
1:D:2293:TYR:CE1	1:D:2319:ILE:HD11	2.52	0.44
1:C:72:LYS:HB2	1:C:72:LYS:HE3	1.75	0.44
1:H:2287:ALA:HB3	1:H:2290:TRP:HB2	1.99	0.44
1:B:2287:ALA:HB3	1:B:2290:TRP:HB2	2.00	0.44
1:E:2227:ARG:HG3	1:E:2240:SER:HB3	1.98	0.44
1:G:2293:TYR:CE1	1:G:2319:ILE:HD11	2.52	0.44
1:D:221:VAL:HA	1:D:248:LYS:O	2.17	0.44
1:A:2293:TYR:CE1	1:A:2319:ILE:HD11	2.52	0.44
1:E:3077:LEU:HG	1:E:3080:ILE:HD12	2.00	0.44
1:B:3140:VAL:HG23	1:B:3188:LEU:HB3	2.00	0.44
1:B:125:ALA:C	1:B:127:GLU:H	2.19	0.44
1:F:3287:ALA:HB3	1:F:3290:TRP:HB2	1.98	0.44
1:B:1066:GLY:O	1:B:1067:PRO:C	2.56	0.44
1:H:69:SER:N	3:H:400:ANP:O1B	2.50	0.44
1:E:1064:ILE:HG23	1:E:1223:LEU:HB3	1.99	0.44
1:B:1062:VAL:HB	1:B:1190:ILE:HG12	1.98	0.44
1:B:3064:ILE:O	1:B:3192:ILE:HA	2.16	0.44
1:C:1145:SER:O	1:C:1146:VAL:C	2.54	0.44
1:G:1305:ALA:O	1:G:1306:THR:O	2.35	0.44
1:C:2084:GLN:HG3	1:C:2090:CYS:SG	2.58	0.44
1:C:2229:GLY:O	1:C:2230:ALA:CB	2.64	0.44
1:B:1090:CYS:HB3	1:B:1140:VAL:HG23	1.99	0.44
1:D:2230:ALA:HA	1:D:2239:GLY:O	2.18	0.44
1:F:92:PHE:O	1:F:116:CYS:HA	2.17	0.44
1:G:2218:TYR:HA	1:G:2218:TYR:HD2	1.73	0.44
1:C:2171:MET:O	1:C:2175:MET:HB2	2.17	0.44
1:H:1324:ARG:HA	1:H:1328:LEU:HD13	1.98	0.44
1:E:3075:LEU:O	1:E:3075:LEU:HD23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:157:GLY:O	1:E:158:GLU:O	2.36	0.44
1:B:1050:ALA:HB1	1:B:1256:LYS:HB3	1.99	0.44
1:F:2128:ILE:HG22	1:F:2132:LEU:CD1	2.47	0.44
1:B:3291:TYR:HE1	1:B:3302:LYS:HA	1.82	0.44
1:G:1062:VAL:HB	1:G:1190:ILE:HG12	2.00	0.44
1:A:160:GLY:C	1:A:163:HIS:HB3	2.37	0.44
1:D:157:GLY:HA3	1:D:1172:SER:CB	2.47	0.44
1:E:2063:GLU:HG3	1:E:2215:LEU:HD21	1.99	0.44
1:B:3185:SER:C	1:B:3187:THR:N	2.70	0.44
1:A:3224:ASP:O	1:A:3244:VAL:HA	2.18	0.44
1:D:3269:ASN:O	1:D:3272:GLY:N	2.51	0.44
1:D:2305:ALA:O	1:D:2306:THR:C	2.55	0.44
1:A:73:THR:HG23	1:A:77:LEU:HD13	1.98	0.44
1:E:3326:LEU:O	1:E:3327:LEU:HG	2.17	0.44
1:C:2253:ALA:HA	1:C:2254:PRO:HD3	1.83	0.44
1:H:3040:ILE:O	1:H:3055:GLY:HA3	2.18	0.44
1:E:2287:ALA:HB3	1:E:2290:TRP:HB2	1.99	0.44
1:D:2063:GLU:HG3	1:D:2215:LEU:HD21	2.00	0.44
1:G:3253:ALA:HA	1:G:3254:PRO:HD3	1.81	0.44
1:C:3140:VAL:HG23	1:C:3188:LEU:HB3	1.99	0.44
1:G:1090:CYS:HB3	1:G:1140:VAL:HG23	1.99	0.44
1:H:45:LEU:HD23	1:H:270:PHE:HD1	1.82	0.44
1:B:1324:ARG:HA	1:B:1328:LEU:HD13	2.00	0.44
1:C:3271:TYR:O	1:C:3275:VAL:HG23	2.18	0.44
1:F:3313:PRO:O	1:F:3316:ALA:HB3	2.17	0.44
1:F:2305:ALA:O	1:F:2306:THR:C	2.54	0.44
1:B:171:MET:O	1:B:175:MET:HB2	2.17	0.44
1:H:1016:GLN:O	1:H:1020:GLN:HB2	2.17	0.44
1:C:171:MET:O	1:C:175:MET:HB2	2.18	0.44
1:A:1202:MET:O	1:B:3116:CYS:O	2.36	0.44
1:C:3077:LEU:HG	1:C:3080:ILE:HD12	2.00	0.44
1:A:2229:GLY:O	1:A:2230:ALA:CB	2.65	0.44
1:F:3090:CYS:SG	1:F:3140:VAL:CG1	3.06	0.44
1:H:92:PHE:O	1:H:116:CYS:HA	2.16	0.44
1:B:115:LEU:HA	1:B:1027:MET:O	2.18	0.44
1:H:3101:PRO:O	1:H:3104:ALA:HB3	2.18	0.44
1:D:3326:LEU:O	1:D:3327:LEU:HG	2.17	0.44
1:C:125:ALA:C	1:C:127:GLU:H	2.21	0.44
1:A:3123:GLU:O	1:A:3124:GLN:C	2.56	0.44
1:E:2048:ASP:O	1:E:2051:LEU:HB2	2.18	0.44
1:C:173:GLN:HB3	1:C:174:ALA:H	1.68	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2300:GLN:CD	1:H:2304:ASN:HB3	2.38	0.44
1:A:115:LEU:CD2	1:A:1028:ARG:HG2	2.48	0.44
1:F:2230:ALA:HA	1:F:2239:GLY:O	2.18	0.44
1:G:2229:GLY:O	1:G:2230:ALA:CB	2.66	0.44
1:F:3224:ASP:O	1:F:3244:VAL:HA	2.18	0.44
1:G:92:PHE:O	1:G:116:CYS:HA	2.17	0.44
1:F:2253:ALA:HA	1:F:2254:PRO:HD3	1.83	0.44
1:H:2128:ILE:HG22	1:H:2132:LEU:CD1	2.48	0.44
1:E:3114:LEU:HD13	1:E:3114:LEU:O	2.18	0.44
1:B:72:LYS:HE3	1:B:72:LYS:HB2	1.74	0.44
1:H:1282:LYS:HG2	1:H:1282:LYS:H	1.58	0.44
1:C:2293:TYR:CE1	1:C:2319:ILE:HD11	2.52	0.44
1:A:3293:TYR:O	1:A:3296:GLU:HB2	2.18	0.44
1:A:2227:ARG:HG3	1:A:2240:SER:HB3	1.99	0.44
1:D:3092:PHE:CE2	1:D:3099:LEU:HD22	2.53	0.44
1:F:1327:LEU:C	1:F:1328:LEU:HD12	2.38	0.44
1:C:2064:ILE:O	1:C:2192:ILE:HA	2.17	0.44
1:E:90:CYS:HG	1:E:140:VAL:HG13	1.82	0.44
1:C:3029:LEU:CD2	1:C:3254:PRO:HD2	2.47	0.44
1:A:2090:CYS:CB	1:A:2140:VAL:HG13	2.47	0.44
1:H:2090:CYS:CB	1:H:2140:VAL:HG13	2.48	0.44
1:B:3300:GLN:NE2	1:C:1300:GLN:H	2.15	0.44
1:H:2060:ARG:HB3	1:H:2220:SER:OG	2.17	0.44
1:C:3040:ILE:O	1:C:3055:GLY:HA3	2.18	0.44
1:A:2223:LEU:HA	1:A:2223:LEU:HD12	1.85	0.44
1:C:3048:ASP:OD1	1:C:3048:ASP:N	2.50	0.44
1:G:1064:ILE:HG23	1:G:1223:LEU:HB3	2.00	0.44
1:G:2233:GLU:HG3	1:G:2238:VAL:HG11	2.00	0.44
1:E:2300:GLN:HE21	1:H:2300:GLN:N	2.16	0.43
1:E:3076:THR:O	1:E:3080:ILE:HG13	2.18	0.43
1:G:3029:LEU:CD2	1:G:3254:PRO:HD2	2.48	0.43
1:B:3029:LEU:CD2	1:B:3254:PRO:HD2	2.48	0.43
1:G:3090:CYS:SG	1:G:3140:VAL:CG1	3.06	0.43
1:D:3140:VAL:HG23	1:D:3188:LEU:HB3	1.99	0.43
1:A:3056:LEU:HA	1:A:3057:PRO:HD3	1.66	0.43
1:A:3090:CYS:SG	1:A:3140:VAL:CG1	3.06	0.43
1:G:3065:TYR:O	1:G:3065:TYR:HD2	2.01	0.43
1:F:2300:GLN:H	1:G:2300:GLN:NE2	2.16	0.43
1:E:3101:PRO:O	1:E:3104:ALA:HB3	2.17	0.43
1:B:2293:TYR:CE1	1:B:2319:ILE:HD11	2.52	0.43
1:C:2233:GLU:HG3	1:C:2238:VAL:HG11	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1153:ALA:O	1:H:1157:GLY:O	2.36	0.43
1:G:2060:ARG:HB3	1:G:2220:SER:OG	2.17	0.43
1:G:2048:ASP:O	1:G:2051:LEU:HB2	2.18	0.43
1:A:1161:ASP:C	1:A:1163:HIS:N	2.70	0.43
1:A:1300:GLN:N	1:D:3300:GLN:NE2	2.64	0.43
1:A:3218:TYR:HD2	1:A:3218:TYR:HA	1.66	0.43
1:D:1305:ALA:O	1:D:1306:THR:O	2.35	0.43
1:H:3140:VAL:HG23	1:H:3188:LEU:HB3	2.01	0.43
1:H:231:VAL:HB	1:H:239:GLY:HA3	2.00	0.43
1:G:2230:ALA:HA	1:G:2239:GLY:O	2.18	0.43
1:C:2128:ILE:HG22	1:C:2132:LEU:CD1	2.47	0.43
1:A:3048:ASP:N	1:A:3048:ASP:OD1	2.51	0.43
1:G:2111:ILE:HD13	1:G:2111:ILE:HA	1.75	0.43
1:C:3051:LEU:HD23	1:C:3051:LEU:HA	1.84	0.43
1:A:3271:TYR:O	1:A:3275:VAL:HG23	2.19	0.43
1:G:171:MET:O	1:G:175:MET:HB2	2.17	0.43
1:A:3132:LEU:HA	1:A:3135:SER:HB2	2.00	0.43
1:B:2305:ALA:O	1:B:2306:THR:C	2.57	0.43
1:D:1050:ALA:HB1	1:D:1256:LYS:HB3	2.00	0.43
1:F:3264:TYR:CE1	3:F:3400:ANP:H1'	2.53	0.43
1:A:3072:LYS:CE	3:A:3400:ANP:O1B	2.59	0.43
1:E:92:PHE:O	1:E:116:CYS:HA	2.17	0.43
1:F:3029:LEU:CD2	1:F:3254:PRO:HD2	2.47	0.43
1:B:3300:GLN:HE22	1:C:1299:GLY:HA2	1.83	0.43
1:H:3109:VAL:HG12	1:H:3110:ASP:N	2.33	0.43
1:F:3171:MET:C	1:F:3173:GLN:H	2.21	0.43
1:C:3326:LEU:O	1:C:3327:LEU:HG	2.17	0.43
1:E:3132:LEU:HA	1:E:3135:SER:HB2	2.00	0.43
1:D:2233:GLU:HG3	1:D:2238:VAL:HG11	2.01	0.43
1:E:3281:GLU:O	1:E:3283:LEU:N	2.51	0.43
1:C:3123:GLU:O	1:C:3124:GLN:C	2.57	0.43
1:C:2305:ALA:O	1:C:2306:THR:C	2.57	0.43
1:D:1154:GLU:HG2	1:D:1159:ILE:HA	2.00	0.43
1:C:164:MET:C	1:C:166:LEU:N	2.71	0.43
1:B:1090:CYS:SG	1:B:1140:VAL:HG22	2.59	0.43
1:B:3224:ASP:O	1:B:3244:VAL:HA	2.18	0.43
1:C:66:GLY:O	1:C:72:LYS:HE2	2.18	0.43
1:B:73:THR:HG23	1:B:77:LEU:HD13	1.99	0.43
1:B:1018:GLU:OE2	1:B:1024:GLY:HA2	2.18	0.43
1:G:2128:ILE:HG22	1:G:2132:LEU:CD1	2.48	0.43
1:C:3177:LYS:HE3	1:F:173:GLN:NE2	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3151:PRO:CB	1:H:3151:PRO:HG2	2.48	0.43
1:D:3185:SER:C	1:D:3187:THR:N	2.71	0.43
1:G:3185:SER:C	1:G:3187:THR:N	2.71	0.43
1:A:3140:VAL:HG23	1:A:3188:LEU:HB3	2.00	0.43
1:A:3065:TYR:O	1:A:3065:TYR:HD2	2.00	0.43
1:F:2171:MET:O	1:F:2175:MET:HB2	2.17	0.43
1:B:2218:TYR:HD2	1:B:2218:TYR:HA	1.73	0.43
1:B:3327:LEU:O	1:B:3328:LEU:HD12	2.17	0.43
1:D:1066:GLY:O	1:D:1067:PRO:C	2.57	0.43
1:G:2122:GLY:O	1:G:2125:ALA:HB3	2.18	0.43
1:F:1048:ASP:HB3	1:F:1054:GLY:HA2	2.01	0.43
1:D:2128:ILE:HG22	1:D:2132:LEU:CD1	2.49	0.43
1:H:1048:ASP:HB3	1:H:1054:GLY:HA2	2.00	0.43
1:C:3281:GLU:O	1:C:3283:LEU:N	2.52	0.43
1:C:1066:GLY:O	1:C:1067:PRO:C	2.56	0.43
1:D:1072:LYS:HB3	1:D:1225:ILE:HG21	2.00	0.43
1:E:1300:GLN:H	1:H:3300:GLN:HE21	1.54	0.43
1:C:2063:GLU:HG3	1:C:2215:LEU:HD21	1.99	0.43
1:D:1090:CYS:HB3	1:D:1140:VAL:HG23	2.00	0.43
1:E:1114:LEU:O	1:E:2028:ARG:HA	2.19	0.43
1:D:2229:GLY:O	1:D:2230:ALA:CB	2.66	0.43
1:D:231:VAL:HB	1:D:239:GLY:HA3	2.00	0.43
1:A:1090:CYS:HB3	1:A:1140:VAL:HG23	1.99	0.43
1:G:1056:LEU:HA	1:G:1057:PRO:HD2	1.81	0.43
1:B:3144:ASP:OD1	1:B:3145:SER:HB2	2.19	0.43
1:C:1067:PRO:O	1:C:1070:SER:OG	2.24	0.43
1:F:3123:GLU:O	1:F:3124:GLN:C	2.56	0.43
1:E:72:LYS:HB2	1:E:72:LYS:HE3	1.73	0.43
1:E:1048:ASP:HB3	1:E:1054:GLY:HA2	2.01	0.43
1:F:3092:PHE:CE2	1:F:3099:LEU:HD22	2.54	0.43
1:B:2300:GLN:HE21	1:C:2300:GLN:CB	2.31	0.43
1:B:2063:GLU:HG3	1:B:2215:LEU:HD21	2.01	0.43
1:G:2063:GLU:HG3	1:G:2215:LEU:HD21	2.01	0.43
1:H:1090:CYS:HB3	1:H:1140:VAL:HG23	2.01	0.43
1:C:3185:SER:C	1:C:3187:THR:N	2.72	0.43
1:F:1097:HIS:CD2	1:F:2248:LYS:HG3	2.53	0.43
1:A:2171:MET:O	1:A:2175:MET:HB2	2.18	0.43
1:B:1066:GLY:HA2	1:B:1067:PRO:HD2	1.85	0.43
1:E:1072:LYS:HB3	1:E:1225:ILE:HG21	2.01	0.43
1:G:3114:LEU:HD13	1:G:3114:LEU:O	2.17	0.43
1:G:2064:ILE:O	1:G:2192:ILE:HA	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3145:SER:C	1:D:3147:ALA:N	2.72	0.43
1:E:118:GLN:HE21	1:E:1254:PRO:HB3	1.84	0.43
1:C:1040:ILE:HD13	1:C:1040:ILE:HA	1.91	0.43
1:C:100:ASP:HB3	1:C:103:TYR:HB3	2.01	0.43
1:H:3281:GLU:O	1:H:3283:LEU:N	2.51	0.43
1:B:1048:ASP:HB3	1:B:1054:GLY:HA2	2.01	0.43
1:D:2048:ASP:O	1:D:2051:LEU:HB2	2.19	0.43
1:A:171:MET:O	1:A:175:MET:HB2	2.19	0.43
1:E:2233:GLU:HG3	1:E:2238:VAL:HG11	2.00	0.43
1:B:3132:LEU:HA	1:B:3135:SER:HB2	2.00	0.43
1:G:100:ASP:HB3	1:G:103:TYR:HB3	2.01	0.43
1:E:1300:GLN:HE22	1:H:3300:GLN:N	2.11	0.43
1:A:1305:ALA:O	1:A:1306:THR:O	2.37	0.43
1:G:3140:VAL:HG23	1:G:3188:LEU:HB3	2.00	0.43
1:B:3056:LEU:HA	1:B:3057:PRO:HD3	1.63	0.43
1:G:3101:PRO:O	1:G:3104:ALA:HB3	2.18	0.43
1:F:2223:LEU:HA	1:F:2223:LEU:HD12	1.83	0.43
1:B:3051:LEU:HD23	1:B:3051:LEU:HA	1.84	0.43
1:B:100:ASP:HB3	1:B:103:TYR:HB3	2.01	0.43
1:E:3232:LYS:NZ	1:H:1235:GLU:HG2	2.34	0.43
1:F:3073:THR:O	1:F:3076:THR:OG1	2.30	0.43
1:A:2305:ALA:O	1:A:2306:THR:C	2.56	0.43
1:A:1209:THR:CG2	1:A:1209:THR:O	2.63	0.43
1:C:3253:ALA:HA	1:C:3254:PRO:HD3	1.80	0.43
1:E:1090:CYS:SG	1:E:1140:VAL:HG22	2.58	0.43
1:H:3224:ASP:O	1:H:3244:VAL:HA	2.19	0.43
1:G:116:CYS:O	1:G:1026:ILE:HA	2.19	0.43
1:A:3084:GLN:O	1:B:226:ARG:HD3	2.18	0.43
1:H:3268:ILE:HG22	1:H:3269:ASN:N	2.33	0.43
1:C:3101:PRO:O	1:C:3104:ALA:HB3	2.19	0.43
1:A:1324:ARG:HA	1:A:1328:LEU:HD13	2.01	0.43
1:B:2254:PRO:HB2	1:B:2255:PHE:CD2	2.54	0.43
1:F:1064:ILE:HG23	1:F:1223:LEU:HB3	2.01	0.43
1:F:1040:ILE:HD13	1:F:1040:ILE:HA	1.92	0.43
1:D:3313:PRO:O	1:D:3316:ALA:HB3	2.19	0.43
1:B:3293:TYR:O	1:B:3296:GLU:HB2	2.19	0.43
1:E:2128:ILE:HG22	1:E:2132:LEU:CD1	2.49	0.43
1:A:3040:ILE:O	1:A:3055:GLY:HA3	2.19	0.43
1:A:1161:ASP:HA	1:A:1166:LEU:HD12	2.01	0.42
1:D:3072:LYS:CE	3:D:3400:ANP:O1B	2.60	0.42
1:G:90:CYS:HG	1:G:140:VAL:HG13	1.80	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2118:GLN:NE2	1:C:3249:ASN:H	2.11	0.42
1:D:3224:ASP:O	1:D:3244:VAL:HA	2.19	0.42
1:E:3144:ASP:OD1	1:E:3145:SER:HB2	2.19	0.42
1:B:2065:TYR:O	1:B:2065:TYR:HD1	2.02	0.42
1:F:2065:TYR:CD1	1:F:2065:TYR:C	2.92	0.42
1:H:2048:ASP:O	1:H:2051:LEU:HB2	2.19	0.42
1:G:72:LYS:HE3	1:G:72:LYS:HB2	1.74	0.42
1:A:2253:ALA:HA	1:A:2254:PRO:HD3	1.83	0.42
1:H:3293:TYR:O	1:H:3296:GLU:HB2	2.19	0.42
1:H:1066:GLY:O	1:H:1067:PRO:C	2.57	0.42
1:H:3132:LEU:HA	1:H:3135:SER:HB2	2.01	0.42
1:A:1163:HIS:O	1:A:1165:GLY:N	2.52	0.42
1:A:1202:MET:HA	1:A:1202:MET:CE	2.49	0.42
1:C:1090:CYS:SG	1:C:1140:VAL:HG22	2.59	0.42
1:A:3185:SER:C	1:A:3187:THR:N	2.72	0.42
1:H:2230:ALA:HA	1:H:2239:GLY:O	2.19	0.42
1:E:2229:GLY:O	1:E:2230:ALA:CB	2.66	0.42
1:C:3090:CYS:SG	1:C:3140:VAL:CG1	3.07	0.42
1:F:3140:VAL:HG23	1:F:3188:LEU:HB3	2.01	0.42
1:F:3056:LEU:CD1	1:F:3190:ILE:HD11	2.48	0.42
1:D:3056:LEU:CD1	1:D:3190:ILE:HD11	2.49	0.42
1:A:1090:CYS:O	1:A:1114:LEU:HD22	2.20	0.42
1:F:231:VAL:HB	1:F:239:GLY:HA3	2.00	0.42
1:F:107:LEU:HD23	1:F:267:GLY:HA3	2.01	0.42
1:A:1064:ILE:HG23	1:A:1223:LEU:HB3	2.00	0.42
1:B:3271:TYR:O	1:B:3275:VAL:HG23	2.19	0.42
1:G:3040:ILE:O	1:G:3055:GLY:HA3	2.18	0.42
1:D:125:ALA:C	1:D:127:GLU:H	2.21	0.42
1:H:171:MET:O	1:H:175:MET:HB2	2.19	0.42
1:B:173:GLN:HB3	1:B:174:ALA:H	1.68	0.42
1:B:3040:ILE:O	1:B:3055:GLY:HA3	2.19	0.42
1:E:71:GLY:HA2	3:E:400:ANP:H5'1	2.01	0.42
1:E:2253:ALA:HA	1:E:2254:PRO:HD3	1.83	0.42
1:B:2301:GLY:O	1:B:2302:LYS:C	2.57	0.42
1:A:1161:ASP:HB3	1:A:1166:LEU:CD1	2.49	0.42
1:A:1170:MET:O	1:A:1170:MET:HG2	2.17	0.42
1:G:3077:LEU:HG	1:G:3080:ILE:HD12	2.00	0.42
1:A:2128:ILE:HG22	1:A:2132:LEU:CD1	2.49	0.42
1:H:156:GLU:HG3	1:H:1176:ARG:CG	2.49	0.42
1:B:231:VAL:HB	1:B:239:GLY:HA3	2.01	0.42
1:C:2090:CYS:CB	1:C:2140:VAL:HG13	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2229:GLY:O	1:B:2230:ALA:CB	2.65	0.42
1:A:92:PHE:O	1:A:116:CYS:HA	2.18	0.42
1:E:1155:ILE:HG22	1:E:1156:GLU:OE2	2.19	0.42
1:H:2218:TYR:HD2	1:H:2218:TYR:HA	1.73	0.42
1:C:2065:TYR:C	1:C:2065:TYR:CD1	2.92	0.42
1:D:3246:VAL:HG12	1:D:3246:VAL:O	2.19	0.42
1:H:2227:ARG:HG3	1:H:2240:SER:HB3	1.99	0.42
1:G:3293:TYR:O	1:G:3296:GLU:HB2	2.19	0.42
1:C:3269:ASN:O	1:C:3272:GLY:N	2.52	0.42
1:D:3281:GLU:O	1:D:3283:LEU:N	2.52	0.42
1:D:2253:ALA:HA	1:D:2254:PRO:HD3	1.83	0.42
1:H:268:ILE:HG22	1:H:269:ASN:N	2.33	0.42
1:A:126:LEU:HA	1:A:129:CYS:SG	2.59	0.42
1:D:3293:TYR:O	1:D:3296:GLU:HB2	2.20	0.42
1:F:1018:GLU:OE2	1:F:1024:GLY:HA2	2.19	0.42
1:H:2233:GLU:HG3	1:H:2238:VAL:HG11	2.01	0.42
1:B:2122:GLY:O	1:B:2125:ALA:HB3	2.19	0.42
1:B:2128:ILE:HG22	1:B:2132:LEU:CD1	2.49	0.42
1:H:2063:GLU:HG3	1:H:2215:LEU:HD21	2.01	0.42
1:F:3306:THR:C	1:F:3308:TRP:H	2.23	0.42
1:G:115:LEU:HA	1:G:1027:MET:O	2.19	0.42
1:D:3144:ASP:OD1	1:D:3145:SER:HB2	2.19	0.42
1:C:118:GLN:HE21	1:C:1249:ASN:H	1.67	0.42
1:F:3326:LEU:O	1:F:3327:LEU:HG	2.19	0.42
1:A:2233:GLU:HG3	1:A:2238:VAL:HG11	2.01	0.42
1:G:3051:LEU:HA	1:G:3051:LEU:HD23	1.85	0.42
1:B:2233:GLU:HG3	1:B:2238:VAL:HG11	2.01	0.42
1:F:1253:ALA:HA	1:F:1254:PRO:HD3	1.90	0.42
1:C:1048:ASP:HB3	1:C:1054:GLY:HA2	2.01	0.42
1:H:2275:VAL:HG21	1:H:2306:THR:HA	2.01	0.42
1:G:3269:ASN:O	1:G:3272:GLY:N	2.52	0.42
1:D:253:ALA:HA	1:D:254:PRO:HD3	1.94	0.42
1:A:1123:GLU:HG3	1:A:1170:MET:HG3	2.02	0.42
1:A:3253:ALA:HA	1:A:3254:PRO:HD3	1.78	0.42
1:C:2230:ALA:HA	1:C:2239:GLY:O	2.18	0.42
1:F:3056:LEU:HD12	1:F:3190:ILE:HD11	2.01	0.42
1:H:92:PHE:CE2	1:H:94:ASP:HB2	2.55	0.42
1:H:3065:TYR:O	1:H:3065:TYR:HD2	2.01	0.42
1:E:3268:ILE:HG22	1:E:3269:ASN:N	2.35	0.42
1:E:3269:ASN:O	1:E:3272:GLY:N	2.53	0.42
1:A:3171:MET:C	1:A:3173:GLN:H	2.23	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3051:LEU:HA	1:D:3051:LEU:HD23	1.86	0.42
1:E:2100:ASP:HA	1:E:2101:PRO:HD2	1.92	0.42
1:F:1072:LYS:HB3	1:F:1225:ILE:HG21	2.01	0.42
1:A:1066:GLY:O	1:A:1067:PRO:C	2.58	0.42
1:D:100:ASP:HB3	1:D:103:TYR:HB3	2.01	0.42
1:H:3077:LEU:HG	1:H:3080:ILE:HD12	2.02	0.42
1:G:1145:SER:HB2	1:G:1192:ILE:HB	2.02	0.42
1:D:1090:CYS:SG	1:D:1140:VAL:HG22	2.59	0.42
1:F:3185:SER:C	1:F:3187:THR:N	2.70	0.42
1:B:2230:ALA:HA	1:B:2239:GLY:O	2.20	0.42
1:C:76:THR:O	1:C:79:VAL:HG22	2.19	0.42
1:A:3101:PRO:O	1:A:3104:ALA:HB3	2.20	0.42
1:G:101:PRO:HG3	1:G:1255:PHE:O	2.19	0.42
1:D:2254:PRO:HB2	1:D:2255:PHE:CD2	2.55	0.42
1:D:2029:LEU:HD23	1:D:2254:PRO:HD2	2.01	0.42
1:C:2223:LEU:HD12	1:C:2223:LEU:HA	1.86	0.42
1:A:3075:LEU:O	1:A:3075:LEU:HD23	2.20	0.42
1:D:1018:GLU:OE2	1:D:1024:GLY:HA2	2.19	0.42
1:B:3123:GLU:O	1:B:3124:GLN:C	2.57	0.42
1:F:100:ASP:HB3	1:F:103:TYR:HB3	2.01	0.42
1:C:2287:ALA:HB3	1:C:2290:TRP:HB2	2.00	0.42
1:E:3299:GLY:HA2	1:H:1300:GLN:HE22	1.85	0.42
1:A:1193:ASN:ND2	1:A:1209:THR:CA	2.83	0.42
1:E:2300:GLN:OE1	1:H:2304:ASN:HB3	2.20	0.42
1:H:1123:GLU:HG3	1:H:1170:MET:HG3	2.02	0.42
1:H:97:HIS:NE2	1:H:1248:LYS:HG3	2.34	0.42
1:A:2125:ALA:HA	1:A:2128:ILE:HD12	2.02	0.42
1:F:2063:GLU:HG3	1:F:2215:LEU:HD21	2.01	0.42
1:D:3029:LEU:CD2	1:D:3254:PRO:HD2	2.47	0.42
1:A:3029:LEU:CD2	1:A:3254:PRO:HD2	2.49	0.42
1:D:3090:CYS:SG	1:D:3140:VAL:CG1	3.08	0.42
1:E:3140:VAL:HG23	1:E:3188:LEU:HB3	2.02	0.42
1:G:76:THR:O	1:G:79:VAL:HG22	2.19	0.42
1:A:231:VAL:HB	1:A:239:GLY:HA3	2.01	0.42
1:E:3311:ASP:OD2	1:F:286:LYS:NZ	2.53	0.42
1:E:3224:ASP:O	1:E:3244:VAL:HA	2.20	0.42
1:C:3224:ASP:O	1:C:3244:VAL:HA	2.19	0.42
1:B:2264:TYR:CD2	1:B:2264:TYR:N	2.88	0.42
1:C:3145:SER:C	1:C:3147:ALA:N	2.69	0.42
1:A:2064:ILE:O	1:A:2192:ILE:HA	2.19	0.42
1:D:3271:TYR:O	1:D:3275:VAL:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:253:ALA:HA	1:H:254:PRO:HD3	1.94	0.42
1:E:126:LEU:HA	1:E:129:CYS:SG	2.60	0.42
1:A:1208:THR:HG21	1:A:1222:ARG:NH2	2.35	0.42
1:D:3044:SER:HA	1:D:3273:GLU:OE1	2.20	0.42
1:H:76:THR:O	1:H:79:VAL:HG22	2.20	0.42
1:G:3171:MET:C	1:G:3173:GLN:H	2.22	0.42
1:B:3109:VAL:HG12	1:B:3110:ASP:N	2.35	0.42
1:H:2065:TYR:CD1	1:H:2065:TYR:C	2.94	0.42
1:E:3123:GLU:O	1:E:3124:GLN:C	2.58	0.42
1:C:1018:GLU:OE2	1:C:1024:GLY:HA2	2.19	0.42
1:F:3132:LEU:HA	1:F:3135:SER:HB2	2.02	0.42
1:F:1123:GLU:HG3	1:F:1170:MET:HG3	2.01	0.42
1:E:3218:TYR:HD2	1:E:3218:TYR:HA	1.66	0.42
1:A:1219:ALA:O	1:A:1248:LYS:NZ	2.45	0.42
1:G:114:LEU:HA	1:G:114:LEU:HD22	1.92	0.42
1:D:2073:THR:HA	1:D:2076:THR:HB	2.02	0.42
1:B:3090:CYS:SG	1:B:3140:VAL:CG1	3.08	0.42
1:A:2218:TYR:HA	1:A:2218:TYR:HD2	1.74	0.42
1:C:1324:ARG:HA	1:C:1328:LEU:HD13	2.02	0.42
1:E:3327:LEU:O	1:E:3328:LEU:HD12	2.20	0.42
1:C:1072:LYS:HB3	1:C:1225:ILE:HG21	2.00	0.42
1:B:3232:LYS:HZ2	1:C:1235:GLU:HG2	1.84	0.42
1:B:3077:LEU:HG	1:B:3080:ILE:HD12	2.02	0.42
1:E:2118:GLN:NE2	1:E:3249:ASN:H	2.13	0.42
1:H:118:GLN:NE2	1:H:1249:ASN:H	2.17	0.42
1:A:1090:CYS:SG	1:A:1140:VAL:HG22	2.60	0.42
1:D:92:PHE:CE2	1:D:94:ASP:HB2	2.54	0.42
1:F:92:PHE:CE2	1:F:94:ASP:HB2	2.55	0.42
1:A:3306:THR:C	1:A:3308:TRP:H	2.22	0.42
1:B:92:PHE:CE2	1:B:94:ASP:HB2	2.55	0.42
1:A:107:LEU:HD23	1:A:267:GLY:HA3	2.01	0.42
1:F:75:LEU:HD23	1:F:75:LEU:C	2.40	0.42
1:F:2065:TYR:HD1	1:F:2065:TYR:O	2.03	0.42
1:E:2275:VAL:HG21	1:E:2306:THR:HA	2.02	0.42
1:F:3051:LEU:HA	1:F:3051:LEU:HD23	1.88	0.42
1:E:111:ILE:HA	1:E:111:ILE:HD13	1.90	0.42
1:D:3232:LYS:HA	1:D:3236:ASN:O	2.20	0.42
1:F:157:GLY:O	1:F:158:GLU:O	2.38	0.42
1:H:3092:PHE:CE2	1:H:3099:LEU:HD22	2.55	0.42
1:E:173:GLN:HB3	1:E:174:ALA:H	1.68	0.42
1:H:126:LEU:HA	1:H:129:CYS:SG	2.60	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3040:ILE:O	1:F:3055:GLY:HA3	2.20	0.42
1:H:3123:GLU:O	1:H:3124:GLN:C	2.57	0.42
1:H:66:GLY:O	1:H:72:LYS:HE2	2.19	0.42
1:H:72:LYS:HB2	1:H:72:LYS:HE3	1.74	0.42
1:C:2014:LEU:C	1:C:2016:GLN:H	2.22	0.42
1:H:150:THR:OG1	1:H:1217:PHE:CE2	2.72	0.41
1:F:1219:ALA:O	1:F:1248:LYS:NZ	2.45	0.41
1:C:2073:THR:HA	1:C:2076:THR:HB	2.02	0.41
1:A:92:PHE:CE2	1:A:94:ASP:HB2	2.54	0.41
1:F:2229:GLY:O	1:F:2230:ALA:CB	2.65	0.41
1:A:2230:ALA:HA	1:A:2239:GLY:O	2.20	0.41
1:E:231:VAL:HB	1:E:239:GLY:HA3	2.02	0.41
1:A:76:THR:O	1:A:79:VAL:HG22	2.20	0.41
1:G:1090:CYS:O	1:G:1114:LEU:HD22	2.19	0.41
1:C:92:PHE:CE2	1:C:94:ASP:HB2	2.55	0.41
1:G:107:LEU:HD23	1:G:267:GLY:HA3	2.01	0.41
1:C:107:LEU:HD23	1:C:267:GLY:HA3	2.01	0.41
1:B:65:TYR:HD2	1:B:223:LEU:O	2.03	0.41
1:D:66:GLY:O	1:D:72:LYS:HE2	2.20	0.41
1:D:1324:ARG:HA	1:D:1328:LEU:HD13	2.01	0.41
1:B:66:GLY:O	1:B:72:LYS:HE2	2.20	0.41
1:F:1324:ARG:HA	1:F:1328:LEU:HD13	2.02	0.41
1:H:2305:ALA:O	1:H:2306:THR:C	2.57	0.41
1:E:2305:ALA:O	1:E:2306:THR:C	2.57	0.41
1:G:1066:GLY:O	1:G:1067:PRO:C	2.57	0.41
1:D:3040:ILE:O	1:D:3055:GLY:HA3	2.19	0.41
1:H:173:GLN:HB3	1:H:174:ALA:H	1.66	0.41
1:B:2100:ASP:HA	1:B:2101:PRO:HD2	1.92	0.41
1:F:114:LEU:O	1:F:1028:ARG:HA	2.21	0.41
1:A:1204:GLY:O	1:A:1205:ASN:CB	2.68	0.41
1:G:93:ILE:HB	1:G:143:VAL:HA	2.02	0.41
1:A:2124:GLN:O	1:A:2128:ILE:HG13	2.20	0.41
1:B:1300:GLN:OE1	1:C:3304:ASN:HB3	2.20	0.41
1:B:2140:VAL:HA	1:B:2188:LEU:O	2.20	0.41
1:E:2230:ALA:HA	1:E:2239:GLY:O	2.20	0.41
1:H:3185:SER:C	1:H:3187:THR:N	2.72	0.41
1:B:3056:LEU:CD1	1:B:3190:ILE:HD11	2.50	0.41
1:F:2300:GLN:H	1:G:2300:GLN:HE22	1.67	0.41
1:A:3144:ASP:OD1	1:A:3145:SER:HB2	2.20	0.41
1:A:2254:PRO:HB2	1:A:2255:PHE:CD2	2.55	0.41
1:D:2111:ILE:HD13	1:D:2111:ILE:HA	1.74	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1072:LYS:HB3	1:G:1225:ILE:HG21	2.01	0.41
1:A:1048:ASP:HB3	1:A:1054:GLY:HA2	2.01	0.41
1:B:1133:ALA:C	1:B:1135:SER:H	2.24	0.41
1:B:1072:LYS:HB3	1:B:1225:ILE:HG21	2.02	0.41
1:F:2233:GLU:HG3	1:F:2238:VAL:HG11	2.01	0.41
1:A:1193:ASN:ND2	1:A:1209:THR:C	2.74	0.41
1:H:1170:MET:O	1:H:1170:MET:HG2	2.18	0.41
1:H:97:HIS:HB3	1:H:1247:VAL:HB	2.01	0.41
1:G:1123:GLU:HG3	1:G:1170:MET:HG3	2.02	0.41
1:H:3218:TYR:HD2	1:H:3218:TYR:HA	1.66	0.41
1:F:66:GLY:O	1:F:72:LYS:HE2	2.21	0.41
1:G:3056:LEU:HA	1:G:3057:PRO:HD3	1.68	0.41
1:C:231:VAL:HB	1:C:239:GLY:HA3	2.01	0.41
1:E:3056:LEU:HA	1:E:3057:PRO:HD3	1.69	0.41
1:G:3072:LYS:HD2	1:G:3193:ASN:O	2.20	0.41
1:G:3264:TYR:CE1	3:G:3400:ANP:H1'	2.56	0.41
1:H:1305:ALA:O	1:H:1306:THR:O	2.38	0.41
1:F:3269:ASN:O	1:F:3272:GLY:N	2.52	0.41
1:G:2254:PRO:HB2	1:G:2255:PHE:CD2	2.55	0.41
1:C:2122:GLY:O	1:C:2125:ALA:HB3	2.19	0.41
1:B:3171:MET:C	1:B:3173:GLN:H	2.23	0.41
1:D:2065:TYR:C	1:D:2065:TYR:CD1	2.94	0.41
1:C:2254:PRO:HB2	1:C:2255:PHE:CD2	2.55	0.41
1:F:114:LEU:HD22	1:F:114:LEU:HA	1.93	0.41
1:B:2223:LEU:HA	1:B:2223:LEU:HD12	1.85	0.41
1:G:1133:ALA:C	1:G:1135:SER:H	2.24	0.41
1:G:1048:ASP:HB3	1:G:1054:GLY:HA2	2.02	0.41
1:C:229:GLY:O	1:C:230:ALA:HB2	2.21	0.41
1:D:1048:ASP:HB3	1:D:1054:GLY:HA2	2.00	0.41
1:E:57:PRO:CG	1:E:251:ILE:HG12	2.50	0.41
1:H:2122:GLY:O	1:H:2125:ALA:HB3	2.21	0.41
1:E:3151:PRO:HB3	1:F:3166:LEU:N	2.35	0.41
1:C:3064:ILE:CG1	1:C:3223:LEU:HB2	2.38	0.41
1:C:1123:GLU:HG3	1:C:1170:MET:HG3	2.02	0.41
1:D:3044:SER:HG	1:D:3045:LEU:H	1.66	0.41
1:H:1253:ALA:HA	1:H:1254:PRO:HD3	1.89	0.41
1:H:1090:CYS:O	1:H:1114:LEU:HD22	2.20	0.41
1:F:2140:VAL:HA	1:F:2188:LEU:O	2.19	0.41
1:A:1111:ILE:HG23	1:A:2029:LEU:HD13	2.02	0.41
1:B:107:LEU:HD23	1:B:267:GLY:HA3	2.00	0.41
1:C:2264:TYR:N	1:C:2264:TYR:CD2	2.88	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2264:TYR:CD2	1:G:2264:TYR:N	2.89	0.41
1:G:3274:LEU:O	1:G:3275:VAL:C	2.59	0.41
1:E:66:GLY:O	1:E:72:LYS:HE2	2.21	0.41
1:F:1066:GLY:O	1:F:1067:PRO:C	2.59	0.41
1:F:57:PRO:CG	1:F:251:ILE:HG12	2.50	0.41
1:G:57:PRO:CG	1:G:251:ILE:HG12	2.50	0.41
1:A:3232:LYS:HA	1:A:3236:ASN:O	2.20	0.41
1:E:1123:GLU:HG3	1:E:1170:MET:HG3	2.03	0.41
1:F:71:GLY:N	3:F:400:ANP:C5'	2.84	0.41
1:D:2140:VAL:HA	1:D:2188:LEU:O	2.20	0.41
1:G:3224:ASP:O	1:G:3244:VAL:HA	2.21	0.41
1:B:3065:TYR:O	1:B:3065:TYR:HD2	2.03	0.41
1:E:107:LEU:HD23	1:E:267:GLY:HA3	2.02	0.41
1:H:3144:ASP:OD1	1:H:3145:SER:HB2	2.20	0.41
1:D:1062:VAL:O	1:D:1190:ILE:HA	2.21	0.41
1:G:2065:TYR:C	1:G:2065:TYR:CD1	2.93	0.41
1:E:2254:PRO:HB2	1:E:2255:PHE:CD2	2.56	0.41
1:G:1018:GLU:OE2	1:G:1024:GLY:HA2	2.20	0.41
1:B:111:ILE:HD13	1:B:111:ILE:HA	1.90	0.41
1:C:114:LEU:HD22	1:C:114:LEU:HA	1.92	0.41
1:A:2111:ILE:HA	1:A:2111:ILE:HD13	1.75	0.41
1:H:2254:PRO:HB2	1:H:2255:PHE:CD2	2.55	0.41
1:E:100:ASP:HB3	1:E:103:TYR:HB3	2.02	0.41
1:C:3293:TYR:O	1:C:3296:GLU:HB2	2.21	0.41
1:D:126:LEU:HA	1:D:129:CYS:SG	2.61	0.41
1:A:2301:GLY:O	1:A:2302:LYS:C	2.59	0.41
1:E:1133:ALA:C	1:E:1135:SER:H	2.24	0.41
1:E:1300:GLN:HE22	1:H:3299:GLY:CA	2.26	0.41
1:D:3077:LEU:HG	1:D:3080:ILE:HD12	2.01	0.41
1:H:1219:ALA:O	1:H:1248:LYS:NZ	2.45	0.41
1:A:2122:GLY:O	1:A:2125:ALA:HB3	2.21	0.41
1:D:1146:VAL:CG1	1:D:1211:GLY:HA3	2.50	0.41
1:E:2084:GLN:HG3	1:E:2090:CYS:SG	2.60	0.41
1:B:2057:PRO:O	1:B:2188:LEU:HD13	2.21	0.41
1:B:1305:ALA:O	1:B:1306:THR:O	2.38	0.41
1:D:3109:VAL:HG12	1:D:3110:ASP:N	2.35	0.41
1:F:2300:GLN:NE2	1:G:2300:GLN:H	2.18	0.41
1:E:2264:TYR:N	1:E:2264:TYR:CD2	2.88	0.41
1:E:3042:THR:OG1	1:E:3048:ASP:OD1	2.27	0.41
1:C:75:LEU:HD23	1:C:75:LEU:C	2.40	0.41
1:F:2254:PRO:HB2	1:F:2255:PHE:CD2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1040:ILE:HD13	1:G:1040:ILE:HA	1.92	0.41
1:H:3271:TYR:O	1:H:3275:VAL:HG23	2.20	0.41
1:B:135:SER:OG	1:B:1013:ALA:HB1	2.20	0.41
1:C:3056:LEU:CD1	1:C:3190:ILE:HD11	2.50	0.41
1:H:1173:GLN:C	1:H:1175:MET:H	2.23	0.41
1:C:93:ILE:HG13	1:C:143:VAL:HG13	2.01	0.41
1:C:93:ILE:HB	1:C:143:VAL:HA	2.03	0.41
1:C:141:ILE:HB	1:C:189:LEU:HG	2.03	0.41
1:A:2063:GLU:HG3	1:A:2215:LEU:HD21	2.01	0.41
1:B:1300:GLN:HE22	1:C:3300:GLN:H	1.66	0.41
1:E:1090:CYS:O	1:E:1114:LEU:HD22	2.20	0.41
1:E:2090:CYS:CB	1:E:2140:VAL:HG13	2.48	0.41
1:D:107:LEU:HD23	1:D:267:GLY:HA3	2.01	0.41
1:F:2300:GLN:HE21	1:G:2300:GLN:HB3	1.85	0.41
1:F:2264:TYR:CD2	1:F:2264:TYR:N	2.88	0.41
1:A:2264:TYR:CD2	1:A:2264:TYR:N	2.89	0.41
1:G:3010:LEU:C	1:G:3012:ALA:H	2.24	0.41
1:F:3144:ASP:OD1	1:F:3145:SER:HB2	2.20	0.41
1:F:1014:LEU:C	1:F:1016:GLN:N	2.74	0.41
1:C:2254:PRO:O	1:C:2255:PHE:HB2	2.21	0.41
1:H:1040:ILE:HA	1:H:1040:ILE:HD13	1.91	0.41
1:F:224:ASP:HB3	1:F:245:LYS:HB3	2.02	0.41
1:E:2014:LEU:C	1:E:2016:GLN:H	2.24	0.41
1:A:229:GLY:O	1:A:230:ALA:HB2	2.21	0.41
1:A:3269:ASN:O	1:A:3272:GLY:N	2.53	0.41
1:G:3313:PRO:O	1:G:3316:ALA:HB3	2.20	0.41
1:B:57:PRO:CG	1:B:251:ILE:HG12	2.51	0.41
1:E:3293:TYR:O	1:E:3296:GLU:HB2	2.21	0.41
1:E:3105:ARG:HH11	1:F:227:ARG:HH22	1.69	0.41
1:B:93:ILE:HG13	1:B:143:VAL:HG13	2.02	0.41
1:H:141:ILE:HB	1:H:189:LEU:HG	2.03	0.41
1:C:1090:CYS:O	1:C:1114:LEU:HD22	2.21	0.41
1:E:76:THR:O	1:E:79:VAL:HG22	2.21	0.41
1:F:1097:HIS:NE2	1:F:2248:LYS:HG3	2.36	0.41
1:C:3144:ASP:OD1	1:C:3145:SER:HB2	2.21	0.41
1:E:3171:MET:C	1:E:3173:GLN:H	2.22	0.41
1:C:3010:LEU:C	1:C:3012:ALA:H	2.24	0.41
1:A:3327:LEU:O	1:A:3328:LEU:HD12	2.20	0.41
1:A:3274:LEU:O	1:A:3275:VAL:C	2.59	0.41
1:D:2122:GLY:O	1:D:2125:ALA:HB3	2.21	0.41
1:B:2142:VAL:HG22	1:B:2190:ILE:HB	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:PRO:CG	1:C:251:ILE:HG12	2.51	0.41
1:C:2301:GLY:O	1:C:2302:LYS:C	2.59	0.41
1:A:100:ASP:HB3	1:A:103:TYR:HB3	2.02	0.41
1:D:3076:THR:O	1:D:3080:ILE:HG13	2.20	0.41
1:G:3044:SER:HB3	1:G:3047:LEU:HB2	2.03	0.41
1:E:2073:THR:HA	1:E:2076:THR:HB	2.03	0.41
1:G:231:VAL:HB	1:G:239:GLY:HA3	2.01	0.41
1:E:3185:SER:C	1:E:3187:THR:N	2.72	0.41
1:H:3090:CYS:SG	1:H:3140:VAL:HG12	2.61	0.41
1:G:1090:CYS:SG	1:G:1140:VAL:HG22	2.60	0.41
1:E:3056:LEU:CD1	1:E:3190:ILE:HD11	2.51	0.41
1:A:3306:THR:C	1:A:3308:TRP:N	2.75	0.41
1:C:3306:THR:C	1:C:3308:TRP:H	2.24	0.41
1:C:2122:GLY:O	1:C:2123:GLU:C	2.59	0.41
1:C:2125:ALA:HA	1:C:2128:ILE:HD12	2.03	0.41
1:D:2264:TYR:N	1:D:2264:TYR:CD2	2.88	0.41
1:C:99:LEU:HD23	1:C:1255:PHE:CZ	2.56	0.41
1:H:75:LEU:C	1:H:75:LEU:HD23	2.41	0.41
1:A:2065:TYR:C	1:A:2065:TYR:CD1	2.93	0.41
1:A:75:LEU:HD23	1:A:75:LEU:C	2.42	0.41
1:F:3010:LEU:C	1:F:3012:ALA:H	2.25	0.41
1:E:158:GLU:O	1:E:159:ILE:O	2.39	0.41
1:C:3274:LEU:O	1:C:3275:VAL:C	2.59	0.41
1:B:2275:VAL:HG21	1:B:2306:THR:HA	2.02	0.41
1:C:3327:LEU:O	1:C:3328:LEU:HD12	2.20	0.41
1:G:2072:LYS:HE3	1:G:2193:ASN:O	2.20	0.41
1:G:2072:LYS:HE2	1:G:2192:ILE:HG22	2.03	0.41
1:E:3232:LYS:HA	1:E:3236:ASN:O	2.21	0.41
1:B:3274:LEU:O	1:B:3275:VAL:C	2.59	0.41
1:B:1006:LYS:HG3	1:B:1007:GLN:H	1.86	0.41
1:E:2111:ILE:HA	1:E:2111:ILE:HD13	1.74	0.41
1:C:1006:LYS:HG3	1:C:1007:GLN:H	1.86	0.41
1:A:71:GLY:HA2	3:A:400:ANP:H5'1	2.03	0.41
1:A:66:GLY:O	1:A:72:LYS:HE2	2.20	0.41
1:A:2057:PRO:O	1:A:2188:LEU:HD13	2.21	0.41
1:H:144:ASP:HA	1:H:145:SER:HA	1.84	0.41
1:A:57:PRO:CG	1:A:251:ILE:HG12	2.50	0.41
1:E:1006:LYS:HG3	1:E:1007:GLN:H	1.86	0.41
1:F:3232:LYS:HA	1:F:3236:ASN:O	2.20	0.41
1:A:178:LEU:O	1:A:182:LEU:HG	2.21	0.41
1:C:1064:ILE:HG23	1:C:1223:LEU:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:178:LEU:O	1:H:182:LEU:HG	2.21	0.41
1:H:3232:LYS:HA	1:H:3236:ASN:O	2.20	0.41
1:D:57:PRO:CG	1:D:251:ILE:HG12	2.51	0.41
1:E:1111:ILE:HA	1:E:1111:ILE:HD13	1.81	0.41
1:G:3246:VAL:HG12	1:G:3246:VAL:O	2.20	0.41
1:G:224:ASP:HB3	1:G:245:LYS:HB3	2.03	0.41
1:H:1133:ALA:C	1:H:1135:SER:H	2.23	0.41
1:H:224:ASP:HB3	1:H:245:LYS:HB3	2.03	0.41
1:B:2014:LEU:C	1:B:2016:GLN:H	2.23	0.41
1:B:93:ILE:HB	1:B:143:VAL:HA	2.03	0.41
1:D:93:ILE:HG13	1:D:143:VAL:HG13	2.03	0.41
1:D:141:ILE:HB	1:D:189:LEU:HG	2.03	0.41
1:D:1090:CYS:O	1:D:1114:LEU:HD22	2.20	0.41
1:E:2140:VAL:HA	1:E:2188:LEU:O	2.21	0.41
1:B:1090:CYS:O	1:B:1114:LEU:HD22	2.21	0.41
1:F:2073:THR:HA	1:F:2076:THR:HB	2.03	0.41
1:G:3327:LEU:O	1:G:3328:LEU:HD12	2.21	0.41
1:G:118:GLN:HE21	1:G:1249:ASN:H	1.68	0.41
1:B:2065:TYR:C	1:B:2065:TYR:HD1	2.24	0.41
1:A:3010:LEU:C	1:A:3012:ALA:H	2.24	0.41
1:C:3075:LEU:HD23	1:C:3075:LEU:O	2.21	0.41
1:B:1040:ILE:HD13	1:B:1040:ILE:HA	1.92	0.41
1:F:111:ILE:HA	1:F:111:ILE:HD13	1.88	0.41
1:E:1040:ILE:HA	1:E:1040:ILE:HD13	1.93	0.41
1:E:1066:GLY:O	1:E:1067:PRO:C	2.59	0.41
1:F:229:GLY:O	1:F:230:ALA:HB2	2.21	0.41
1:H:3313:PRO:O	1:H:3316:ALA:HB3	2.21	0.41
1:E:2142:VAL:HG22	1:E:2190:ILE:HB	2.04	0.41
1:E:1219:ALA:O	1:E:1248:LYS:NZ	2.45	0.40
1:A:3151:PRO:HG2	1:B:3151:PRO:CG	2.45	0.40
1:B:76:THR:O	1:B:79:VAL:HG22	2.21	0.40
1:H:2308:TRP:CE3	1:H:2309:LEU:HD23	2.56	0.40
1:F:2091:ALA:HA	1:F:2115:LEU:HB2	2.02	0.40
1:C:3171:MET:C	1:C:3173:GLN:H	2.23	0.40
1:E:75:LEU:HD23	1:E:75:LEU:C	2.42	0.40
1:F:2254:PRO:O	1:F:2255:PHE:HB2	2.20	0.40
1:H:2072:LYS:HE2	1:H:2192:ILE:HG22	2.03	0.40
1:E:1062:VAL:O	1:E:1190:ILE:HA	2.21	0.40
1:F:2125:ALA:HA	1:F:2128:ILE:HD12	2.03	0.40
1:D:2301:GLY:O	1:D:2302:LYS:C	2.60	0.40
1:B:3284:ILE:HG23	1:B:3292:SER:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1133:ALA:C	1:C:1135:SER:H	2.24	0.40
1:H:100:ASP:HB3	1:H:103:TYR:HB3	2.02	0.40
1:C:144:ASP:HA	1:C:145:SER:HA	1.81	0.40
1:D:1133:ALA:C	1:D:1135:SER:H	2.24	0.40
1:G:2301:GLY:O	1:G:2302:LYS:C	2.59	0.40
1:C:178:LEU:O	1:C:182:LEU:HG	2.22	0.40
1:E:1063:GLU:OE1	1:E:1222:ARG:HD3	2.22	0.40
1:D:1123:GLU:HG3	1:D:1170:MET:HG3	2.02	0.40
1:H:1145:SER:HB2	1:H:1192:ILE:HB	2.03	0.40
1:F:1145:SER:HB2	1:F:1192:ILE:HB	2.02	0.40
1:H:1090:CYS:SG	1:H:1140:VAL:HG22	2.61	0.40
1:G:2090:CYS:CB	1:G:2140:VAL:HG13	2.47	0.40
1:B:2084:GLN:HG3	1:B:2090:CYS:SG	2.61	0.40
1:G:3056:LEU:CD1	1:G:3190:ILE:HD11	2.51	0.40
1:D:76:THR:O	1:D:79:VAL:HG22	2.20	0.40
1:H:1056:LEU:HA	1:H:1057:PRO:HD2	1.80	0.40
1:F:2218:TYR:HD2	1:F:2218:TYR:HA	1.73	0.40
1:D:2064:ILE:HG12	1:D:2223:LEU:HB2	2.03	0.40
1:E:2065:TYR:CD1	1:E:2065:TYR:C	2.94	0.40
1:E:3010:LEU:C	1:E:3012:ALA:H	2.25	0.40
1:H:65:TYR:HD2	1:H:223:LEU:O	2.04	0.40
1:C:2065:TYR:O	1:C:2065:TYR:HD1	2.03	0.40
1:H:2064:ILE:HG12	1:H:2223:LEU:HB2	2.03	0.40
1:G:2125:ALA:HA	1:G:2128:ILE:HD12	2.04	0.40
1:C:3269:ASN:O	1:C:3270:PHE:C	2.60	0.40
1:G:112:ASP:HA	1:G:1030:GLY:H	1.86	0.40
1:F:135:SER:OG	1:F:1013:ALA:HB1	2.21	0.40
1:C:3232:LYS:HA	1:C:3236:ASN:O	2.21	0.40
1:E:224:ASP:HB3	1:E:245:LYS:HB3	2.04	0.40
1:E:2223:LEU:HD12	1:E:2223:LEU:HA	1.85	0.40
1:D:1173:GLN:C	1:D:1175:MET:H	2.25	0.40
1:H:57:PRO:CG	1:H:251:ILE:HG12	2.51	0.40
1:D:224:ASP:HB3	1:D:245:LYS:HB3	2.03	0.40
1:H:3056:LEU:CD1	1:H:3190:ILE:HD11	2.52	0.40
1:E:1300:GLN:N	1:H:3300:GLN:HE22	2.11	0.40
1:F:90:CYS:HG	1:F:140:VAL:HG13	1.84	0.40
1:A:141:ILE:HB	1:A:189:LEU:HG	2.03	0.40
1:E:92:PHE:CE2	1:E:94:ASP:HB2	2.56	0.40
1:F:161:ASP:H	1:F:163:HIS:N	2.19	0.40
1:F:1090:CYS:SG	1:F:1140:VAL:HG22	2.61	0.40
1:C:2140:VAL:HA	1:C:2188:LEU:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2084:GLN:HG3	1:F:2090:CYS:SG	2.61	0.40
1:E:112:ASP:HA	1:E:1030:GLY:CA	2.51	0.40
1:F:2122:GLY:O	1:F:2123:GLU:C	2.58	0.40
1:B:1062:VAL:O	1:B:1190:ILE:HA	2.21	0.40
1:H:1014:LEU:C	1:H:1016:GLN:N	2.75	0.40
1:B:3232:LYS:HA	1:B:3236:ASN:O	2.20	0.40
1:F:1066:GLY:HA2	1:F:1067:PRO:HD2	1.89	0.40
1:G:2223:LEU:HD12	1:G:2223:LEU:HA	1.86	0.40
1:B:3246:VAL:HG12	1:B:3246:VAL:O	2.21	0.40
1:G:1150:THR:HA	1:G:1151:PRO:HD3	1.60	0.40
1:D:1100:ASP:HA	1:D:1101:PRO:HD2	1.98	0.40
1:F:2014:LEU:C	1:F:2016:GLN:H	2.24	0.40
1:A:1072:LYS:HB3	1:A:1225:ILE:HG21	2.04	0.40
1:D:3132:LEU:HA	1:D:3135:SER:HB2	2.01	0.40
1:A:2014:LEU:C	1:A:2016:GLN:H	2.24	0.40
1:G:3232:LYS:HA	1:G:3236:ASN:O	2.21	0.40
1:G:2142:VAL:HG22	1:G:2190:ILE:HB	2.03	0.40
1:A:1074:THR:N	3:A:1400:ANP:O1A	2.50	0.40
1:H:1114:LEU:HD12	1:H:2029:LEU:CD1	2.52	0.40
1:F:1090:CYS:O	1:F:1114:LEU:HD22	2.21	0.40
1:F:76:THR:O	1:F:79:VAL:HG22	2.20	0.40
1:E:3306:THR:C	1:E:3308:TRP:H	2.25	0.40
1:H:3171:MET:C	1:H:3173:GLN:H	2.23	0.40
1:H:2264:TYR:CD2	1:H:2264:TYR:N	2.89	0.40
1:C:1254:PRO:HB2	1:C:1255:PHE:CD2	2.57	0.40
1:H:111:ILE:HD13	1:H:111:ILE:HA	1.87	0.40
1:H:2057:PRO:O	1:H:2188:LEU:HD13	2.22	0.40
1:A:3284:ILE:HG23	1:A:3292:SER:O	2.22	0.40
1:D:2142:VAL:HG22	1:D:2190:ILE:HB	2.03	0.40
1:H:2301:GLY:O	1:H:2302:LYS:C	2.60	0.40
1:A:2122:GLY:O	1:A:2123:GLU:C	2.59	0.40
1:A:3077:LEU:HG	1:A:3080:ILE:HD12	2.03	0.40
1:G:2073:THR:HA	1:G:2076:THR:HB	2.02	0.40
1:G:92:PHE:CE2	1:G:94:ASP:HB2	2.56	0.40
1:G:3220:SER:O	1:G:3221:VAL:HG23	2.22	0.40
1:E:3274:LEU:O	1:E:3275:VAL:C	2.60	0.40
1:G:2275:VAL:HG21	1:G:2306:THR:HA	2.03	0.40
1:E:2125:ALA:HA	1:E:2128:ILE:HD12	2.03	0.40
1:B:2125:ALA:HA	1:B:2128:ILE:HD12	2.04	0.40
1:F:3075:LEU:O	1:F:3075:LEU:HD23	2.21	0.40
1:E:2103:TYR:HE1	1:E:2265:GLY:H	1.70	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LEU:HA	1:B:129:CYS:SG	2.61	0.40
1:D:1006:LYS:HG3	1:D:1007:GLN:H	1.86	0.40
1:C:135:SER:OG	1:C:1013:ALA:HB1	2.21	0.40
1:A:1173:GLN:C	1:A:1175:MET:H	2.25	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1161:ASP:OD1	1:C:1314:GLU:OE2[4_456]	2.05	0.15

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	A	1172/1357 (86%)	923 (79%)	191 (16%)	58 (5%)	3	32
1	B	1139/1357 (84%)	915 (80%)	172 (15%)	52 (5%)	3	33
1	C	1155/1357 (85%)	919 (80%)	178 (15%)	58 (5%)	3	31
1	D	1155/1357 (85%)	923 (80%)	179 (16%)	53 (5%)	3	33
1	E	1141/1357 (84%)	910 (80%)	178 (16%)	53 (5%)	3	33
1	F	1155/1357 (85%)	913 (79%)	188 (16%)	54 (5%)	3	33
1	G	1145/1357 (84%)	914 (80%)	179 (16%)	52 (4%)	3	34
1	H	1151/1357 (85%)	914 (79%)	180 (16%)	57 (5%)	3	31
All	All	9213/10856 (85%)	7331 (80%)	1445 (16%)	437 (5%)	3	33

All (437) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	99	LEU
1	A	238	VAL
1	A	1099	LEU
1	A	1146	VAL
1	A	1173	GLN
1	A	1203	PHE
1	A	1282	LYS
1	A	2099	LEU
1	A	2173	GLN
1	A	3033	ARG
1	A	3099	LEU
1	A	3213	ASN
1	A	3214	ALA
1	A	3230	ALA
1	B	88	LYS
1	B	99	LEU
1	B	157	GLY
1	B	163	HIS
1	B	238	VAL
1	B	1099	LEU
1	B	1146	VAL
1	B	1173	GLN
1	B	1282	LYS
1	B	2099	LEU
1	B	2173	GLN
1	B	3033	ARG
1	B	3099	LEU
1	B	3213	ASN
1	B	3214	ALA
1	B	3230	ALA
1	C	88	LYS
1	C	99	LEU
1	C	238	VAL
1	C	1099	LEU
1	C	1146	VAL
1	C	1173	GLN
1	C	1282	LYS
1	C	2099	LEU
1	C	2173	GLN
1	C	3033	ARG
1	C	3099	LEU
1	C	3213	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	3214	ALA
1	C	3230	ALA
1	D	88	LYS
1	D	99	LEU
1	D	159	ILE
1	D	238	VAL
1	D	1099	LEU
1	D	1146	VAL
1	D	1159	ILE
1	D	1173	GLN
1	D	1282	LYS
1	D	2099	LEU
1	D	2173	GLN
1	D	3033	ARG
1	D	3099	LEU
1	D	3213	ASN
1	D	3214	ALA
1	D	3230	ALA
1	E	88	LYS
1	E	99	LEU
1	E	158	GLU
1	E	163	HIS
1	E	238	VAL
1	E	1099	LEU
1	E	1146	VAL
1	E	1173	GLN
1	E	1282	LYS
1	E	2099	LEU
1	E	2173	GLN
1	E	3033	ARG
1	E	3099	LEU
1	E	3213	ASN
1	E	3214	ALA
1	E	3230	ALA
1	F	88	LYS
1	F	99	LEU
1	F	158	GLU
1	F	238	VAL
1	F	1099	LEU
1	F	1146	VAL
1	F	1159	ILE
1	F	1161	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	1173	GLN
1	F	1282	LYS
1	F	2099	LEU
1	F	2173	GLN
1	F	3033	ARG
1	F	3099	LEU
1	F	3213	ASN
1	F	3214	ALA
1	F	3230	ALA
1	G	88	LYS
1	G	99	LEU
1	G	163	HIS
1	G	238	VAL
1	G	1099	LEU
1	G	1146	VAL
1	G	1173	GLN
1	G	1282	LYS
1	G	2099	LEU
1	G	2173	GLN
1	G	3033	ARG
1	G	3099	LEU
1	G	3213	ASN
1	G	3214	ALA
1	G	3230	ALA
1	H	88	LYS
1	H	99	LEU
1	H	238	VAL
1	H	1099	LEU
1	H	1146	VAL
1	H	1163	HIS
1	H	1164	MET
1	H	1173	GLN
1	H	1282	LYS
1	H	2099	LEU
1	H	2173	GLN
1	H	3033	ARG
1	H	3099	LEU
1	H	3213	ASN
1	H	3214	ALA
1	H	3230	ALA
1	A	136	GLY
1	A	173	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1163	HIS
1	A	1167	ALA
1	A	1195	ILE
1	A	2230	ALA
1	A	3282	LYS
1	A	3307	ALA
1	B	136	GLY
1	B	173	GLN
1	B	1167	ALA
1	B	2230	ALA
1	B	3282	LYS
1	B	3306	THR
1	B	3307	ALA
1	C	136	GLY
1	C	159	ILE
1	C	161	ASP
1	C	165	GLY
1	C	173	GLN
1	C	1159	ILE
1	C	1164	MET
1	C	1165	GLY
1	C	1167	ALA
1	C	2230	ALA
1	C	3282	LYS
1	C	3307	ALA
1	D	136	GLY
1	D	173	GLN
1	D	1167	ALA
1	D	2230	ALA
1	D	3282	LYS
1	D	3306	THR
1	D	3307	ALA
1	E	136	GLY
1	E	173	GLN
1	E	1167	ALA
1	E	2230	ALA
1	E	3282	LYS
1	E	3306	THR
1	E	3307	ALA
1	F	136	GLY
1	F	173	GLN
1	F	1164	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	1167	ALA
1	F	2230	ALA
1	F	3282	LYS
1	F	3307	ALA
1	G	136	GLY
1	G	173	GLN
1	G	1167	ALA
1	G	2230	ALA
1	G	3282	LYS
1	G	3307	ALA
1	H	136	GLY
1	H	173	GLN
1	H	1160	GLY
1	H	1167	ALA
1	H	2230	ALA
1	H	3282	LYS
1	H	3306	THR
1	H	3307	ALA
1	A	126	LEU
1	A	264	TYR
1	A	1067	PRO
1	A	1160	GLY
1	A	1162	SER
1	A	2294	LYS
1	A	3011	ALA
1	A	3172	SER
1	A	3186	ASN
1	A	3303	ALA
1	A	3306	THR
1	B	126	LEU
1	B	264	TYR
1	B	1067	PRO
1	B	2294	LYS
1	B	3011	ALA
1	B	3186	ASN
1	B	3303	ALA
1	C	126	LEU
1	C	264	TYR
1	C	1067	PRO
1	C	2294	LYS
1	C	3011	ALA
1	C	3172	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	3186	ASN
1	C	3303	ALA
1	C	3306	THR
1	D	126	LEU
1	D	163	HIS
1	D	264	TYR
1	D	1067	PRO
1	D	1306	THR
1	D	2294	LYS
1	D	3011	ALA
1	D	3186	ASN
1	D	3303	ALA
1	E	126	LEU
1	E	264	TYR
1	E	1067	PRO
1	E	2294	LYS
1	E	3186	ASN
1	E	3303	ALA
1	F	126	LEU
1	F	264	TYR
1	F	1067	PRO
1	F	2294	LYS
1	F	3011	ALA
1	F	3172	SER
1	F	3186	ASN
1	F	3303	ALA
1	F	3306	THR
1	G	126	LEU
1	G	264	TYR
1	G	1067	PRO
1	G	2294	LYS
1	G	3011	ALA
1	G	3172	SER
1	G	3186	ASN
1	G	3303	ALA
1	G	3306	THR
1	H	126	LEU
1	H	264	TYR
1	H	1067	PRO
1	H	1306	THR
1	H	2294	LYS
1	H	3011	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	3172	SER
1	H	3186	ASN
1	H	3303	ALA
1	A	164	MET
1	A	172	SER
1	A	174	ALA
1	A	1205	ASN
1	A	1306	THR
1	A	1320	GLU
1	A	3014	LEU
1	A	3072	LYS
1	A	3167	ALA
1	B	174	ALA
1	B	1306	THR
1	B	3014	LEU
1	B	3072	LYS
1	B	3146	VAL
1	B	3167	ALA
1	B	3172	SER
1	C	172	SER
1	C	174	ALA
1	C	1306	THR
1	C	3014	LEU
1	C	3072	LYS
1	C	3167	ALA
1	D	174	ALA
1	D	1164	MET
1	D	1320	GLU
1	D	3014	LEU
1	D	3072	LYS
1	D	3167	ALA
1	D	3172	SER
1	E	174	ALA
1	E	1306	THR
1	E	1320	GLU
1	E	3011	ALA
1	E	3014	LEU
1	E	3072	LYS
1	E	3167	ALA
1	E	3172	SER
1	F	163	HIS
1	F	172	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	174	ALA
1	F	1306	THR
1	F	1320	GLU
1	F	3014	LEU
1	F	3072	LYS
1	F	3167	ALA
1	G	172	SER
1	G	174	ALA
1	G	1306	THR
1	G	3014	LEU
1	G	3072	LYS
1	G	3167	ALA
1	H	163	HIS
1	H	172	SER
1	H	174	ALA
1	H	1158	GLU
1	H	3014	LEU
1	H	3072	LYS
1	H	3167	ALA
1	A	230	ALA
1	A	1252	ALA
1	A	3146	VAL
1	B	172	SER
1	B	1252	ALA
1	B	1320	GLU
1	B	3088	LYS
1	B	3173	GLN
1	C	118	GLN
1	C	163	HIS
1	C	230	ALA
1	C	1252	ALA
1	C	1320	GLU
1	C	2187	THR
1	C	3146	VAL
1	C	3173	GLN
1	D	118	GLN
1	D	172	SER
1	D	230	ALA
1	D	3146	VAL
1	D	3173	GLN
1	E	118	GLN
1	E	172	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	230	ALA
1	E	1252	ALA
1	E	2187	THR
1	E	3088	LYS
1	E	3146	VAL
1	E	3173	GLN
1	F	118	GLN
1	F	230	ALA
1	G	118	GLN
1	G	158	GLU
1	G	230	ALA
1	G	1252	ALA
1	G	1320	GLU
1	G	2187	THR
1	G	3146	VAL
1	G	3173	GLN
1	H	165	GLY
1	H	230	ALA
1	H	1252	ALA
1	H	1320	GLU
1	H	3088	LYS
1	H	3146	VAL
1	H	3173	GLN
1	A	118	GLN
1	A	2252	ALA
1	A	3088	LYS
1	A	3173	GLN
1	B	118	GLN
1	B	230	ALA
1	B	2187	THR
1	C	2252	ALA
1	C	3088	LYS
1	D	1252	ALA
1	D	2187	THR
1	D	3088	LYS
1	E	2252	ALA
1	F	1252	ALA
1	F	2174	ALA
1	F	3146	VAL
1	F	3173	GLN
1	G	2252	ALA
1	G	3088	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	118	GLN
1	H	1174	ALA
1	H	2252	ALA
1	A	1057	PRO
1	B	1057	PRO
1	C	1155	ILE
1	D	1057	PRO
1	E	1057	PRO
1	E	2026	ILE
1	F	1057	PRO
1	G	1057	PRO
1	H	1057	PRO
1	H	3067	PRO
1	A	212	GLY
1	A	2026	ILE
1	B	212	GLY
1	C	212	GLY
1	C	1057	PRO
1	D	212	GLY
1	D	2026	ILE
1	D	3067	PRO
1	E	212	GLY
1	E	3067	PRO
1	F	212	GLY
1	G	212	GLY
1	G	2026	ILE
1	H	212	GLY
1	A	313	PRO
1	A	3067	PRO
1	B	2026	ILE
1	B	3067	PRO
1	C	313	PRO
1	C	2026	ILE
1	F	159	ILE
1	F	2026	ILE
1	F	3067	PRO
1	H	2026	ILE
1	A	3102	ILE
1	A	3212	GLY
1	B	313	PRO
1	B	3212	GLY
1	C	3067	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	3212	GLY
1	D	313	PRO
1	D	3212	GLY
1	E	313	PRO
1	E	3102	ILE
1	E	3212	GLY
1	F	313	PRO
1	F	3212	GLY
1	G	313	PRO
1	G	3067	PRO
1	G	3212	GLY
1	H	313	PRO
1	H	3102	ILE
1	H	3212	GLY
1	A	1200	GLY
1	B	3102	ILE

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	A	930/1065 (87%)	813 (87%)	117 (13%)	5	31
1	B	908/1065 (85%)	801 (88%)	107 (12%)	6	35
1	C	917/1065 (86%)	805 (88%)	112 (12%)	6	33
1	D	917/1065 (86%)	810 (88%)	107 (12%)	7	35
1	E	910/1065 (85%)	801 (88%)	109 (12%)	6	33
1	F	917/1065 (86%)	812 (88%)	105 (12%)	7	35
1	G	911/1065 (86%)	800 (88%)	111 (12%)	6	33
1	H	916/1065 (86%)	806 (88%)	110 (12%)	6	33
All	All	7326/8520 (86%)	6448 (88%)	878 (12%)	6	33

All (878) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	45	LEU
1	A	65	TYR
1	A	72	LYS
1	A	73	THR
1	A	113	ASN
1	A	114	LEU
1	A	116	CYS
1	A	117	SER
1	A	140	VAL
1	A	143	VAL
1	A	149	LEU
1	A	159	ILE
1	A	163	HIS
1	A	164	MET
1	A	173	GLN
1	A	189	LEU
1	A	194	GLN
1	A	223	LEU
1	A	238	VAL
1	A	277	LEU
1	A	1006	LYS
1	A	1023	LYS
1	A	1033	ARG
1	A	1035	MET
1	A	1036	ASP
1	A	1045	LEU
1	A	1065	TYR
1	A	1070	SER
1	A	1073	THR
1	A	1078	GLN
1	A	1079	VAL
1	A	1116	CYS
1	A	1123	GLU
1	A	1141	ILE
1	A	1149	LEU
1	A	1150	THR
1	A	1152	LYS
1	A	1156	GLU
1	A	1159	ILE
1	A	1161	ASP
1	A	1170	MET
1	A	1173	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1176	ARG
1	A	1192	ILE
1	A	1201	VAL
1	A	1207	GLU
1	A	1210	THR
1	A	1221	VAL
1	A	1231	VAL
1	A	1247	VAL
1	A	1270	PHE
1	A	1277	LEU
1	A	1282	LYS
1	A	1284	ILE
1	A	1296	GLU
1	A	1312	ASN
1	A	1314	GLU
1	A	1317	LYS
1	A	2016	GLN
1	A	2023	LYS
1	A	2025	SER
1	A	2036	ASP
1	A	2045	LEU
1	A	2065	TYR
1	A	2073	THR
1	A	2076	THR
1	A	2078	GLN
1	A	2089	THR
1	A	2090	CYS
1	A	2130	ASP
1	A	2140	VAL
1	A	2149	LEU
1	A	2152	LYS
1	A	2166	LEU
1	A	2223	LEU
1	A	2235	GLU
1	A	2236	ASN
1	A	2247	VAL
1	A	2264	TYR
1	A	2296	GLU
1	A	2311	ASP
1	A	2312	ASN
1	A	2315	THR
1	A	3006	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	3032	ASP
1	A	3036	ASP
1	A	3045	LEU
1	A	3048	ASP
1	A	3065	TYR
1	A	3068	GLU
1	A	3072	LYS
1	A	3077	LEU
1	A	3089	THR
1	A	3099	LEU
1	A	3107	LEU
1	A	3112	ASP
1	A	3114	LEU
1	A	3127	GLU
1	A	3135	SER
1	A	3143	VAL
1	A	3166	LEU
1	A	3173	GLN
1	A	3184	GLN
1	A	3186	ASN
1	A	3189	LEU
1	A	3218	TYR
1	A	3223	LEU
1	A	3236	ASN
1	A	3237	VAL
1	A	3247	VAL
1	A	3254	PRO
1	A	3270	PHE
1	A	3274	LEU
1	A	3296	GLU
1	A	3311	ASP
1	A	3326	LEU
1	B	37	VAL
1	B	45	LEU
1	B	65	TYR
1	B	72	LYS
1	B	73	THR
1	B	113	ASN
1	B	114	LEU
1	B	116	CYS
1	B	117	SER
1	B	140	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	143	VAL
1	B	149	LEU
1	B	156	GLU
1	B	163	HIS
1	B	164	MET
1	B	173	GLN
1	B	189	LEU
1	B	194	GLN
1	B	223	LEU
1	B	238	VAL
1	B	277	LEU
1	B	1006	LYS
1	B	1023	LYS
1	B	1033	ARG
1	B	1035	MET
1	B	1036	ASP
1	B	1045	LEU
1	B	1065	TYR
1	B	1073	THR
1	B	1078	GLN
1	B	1079	VAL
1	B	1116	CYS
1	B	1123	GLU
1	B	1141	ILE
1	B	1149	LEU
1	B	1150	THR
1	B	1152	LYS
1	B	1170	MET
1	B	1173	GLN
1	B	1176	ARG
1	B	1192	ILE
1	B	1221	VAL
1	B	1231	VAL
1	B	1247	VAL
1	B	1270	PHE
1	B	1277	LEU
1	B	1282	LYS
1	B	1284	ILE
1	B	1296	GLU
1	B	1312	ASN
1	B	1314	GLU
1	B	1317	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2016	GLN
1	B	2023	LYS
1	B	2025	SER
1	B	2036	ASP
1	B	2045	LEU
1	B	2065	TYR
1	B	2073	THR
1	B	2076	THR
1	B	2078	GLN
1	B	2089	THR
1	B	2090	CYS
1	B	2130	ASP
1	B	2140	VAL
1	B	2149	LEU
1	B	2152	LYS
1	B	2166	LEU
1	B	2223	LEU
1	B	2235	GLU
1	B	2236	ASN
1	B	2247	VAL
1	B	2264	TYR
1	B	2296	GLU
1	B	2311	ASP
1	B	2312	ASN
1	B	2315	THR
1	B	3006	LYS
1	B	3032	ASP
1	B	3036	ASP
1	B	3045	LEU
1	B	3048	ASP
1	B	3065	TYR
1	B	3068	GLU
1	B	3072	LYS
1	B	3077	LEU
1	B	3099	LEU
1	B	3107	LEU
1	B	3114	LEU
1	B	3127	GLU
1	B	3135	SER
1	B	3143	VAL
1	B	3166	LEU
1	B	3173	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	3184	GLN
1	B	3186	ASN
1	B	3189	LEU
1	B	3223	LEU
1	B	3236	ASN
1	B	3237	VAL
1	B	3247	VAL
1	B	3254	PRO
1	B	3270	PHE
1	B	3274	LEU
1	B	3296	GLU
1	B	3311	ASP
1	B	3326	LEU
1	C	37	VAL
1	C	45	LEU
1	C	65	TYR
1	C	72	LYS
1	C	73	THR
1	C	113	ASN
1	C	114	LEU
1	C	116	CYS
1	C	117	SER
1	C	140	VAL
1	C	143	VAL
1	C	149	LEU
1	C	159	ILE
1	C	162	SER
1	C	164	MET
1	C	173	GLN
1	C	189	LEU
1	C	194	GLN
1	C	223	LEU
1	C	238	VAL
1	C	277	LEU
1	C	1006	LYS
1	C	1023	LYS
1	C	1033	ARG
1	C	1035	MET
1	C	1036	ASP
1	C	1045	LEU
1	C	1065	TYR
1	C	1073	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1078	GLN
1	C	1079	VAL
1	C	1116	CYS
1	C	1123	GLU
1	C	1141	ILE
1	C	1150	THR
1	C	1152	LYS
1	C	1158	GLU
1	C	1159	ILE
1	C	1164	MET
1	C	1170	MET
1	C	1173	GLN
1	C	1176	ARG
1	C	1192	ILE
1	C	1221	VAL
1	C	1231	VAL
1	C	1247	VAL
1	C	1270	PHE
1	C	1277	LEU
1	C	1282	LYS
1	C	1284	ILE
1	C	1296	GLU
1	C	1312	ASN
1	C	1314	GLU
1	C	1317	LYS
1	C	2016	GLN
1	C	2023	LYS
1	C	2025	SER
1	C	2036	ASP
1	C	2045	LEU
1	C	2065	TYR
1	C	2073	THR
1	C	2076	THR
1	C	2078	GLN
1	C	2089	THR
1	C	2090	CYS
1	C	2130	ASP
1	C	2140	VAL
1	C	2149	LEU
1	C	2152	LYS
1	C	2156	GLU
1	C	2166	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	2223	LEU
1	C	2235	GLU
1	C	2236	ASN
1	C	2247	VAL
1	C	2264	TYR
1	C	2296	GLU
1	C	2311	ASP
1	C	2312	ASN
1	C	2315	THR
1	C	3006	LYS
1	C	3032	ASP
1	C	3036	ASP
1	C	3045	LEU
1	C	3048	ASP
1	C	3065	TYR
1	C	3068	GLU
1	C	3072	LYS
1	C	3077	LEU
1	C	3099	LEU
1	C	3107	LEU
1	C	3112	ASP
1	C	3114	LEU
1	C	3127	GLU
1	C	3135	SER
1	C	3143	VAL
1	C	3166	LEU
1	C	3173	GLN
1	C	3184	GLN
1	C	3186	ASN
1	C	3189	LEU
1	C	3218	TYR
1	C	3223	LEU
1	C	3236	ASN
1	C	3237	VAL
1	C	3247	VAL
1	C	3254	PRO
1	C	3270	PHE
1	C	3274	LEU
1	C	3296	GLU
1	C	3311	ASP
1	C	3326	LEU
1	D	37	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	45	LEU
1	D	65	TYR
1	D	72	LYS
1	D	73	THR
1	D	113	ASN
1	D	114	LEU
1	D	116	CYS
1	D	117	SER
1	D	140	VAL
1	D	143	VAL
1	D	149	LEU
1	D	161	ASP
1	D	164	MET
1	D	173	GLN
1	D	189	LEU
1	D	194	GLN
1	D	223	LEU
1	D	238	VAL
1	D	277	LEU
1	D	1006	LYS
1	D	1023	LYS
1	D	1033	ARG
1	D	1035	MET
1	D	1036	ASP
1	D	1045	LEU
1	D	1065	TYR
1	D	1073	THR
1	D	1078	GLN
1	D	1079	VAL
1	D	1116	CYS
1	D	1123	GLU
1	D	1141	ILE
1	D	1149	LEU
1	D	1150	THR
1	D	1152	LYS
1	D	1164	MET
1	D	1170	MET
1	D	1173	GLN
1	D	1176	ARG
1	D	1192	ILE
1	D	1221	VAL
1	D	1231	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1247	VAL
1	D	1270	PHE
1	D	1277	LEU
1	D	1282	LYS
1	D	1284	ILE
1	D	1296	GLU
1	D	1312	ASN
1	D	1314	GLU
1	D	1317	LYS
1	D	2016	GLN
1	D	2023	LYS
1	D	2025	SER
1	D	2036	ASP
1	D	2045	LEU
1	D	2065	TYR
1	D	2073	THR
1	D	2076	THR
1	D	2078	GLN
1	D	2089	THR
1	D	2090	CYS
1	D	2130	ASP
1	D	2140	VAL
1	D	2149	LEU
1	D	2152	LYS
1	D	2166	LEU
1	D	2223	LEU
1	D	2235	GLU
1	D	2236	ASN
1	D	2247	VAL
1	D	2264	TYR
1	D	2296	GLU
1	D	2311	ASP
1	D	2312	ASN
1	D	2315	THR
1	D	3006	LYS
1	D	3032	ASP
1	D	3036	ASP
1	D	3045	LEU
1	D	3048	ASP
1	D	3065	TYR
1	D	3068	GLU
1	D	3072	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	3077	LEU
1	D	3089	THR
1	D	3099	LEU
1	D	3107	LEU
1	D	3114	LEU
1	D	3127	GLU
1	D	3135	SER
1	D	3143	VAL
1	D	3166	LEU
1	D	3173	GLN
1	D	3184	GLN
1	D	3186	ASN
1	D	3189	LEU
1	D	3223	LEU
1	D	3236	ASN
1	D	3237	VAL
1	D	3247	VAL
1	D	3270	PHE
1	D	3274	LEU
1	D	3296	GLU
1	D	3311	ASP
1	D	3326	LEU
1	E	37	VAL
1	E	45	LEU
1	E	65	TYR
1	E	72	LYS
1	E	73	THR
1	E	113	ASN
1	E	114	LEU
1	E	116	CYS
1	E	117	SER
1	E	140	VAL
1	E	143	VAL
1	E	149	LEU
1	E	156	GLU
1	E	158	GLU
1	E	159	ILE
1	E	162	SER
1	E	164	MET
1	E	173	GLN
1	E	189	LEU
1	E	194	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	223	LEU
1	E	238	VAL
1	E	277	LEU
1	E	1006	LYS
1	E	1023	LYS
1	E	1033	ARG
1	E	1035	MET
1	E	1036	ASP
1	E	1045	LEU
1	E	1065	TYR
1	E	1073	THR
1	E	1078	GLN
1	E	1079	VAL
1	E	1116	CYS
1	E	1123	GLU
1	E	1141	ILE
1	E	1149	LEU
1	E	1150	THR
1	E	1152	LYS
1	E	1170	MET
1	E	1173	GLN
1	E	1176	ARG
1	E	1192	ILE
1	E	1221	VAL
1	E	1231	VAL
1	E	1247	VAL
1	E	1270	PHE
1	E	1277	LEU
1	E	1282	LYS
1	E	1284	ILE
1	E	1296	GLU
1	E	1312	ASN
1	E	1314	GLU
1	E	1317	LYS
1	E	2016	GLN
1	E	2023	LYS
1	E	2025	SER
1	E	2036	ASP
1	E	2045	LEU
1	E	2065	TYR
1	E	2073	THR
1	E	2076	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	2078	GLN
1	E	2089	THR
1	E	2090	CYS
1	E	2130	ASP
1	E	2140	VAL
1	E	2149	LEU
1	E	2152	LYS
1	E	2166	LEU
1	E	2223	LEU
1	E	2235	GLU
1	E	2236	ASN
1	E	2247	VAL
1	E	2264	TYR
1	E	2296	GLU
1	E	2311	ASP
1	E	2312	ASN
1	E	2315	THR
1	E	3006	LYS
1	E	3032	ASP
1	E	3036	ASP
1	E	3045	LEU
1	E	3048	ASP
1	E	3065	TYR
1	E	3068	GLU
1	E	3072	LYS
1	E	3077	LEU
1	E	3099	LEU
1	E	3107	LEU
1	E	3112	ASP
1	E	3114	LEU
1	E	3127	GLU
1	E	3135	SER
1	E	3143	VAL
1	E	3166	LEU
1	E	3173	GLN
1	E	3184	GLN
1	E	3186	ASN
1	E	3189	LEU
1	E	3223	LEU
1	E	3236	ASN
1	E	3237	VAL
1	E	3247	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	3254	PRO
1	E	3270	PHE
1	E	3274	LEU
1	E	3296	GLU
1	E	3311	ASP
1	F	37	VAL
1	F	45	LEU
1	F	65	TYR
1	F	72	LYS
1	F	73	THR
1	F	113	ASN
1	F	114	LEU
1	F	116	CYS
1	F	117	SER
1	F	140	VAL
1	F	143	VAL
1	F	149	LEU
1	F	173	GLN
1	F	189	LEU
1	F	194	GLN
1	F	223	LEU
1	F	238	VAL
1	F	277	LEU
1	F	1006	LYS
1	F	1023	LYS
1	F	1033	ARG
1	F	1035	MET
1	F	1036	ASP
1	F	1045	LEU
1	F	1065	TYR
1	F	1073	THR
1	F	1078	GLN
1	F	1079	VAL
1	F	1116	CYS
1	F	1123	GLU
1	F	1141	ILE
1	F	1149	LEU
1	F	1150	THR
1	F	1152	LYS
1	F	1161	ASP
1	F	1170	MET
1	F	1173	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	1176	ARG
1	F	1221	VAL
1	F	1231	VAL
1	F	1247	VAL
1	F	1270	PHE
1	F	1277	LEU
1	F	1282	LYS
1	F	1284	ILE
1	F	1296	GLU
1	F	1312	ASN
1	F	1314	GLU
1	F	1317	LYS
1	F	2016	GLN
1	F	2023	LYS
1	F	2025	SER
1	F	2036	ASP
1	F	2045	LEU
1	F	2065	TYR
1	F	2073	THR
1	F	2076	THR
1	F	2078	GLN
1	F	2089	THR
1	F	2090	CYS
1	F	2130	ASP
1	F	2140	VAL
1	F	2149	LEU
1	F	2152	LYS
1	F	2166	LEU
1	F	2223	LEU
1	F	2235	GLU
1	F	2236	ASN
1	F	2247	VAL
1	F	2264	TYR
1	F	2296	GLU
1	F	2311	ASP
1	F	2312	ASN
1	F	2315	THR
1	F	3006	LYS
1	F	3032	ASP
1	F	3036	ASP
1	F	3045	LEU
1	F	3048	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	3065	TYR
1	F	3068	GLU
1	F	3072	LYS
1	F	3077	LEU
1	F	3099	LEU
1	F	3107	LEU
1	F	3112	ASP
1	F	3114	LEU
1	F	3127	GLU
1	F	3135	SER
1	F	3143	VAL
1	F	3166	LEU
1	F	3173	GLN
1	F	3184	GLN
1	F	3186	ASN
1	F	3189	LEU
1	F	3223	LEU
1	F	3236	ASN
1	F	3237	VAL
1	F	3247	VAL
1	F	3254	PRO
1	F	3270	PHE
1	F	3274	LEU
1	F	3296	GLU
1	F	3311	ASP
1	F	3326	LEU
1	G	37	VAL
1	G	45	LEU
1	G	65	TYR
1	G	72	LYS
1	G	73	THR
1	G	113	ASN
1	G	114	LEU
1	G	116	CYS
1	G	117	SER
1	G	140	VAL
1	G	143	VAL
1	G	149	LEU
1	G	159	ILE
1	G	162	SER
1	G	163	HIS
1	G	173	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	189	LEU
1	G	194	GLN
1	G	223	LEU
1	G	238	VAL
1	G	277	LEU
1	G	1006	LYS
1	G	1023	LYS
1	G	1033	ARG
1	G	1035	MET
1	G	1036	ASP
1	G	1045	LEU
1	G	1065	TYR
1	G	1073	THR
1	G	1078	GLN
1	G	1079	VAL
1	G	1116	CYS
1	G	1123	GLU
1	G	1141	ILE
1	G	1149	LEU
1	G	1150	THR
1	G	1152	LYS
1	G	1170	MET
1	G	1173	GLN
1	G	1176	ARG
1	G	1192	ILE
1	G	1221	VAL
1	G	1231	VAL
1	G	1247	VAL
1	G	1270	PHE
1	G	1277	LEU
1	G	1282	LYS
1	G	1284	ILE
1	G	1296	GLU
1	G	1312	ASN
1	G	1314	GLU
1	G	1317	LYS
1	G	2016	GLN
1	G	2023	LYS
1	G	2025	SER
1	G	2036	ASP
1	G	2045	LEU
1	G	2065	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	2073	THR
1	G	2076	THR
1	G	2078	GLN
1	G	2079	VAL
1	G	2089	THR
1	G	2090	CYS
1	G	2130	ASP
1	G	2140	VAL
1	G	2149	LEU
1	G	2152	LYS
1	G	2166	LEU
1	G	2223	LEU
1	G	2235	GLU
1	G	2236	ASN
1	G	2247	VAL
1	G	2264	TYR
1	G	2296	GLU
1	G	2311	ASP
1	G	2312	ASN
1	G	2315	THR
1	G	3006	LYS
1	G	3032	ASP
1	G	3036	ASP
1	G	3045	LEU
1	G	3048	ASP
1	G	3065	TYR
1	G	3068	GLU
1	G	3072	LYS
1	G	3077	LEU
1	G	3089	THR
1	G	3099	LEU
1	G	3107	LEU
1	G	3112	ASP
1	G	3114	LEU
1	G	3127	GLU
1	G	3135	SER
1	G	3143	VAL
1	G	3166	LEU
1	G	3173	GLN
1	G	3184	GLN
1	G	3186	ASN
1	G	3189	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	3218	TYR
1	G	3223	LEU
1	G	3236	ASN
1	G	3237	VAL
1	G	3247	VAL
1	G	3254	PRO
1	G	3270	PHE
1	G	3274	LEU
1	G	3296	GLU
1	G	3311	ASP
1	G	3326	LEU
1	H	37	VAL
1	H	45	LEU
1	H	65	TYR
1	H	72	LYS
1	H	73	THR
1	H	113	ASN
1	H	114	LEU
1	H	116	CYS
1	H	117	SER
1	H	140	VAL
1	H	143	VAL
1	H	149	LEU
1	H	158	GLU
1	H	159	ILE
1	H	164	MET
1	H	173	GLN
1	H	189	LEU
1	H	194	GLN
1	H	223	LEU
1	H	238	VAL
1	H	277	LEU
1	H	1006	LYS
1	H	1023	LYS
1	H	1033	ARG
1	H	1035	MET
1	H	1036	ASP
1	H	1045	LEU
1	H	1065	TYR
1	H	1073	THR
1	H	1078	GLN
1	H	1079	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	1116	CYS
1	H	1123	GLU
1	H	1141	ILE
1	H	1149	LEU
1	H	1150	THR
1	H	1152	LYS
1	H	1162	SER
1	H	1163	HIS
1	H	1170	MET
1	H	1173	GLN
1	H	1176	ARG
1	H	1192	ILE
1	H	1221	VAL
1	H	1231	VAL
1	H	1247	VAL
1	H	1270	PHE
1	H	1277	LEU
1	H	1282	LYS
1	H	1284	ILE
1	H	1296	GLU
1	H	1312	ASN
1	H	1314	GLU
1	H	1317	LYS
1	H	2016	GLN
1	H	2023	LYS
1	H	2025	SER
1	H	2036	ASP
1	H	2045	LEU
1	H	2065	TYR
1	H	2073	THR
1	H	2076	THR
1	H	2078	GLN
1	H	2089	THR
1	H	2090	CYS
1	H	2130	ASP
1	H	2140	VAL
1	H	2149	LEU
1	H	2152	LYS
1	H	2166	LEU
1	H	2223	LEU
1	H	2235	GLU
1	H	2236	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	2247	VAL
1	H	2264	TYR
1	H	2296	GLU
1	H	2311	ASP
1	H	2312	ASN
1	H	2315	THR
1	H	3006	LYS
1	H	3032	ASP
1	H	3036	ASP
1	H	3045	LEU
1	H	3048	ASP
1	H	3065	TYR
1	H	3068	GLU
1	H	3072	LYS
1	H	3077	LEU
1	H	3099	LEU
1	H	3107	LEU
1	H	3112	ASP
1	H	3114	LEU
1	H	3127	GLU
1	H	3135	SER
1	H	3143	VAL
1	H	3166	LEU
1	H	3173	GLN
1	H	3184	GLN
1	H	3186	ASN
1	H	3189	LEU
1	H	3223	LEU
1	H	3236	ASN
1	H	3237	VAL
1	H	3247	VAL
1	H	3254	PRO
1	H	3270	PHE
1	H	3274	LEU
1	H	3296	GLU
1	H	3311	ASP
1	H	3326	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	118	GLN
1	A	173	GLN
1	A	181	ASN
1	A	1193	ASN
1	A	1213	ASN
1	A	1300	GLN
1	A	2020	GLN
1	A	2118	GLN
1	A	2181	ASN
1	A	2236	ASN
1	A	2300	GLN
1	A	3124	GLN
1	A	3181	ASN
1	A	3300	GLN
1	A	3304	ASN
1	B	97	HIS
1	B	118	GLN
1	B	173	GLN
1	B	181	ASN
1	B	1118	GLN
1	B	1300	GLN
1	B	2118	GLN
1	B	2181	ASN
1	B	2236	ASN
1	B	2300	GLN
1	B	3124	GLN
1	B	3181	ASN
1	B	3300	GLN
1	B	3304	ASN
1	C	97	HIS
1	C	118	GLN
1	C	173	GLN
1	C	181	ASN
1	C	1118	GLN
1	C	1300	GLN
1	C	2020	GLN
1	C	2118	GLN
1	C	2181	ASN
1	C	2236	ASN
1	C	2300	GLN
1	C	3124	GLN
1	C	3181	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	3300	GLN
1	C	3304	ASN
1	D	173	GLN
1	D	181	ASN
1	D	1118	GLN
1	D	1300	GLN
1	D	2118	GLN
1	D	2181	ASN
1	D	2236	ASN
1	D	2300	GLN
1	D	3124	GLN
1	D	3181	ASN
1	D	3300	GLN
1	D	3304	ASN
1	E	97	HIS
1	E	118	GLN
1	E	173	GLN
1	E	181	ASN
1	E	1118	GLN
1	E	1300	GLN
1	E	2118	GLN
1	E	2181	ASN
1	E	2236	ASN
1	E	2300	GLN
1	E	3124	GLN
1	E	3181	ASN
1	E	3300	GLN
1	E	3304	ASN
1	F	97	HIS
1	F	118	GLN
1	F	173	GLN
1	F	181	ASN
1	F	1163	HIS
1	F	1213	ASN
1	F	1300	GLN
1	F	2020	GLN
1	F	2118	GLN
1	F	2181	ASN
1	F	2236	ASN
1	F	2300	GLN
1	F	3113	ASN
1	F	3124	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	3181	ASN
1	F	3300	GLN
1	F	3304	ASN
1	G	97	HIS
1	G	118	GLN
1	G	173	GLN
1	G	181	ASN
1	G	1118	GLN
1	G	1300	GLN
1	G	2118	GLN
1	G	2181	ASN
1	G	2236	ASN
1	G	2300	GLN
1	G	3124	GLN
1	G	3181	ASN
1	G	3300	GLN
1	G	3304	ASN
1	H	97	HIS
1	H	118	GLN
1	H	173	GLN
1	H	181	ASN
1	H	1213	ASN
1	H	1300	GLN
1	H	2020	GLN
1	H	2118	GLN
1	H	2181	ASN
1	H	2236	ASN
1	H	2300	GLN
1	H	3124	GLN
1	H	3181	ASN
1	H	3300	GLN
1	H	3304	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 64 ligands modelled in this entry, 32 are monoatomic - leaving 32 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	ANP	A	1400	-	27,33,33	2.17	7 (25%)	30,52,52	2.26	6 (20%)
3	ANP	A	2400	-	27,33,33	2.29	8 (29%)	30,52,52	2.31	6 (20%)
3	ANP	A	3400	-	27,33,33	2.15	7 (25%)	30,52,52	2.61	9 (30%)
3	ANP	A	400	-	27,33,33	2.30	9 (33%)	30,52,52	2.12	5 (16%)
3	ANP	B	1400	-	27,33,33	2.25	8 (29%)	30,52,52	2.33	7 (23%)
3	ANP	B	2400	-	27,33,33	2.25	8 (29%)	30,52,52	2.28	6 (20%)
3	ANP	B	3400	-	27,33,33	2.10	7 (25%)	30,52,52	2.70	9 (30%)
3	ANP	B	400	-	27,33,33	2.26	8 (29%)	30,52,52	2.12	6 (20%)
3	ANP	C	1400	-	27,33,33	2.38	8 (29%)	30,52,52	2.32	7 (23%)
3	ANP	C	2400	-	27,33,33	2.18	8 (29%)	30,52,52	2.29	7 (23%)
3	ANP	C	3400	-	27,33,33	2.33	6 (22%)	30,52,52	2.65	9 (30%)
3	ANP	C	400	-	27,33,33	2.06	7 (25%)	30,52,52	2.17	6 (20%)
3	ANP	D	1400	-	27,33,33	2.23	7 (25%)	30,52,52	2.29	6 (20%)
3	ANP	D	2400	-	27,33,33	2.25	8 (29%)	30,52,52	2.26	6 (20%)
3	ANP	D	3400	-	27,33,33	2.14	7 (25%)	30,52,52	2.69	9 (30%)
3	ANP	D	400	-	27,33,33	2.31	7 (25%)	30,52,52	2.10	6 (20%)
3	ANP	E	1400	-	27,33,33	2.29	7 (25%)	30,52,52	2.33	6 (20%)
3	ANP	E	2400	-	27,33,33	2.31	9 (33%)	30,52,52	2.29	6 (20%)
3	ANP	E	3400	2	27,33,33	1.99	6 (22%)	30,52,52	2.68	9 (30%)
3	ANP	E	400	-	27,33,33	2.22	9 (33%)	30,52,52	2.15	5 (16%)
3	ANP	F	1400	-	27,33,33	2.34	8 (29%)	30,52,52	2.30	6 (20%)
3	ANP	F	2400	-	27,33,33	2.11	8 (29%)	30,52,52	2.32	6 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ANP	F	3400	-	27,33,33	2.18	9 (33%)	30,52,52	2.65	9 (30%)
3	ANP	F	400	-	27,33,33	2.16	7 (25%)	30,52,52	2.07	6 (20%)
3	ANP	G	1400	-	27,33,33	2.26	8 (29%)	30,52,52	2.26	6 (20%)
3	ANP	G	2400	-	27,33,33	2.31	8 (29%)	30,52,52	2.29	7 (23%)
3	ANP	G	3400	-	27,33,33	2.34	7 (25%)	30,52,52	2.71	10 (33%)
3	ANP	G	400	-	27,33,33	2.20	7 (25%)	30,52,52	2.12	6 (20%)
3	ANP	H	1400	-	27,33,33	2.34	8 (29%)	30,52,52	2.23	7 (23%)
3	ANP	H	2400	-	27,33,33	2.24	8 (29%)	30,52,52	2.31	7 (23%)
3	ANP	H	3400	-	27,33,33	2.23	6 (22%)	30,52,52	2.81	9 (30%)
3	ANP	H	400	-	27,33,33	2.18	8 (29%)	30,52,52	2.11	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	A	1400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	A	2400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	A	3400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	A	400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	B	1400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	B	2400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	B	3400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	B	400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	C	1400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	C	2400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	C	3400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	C	400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	D	1400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	D	2400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	D	3400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	D	400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	E	1400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	E	2400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	E	3400	2	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	E	400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	F	1400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	F	2400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	F	3400	-	1/1/7/8	0/12/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ANP	F	400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	G	1400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	G	2400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	G	3400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	G	400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	H	1400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	H	2400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	H	3400	-	1/1/7/8	0/12/38/38	0/3/3/3
3	ANP	H	400	-	1/1/7/8	0/12/38/38	0/3/3/3

All (243) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3400	ANP	PB-O2B	-2.46	1.49	1.56
3	A	3400	ANP	PB-O2B	-2.46	1.49	1.56
3	A	400	ANP	PG-O2G	-2.32	1.50	1.56
3	C	400	ANP	PG-O2G	-2.21	1.50	1.56
3	G	400	ANP	PG-O2G	-2.21	1.50	1.56
3	B	3400	ANP	PB-O2B	-2.20	1.50	1.56
3	B	400	ANP	PG-O2G	-2.19	1.50	1.56
3	D	3400	ANP	PB-O2B	-2.12	1.50	1.56
3	F	1400	ANP	PG-O2G	-2.06	1.50	1.56
3	G	2400	ANP	PG-O3G	-2.05	1.51	1.56
3	E	400	ANP	PG-O2G	-2.05	1.51	1.56
3	E	400	ANP	PG-O3G	-2.05	1.51	1.56
3	E	2400	ANP	PG-O3G	-2.04	1.51	1.56
3	B	1400	ANP	PB-O2B	-2.04	1.51	1.56
3	F	2400	ANP	PG-O2G	-2.04	1.51	1.56
3	H	400	ANP	PG-O2G	-2.04	1.51	1.56
3	F	3400	ANP	PG-O2G	-2.01	1.51	1.56
3	A	400	ANP	PG-O3G	-2.00	1.51	1.56
3	A	2400	ANP	O4'-C1'	2.02	1.43	1.41
3	C	1400	ANP	O4'-C1'	2.02	1.43	1.41
3	C	2400	ANP	O4'-C1'	2.02	1.43	1.41
3	B	2400	ANP	O4'-C1'	2.02	1.43	1.41
3	E	400	ANP	C2-N3	2.04	1.35	1.32
3	C	2400	ANP	PB-O3A	2.05	1.61	1.59
3	H	1400	ANP	O4'-C1'	2.05	1.43	1.41
3	B	1400	ANP	C2-N3	2.07	1.35	1.32
3	F	2400	ANP	C2-N3	2.08	1.35	1.32
3	H	2400	ANP	C2-N3	2.08	1.35	1.32
3	B	400	ANP	C2-N3	2.09	1.35	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2400	ANP	C2-N3	2.09	1.35	1.32
3	A	2400	ANP	C2-N3	2.10	1.35	1.32
3	G	1400	ANP	O4'-C1'	2.10	1.43	1.41
3	B	1400	ANP	O4'-C1'	2.11	1.43	1.41
3	D	1400	ANP	C2-N3	2.11	1.35	1.32
3	F	2400	ANP	PB-O3A	2.12	1.61	1.59
3	C	400	ANP	C2-N3	2.14	1.36	1.32
3	H	2400	ANP	O4'-C1'	2.15	1.43	1.41
3	G	400	ANP	C2-N3	2.15	1.36	1.32
3	H	400	ANP	C2-N3	2.16	1.36	1.32
3	G	3400	ANP	O4'-C1'	2.17	1.43	1.41
3	D	2400	ANP	O4'-C1'	2.18	1.44	1.41
3	D	2400	ANP	C2-N3	2.19	1.36	1.32
3	H	2400	ANP	PB-O3A	2.20	1.61	1.59
3	F	400	ANP	C2-N3	2.20	1.36	1.32
3	B	3400	ANP	PB-O1B	2.21	1.48	1.46
3	C	2400	ANP	C2-N3	2.21	1.36	1.32
3	C	1400	ANP	C2-N3	2.21	1.36	1.32
3	D	400	ANP	O4'-C1'	2.22	1.44	1.41
3	E	2400	ANP	C2-N3	2.22	1.36	1.32
3	A	1400	ANP	C2-N3	2.22	1.36	1.32
3	E	2400	ANP	O4'-C1'	2.22	1.44	1.41
3	H	1400	ANP	C2-N3	2.22	1.36	1.32
3	G	1400	ANP	C2-N3	2.24	1.36	1.32
3	A	400	ANP	C2-N3	2.24	1.36	1.32
3	E	1400	ANP	C2-N3	2.24	1.36	1.32
3	D	3400	ANP	PB-O1B	2.25	1.48	1.46
3	G	2400	ANP	PB-O3A	2.26	1.61	1.59
3	G	2400	ANP	C2-N3	2.28	1.36	1.32
3	F	3400	ANP	C2-N3	2.35	1.36	1.32
3	G	3400	ANP	C2-N3	2.39	1.36	1.32
3	E	3400	ANP	C2-N3	2.44	1.36	1.32
3	F	1400	ANP	C2-N3	2.44	1.36	1.32
3	A	2400	ANP	PB-O3A	2.46	1.62	1.59
3	H	400	ANP	PB-O3A	2.49	1.62	1.59
3	A	3400	ANP	PB-O1B	2.49	1.48	1.46
3	B	400	ANP	PB-O3A	2.50	1.62	1.59
3	B	2400	ANP	PB-O3A	2.51	1.62	1.59
3	E	2400	ANP	PB-O3A	2.57	1.62	1.59
3	H	1400	ANP	PB-O3A	2.58	1.62	1.59
3	E	400	ANP	PB-O3A	2.64	1.62	1.59
3	D	1400	ANP	PB-O3A	2.66	1.62	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3400	ANP	O4'-C1'	2.66	1.44	1.41
3	H	3400	ANP	C2-N3	2.68	1.36	1.32
3	D	2400	ANP	PB-O3A	2.69	1.62	1.59
3	F	400	ANP	PB-O3A	2.72	1.62	1.59
3	A	3400	ANP	C2-N3	2.74	1.37	1.32
3	C	3400	ANP	C2-N3	2.79	1.37	1.32
3	G	1400	ANP	PB-O3A	2.80	1.62	1.59
3	A	1400	ANP	PB-O3A	2.83	1.62	1.59
3	D	400	ANP	PB-O3A	2.91	1.62	1.59
3	D	3400	ANP	C2-N3	2.95	1.37	1.32
3	E	1400	ANP	PB-O3A	2.97	1.62	1.59
3	B	3400	ANP	C2-N3	3.10	1.37	1.32
3	C	1400	ANP	PB-O3A	3.10	1.63	1.59
3	H	3400	ANP	PB-O1B	3.13	1.49	1.46
3	F	1400	ANP	PB-O3A	3.16	1.63	1.59
3	A	400	ANP	PB-O3A	3.30	1.63	1.59
3	E	3400	ANP	PB-O1B	3.32	1.49	1.46
3	E	3400	ANP	C5-C4	3.40	1.48	1.40
3	E	400	ANP	C5-C4	3.46	1.48	1.40
3	C	3400	ANP	PB-O1B	3.52	1.50	1.46
3	H	400	ANP	C5-C4	3.56	1.48	1.40
3	A	1400	ANP	C5-C4	3.57	1.48	1.40
3	B	2400	ANP	C5-C4	3.57	1.48	1.40
3	F	3400	ANP	PB-O1B	3.61	1.50	1.46
3	G	1400	ANP	C5-C4	3.63	1.48	1.40
3	C	1400	ANP	C5-C4	3.65	1.48	1.40
3	A	2400	ANP	C5-C4	3.67	1.48	1.40
3	F	2400	ANP	C5-C4	3.68	1.48	1.40
3	C	2400	ANP	C5-C4	3.69	1.48	1.40
3	D	2400	ANP	C5-C4	3.70	1.48	1.40
3	G	400	ANP	C5-C4	3.70	1.48	1.40
3	A	400	ANP	C5-C4	3.71	1.48	1.40
3	C	400	ANP	C5-C4	3.71	1.48	1.40
3	B	1400	ANP	C5-C4	3.72	1.48	1.40
3	E	1400	ANP	C5-C4	3.73	1.48	1.40
3	H	2400	ANP	C5-C4	3.75	1.48	1.40
3	B	3400	ANP	C5-C4	3.78	1.49	1.40
3	D	1400	ANP	C5-C4	3.79	1.49	1.40
3	H	3400	ANP	C5-C4	3.81	1.49	1.40
3	G	2400	ANP	C5-C4	3.81	1.49	1.40
3	F	1400	ANP	C5-C4	3.81	1.49	1.40
3	E	2400	ANP	C5-C4	3.82	1.49	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3400	ANP	C5-C4	3.83	1.49	1.40
3	D	400	ANP	C5-C4	3.90	1.49	1.40
3	H	1400	ANP	C5-C4	3.91	1.49	1.40
3	F	2400	ANP	PB-O1B	3.91	1.50	1.46
3	C	400	ANP	PB-N3B	3.91	1.73	1.63
3	F	400	ANP	C5-C4	3.94	1.49	1.40
3	G	3400	ANP	PB-O1B	3.96	1.50	1.46
3	C	400	ANP	PG-O1G	3.97	1.50	1.46
3	B	400	ANP	C5-C4	4.00	1.49	1.40
3	E	3400	ANP	PB-N3B	4.11	1.74	1.63
3	D	3400	ANP	PB-N3B	4.12	1.74	1.63
3	C	3400	ANP	C5-C4	4.14	1.49	1.40
3	E	400	ANP	PB-O1B	4.15	1.50	1.46
3	G	3400	ANP	C5-C4	4.15	1.49	1.40
3	F	400	ANP	PB-O1B	4.15	1.50	1.46
3	A	400	ANP	PB-O1B	4.16	1.50	1.46
3	C	2400	ANP	PB-O1B	4.17	1.50	1.46
3	D	3400	ANP	C5-C4	4.20	1.50	1.40
3	A	3400	ANP	PB-N3B	4.22	1.74	1.63
3	H	400	ANP	PB-O1B	4.22	1.50	1.46
3	A	1400	ANP	PB-N3B	4.23	1.74	1.63
3	A	3400	ANP	PG-N3B	4.23	1.74	1.63
3	B	400	ANP	PB-N3B	4.24	1.74	1.63
3	G	400	ANP	PB-O1B	4.29	1.51	1.46
3	C	400	ANP	PB-O1B	4.31	1.51	1.46
3	F	400	ANP	PB-N3B	4.35	1.74	1.63
3	A	3400	ANP	C5-C4	4.35	1.50	1.40
3	F	2400	ANP	PB-N3B	4.37	1.74	1.63
3	F	2400	ANP	PG-O1G	4.37	1.51	1.46
3	F	400	ANP	PG-O1G	4.40	1.51	1.46
3	E	1400	ANP	PB-O1B	4.41	1.51	1.46
3	D	2400	ANP	PB-O1B	4.43	1.51	1.46
3	H	400	ANP	PB-N3B	4.44	1.75	1.63
3	G	1400	ANP	PB-N3B	4.47	1.75	1.63
3	A	1400	ANP	PG-O1G	4.48	1.51	1.46
3	D	1400	ANP	PG-O1G	4.49	1.51	1.46
3	C	2400	ANP	PB-N3B	4.49	1.75	1.63
3	B	1400	ANP	PB-N3B	4.52	1.75	1.63
3	D	1400	ANP	PB-N3B	4.53	1.75	1.63
3	D	400	ANP	PG-O1G	4.54	1.51	1.46
3	C	400	ANP	PG-N3B	4.55	1.75	1.63
3	F	3400	ANP	PG-N3B	4.56	1.75	1.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	3400	ANP	PG-N3B	4.57	1.75	1.63
3	G	2400	ANP	PG-O1G	4.58	1.51	1.46
3	H	2400	ANP	PB-O1B	4.59	1.51	1.46
3	A	1400	ANP	PG-N3B	4.60	1.75	1.63
3	H	2400	ANP	PG-O1G	4.61	1.51	1.46
3	G	400	ANP	PG-O1G	4.61	1.51	1.46
3	B	2400	ANP	PB-O1B	4.63	1.51	1.46
3	D	2400	ANP	PG-O1G	4.63	1.51	1.46
3	A	1400	ANP	PB-O1B	4.64	1.51	1.46
3	D	2400	ANP	PB-N3B	4.64	1.75	1.63
3	H	2400	ANP	PB-N3B	4.65	1.75	1.63
3	B	3400	ANP	PB-N3B	4.65	1.75	1.63
3	D	400	ANP	PB-O1B	4.67	1.51	1.46
3	C	2400	ANP	PG-O1G	4.67	1.51	1.46
3	F	400	ANP	PG-N3B	4.68	1.75	1.63
3	B	2400	ANP	PB-N3B	4.68	1.75	1.63
3	E	3400	ANP	PG-O1G	4.68	1.51	1.46
3	H	400	ANP	PG-O1G	4.69	1.51	1.46
3	G	400	ANP	PB-N3B	4.69	1.75	1.63
3	A	2400	ANP	PB-O1B	4.69	1.51	1.46
3	E	400	ANP	PB-N3B	4.71	1.75	1.63
3	G	2400	ANP	PB-N3B	4.71	1.75	1.63
3	B	400	ANP	PG-O1G	4.72	1.51	1.46
3	F	3400	ANP	PB-N3B	4.72	1.75	1.63
3	G	1400	ANP	PB-O1B	4.72	1.51	1.46
3	F	1400	ANP	PB-O1B	4.73	1.51	1.46
3	G	1400	ANP	PG-N3B	4.74	1.75	1.63
3	E	1400	ANP	PB-N3B	4.74	1.75	1.63
3	E	2400	ANP	PB-O1B	4.74	1.51	1.46
3	D	1400	ANP	PB-O1B	4.75	1.51	1.46
3	F	2400	ANP	PG-N3B	4.75	1.75	1.63
3	B	400	ANP	PB-O1B	4.75	1.51	1.46
3	B	1400	ANP	PB-O1B	4.76	1.51	1.46
3	B	2400	ANP	PG-O1G	4.77	1.51	1.46
3	F	1400	ANP	PB-N3B	4.78	1.76	1.63
3	A	2400	ANP	PB-N3B	4.78	1.76	1.63
3	B	3400	ANP	PG-O1G	4.79	1.51	1.46
3	E	2400	ANP	PG-O1G	4.79	1.51	1.46
3	A	400	ANP	PG-N3B	4.80	1.76	1.63
3	E	2400	ANP	PB-N3B	4.80	1.76	1.63
3	H	3400	ANP	PG-O1G	4.83	1.51	1.46
3	B	1400	ANP	PG-O1G	4.84	1.51	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1400	ANP	PG-N3B	4.84	1.76	1.63
3	H	1400	ANP	PB-N3B	4.85	1.76	1.63
3	H	400	ANP	PG-N3B	4.85	1.76	1.63
3	F	3400	ANP	PG-O1G	4.86	1.51	1.46
3	C	1400	ANP	PB-N3B	4.87	1.76	1.63
3	E	400	ANP	PG-O1G	4.88	1.51	1.46
3	D	1400	ANP	PG-N3B	4.89	1.76	1.63
3	D	400	ANP	PG-N3B	4.90	1.76	1.63
3	C	2400	ANP	PG-N3B	4.93	1.76	1.63
3	A	400	ANP	PB-N3B	4.93	1.76	1.63
3	B	400	ANP	PG-N3B	4.94	1.76	1.63
3	H	1400	ANP	PG-O1G	4.94	1.51	1.46
3	B	3400	ANP	PG-N3B	4.97	1.76	1.63
3	E	400	ANP	PG-N3B	4.98	1.76	1.63
3	H	1400	ANP	PB-O1B	4.98	1.51	1.46
3	D	400	ANP	PB-N3B	4.99	1.76	1.63
3	F	1400	ANP	PG-N3B	4.99	1.76	1.63
3	A	2400	ANP	PG-O1G	4.99	1.51	1.46
3	G	400	ANP	PG-N3B	5.00	1.76	1.63
3	H	2400	ANP	PG-N3B	5.00	1.76	1.63
3	D	3400	ANP	PG-O1G	5.03	1.51	1.46
3	E	1400	ANP	PG-O1G	5.07	1.51	1.46
3	B	2400	ANP	PG-N3B	5.08	1.76	1.63
3	E	2400	ANP	PG-N3B	5.10	1.76	1.63
3	F	1400	ANP	PG-O1G	5.10	1.52	1.46
3	A	2400	ANP	PG-N3B	5.11	1.76	1.63
3	D	2400	ANP	PG-N3B	5.14	1.76	1.63
3	D	3400	ANP	PG-N3B	5.14	1.76	1.63
3	A	400	ANP	PG-O1G	5.14	1.52	1.46
3	G	2400	ANP	PB-O1B	5.16	1.52	1.46
3	C	1400	ANP	PB-O1B	5.16	1.52	1.46
3	C	1400	ANP	PG-N3B	5.17	1.77	1.63
3	B	1400	ANP	PG-N3B	5.19	1.77	1.63
3	G	1400	ANP	PG-O1G	5.20	1.52	1.46
3	C	3400	ANP	PG-O1G	5.20	1.52	1.46
3	G	2400	ANP	PG-N3B	5.21	1.77	1.63
3	H	3400	ANP	PB-N3B	5.21	1.77	1.63
3	H	1400	ANP	PG-N3B	5.24	1.77	1.63
3	C	1400	ANP	PG-O1G	5.26	1.52	1.46
3	G	3400	ANP	PB-N3B	5.27	1.77	1.63
3	C	3400	ANP	PB-N3B	5.38	1.77	1.63
3	G	3400	ANP	PG-N3B	5.42	1.77	1.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	3400	ANP	PG-O1G	5.46	1.52	1.46
3	H	3400	ANP	PG-N3B	5.47	1.77	1.63
3	A	3400	ANP	PG-O1G	5.49	1.52	1.46
3	C	3400	ANP	PG-N3B	5.83	1.78	1.63

All (220) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	2400	ANP	N3-C2-N1	-8.07	122.72	128.89
3	H	2400	ANP	N3-C2-N1	-7.90	122.84	128.89
3	A	2400	ANP	N3-C2-N1	-7.90	122.85	128.89
3	E	1400	ANP	N3-C2-N1	-7.80	122.92	128.89
3	E	2400	ANP	N3-C2-N1	-7.78	122.94	128.89
3	C	2400	ANP	N3-C2-N1	-7.77	122.95	128.89
3	B	2400	ANP	N3-C2-N1	-7.71	122.99	128.89
3	G	2400	ANP	N3-C2-N1	-7.69	123.01	128.89
3	C	1400	ANP	N3-C2-N1	-7.64	123.05	128.89
3	D	1400	ANP	N3-C2-N1	-7.62	123.06	128.89
3	B	3400	ANP	O1G-PG-N3B	-7.61	100.23	111.90
3	B	1400	ANP	N3-C2-N1	-7.58	123.09	128.89
3	D	2400	ANP	N3-C2-N1	-7.57	123.10	128.89
3	E	400	ANP	N3-C2-N1	-7.55	123.11	128.89
3	B	400	ANP	N3-C2-N1	-7.55	123.11	128.89
3	G	1400	ANP	N3-C2-N1	-7.53	123.12	128.89
3	A	400	ANP	N3-C2-N1	-7.45	123.19	128.89
3	H	400	ANP	N3-C2-N1	-7.45	123.19	128.89
3	A	1400	ANP	N3-C2-N1	-7.45	123.19	128.89
3	F	1400	ANP	N3-C2-N1	-7.42	123.21	128.89
3	C	400	ANP	N3-C2-N1	-7.42	123.22	128.89
3	H	1400	ANP	N3-C2-N1	-7.38	123.24	128.89
3	D	400	ANP	N3-C2-N1	-7.26	123.34	128.89
3	F	3400	ANP	O1G-PG-N3B	-7.23	100.81	111.90
3	H	3400	ANP	O1G-PG-N3B	-7.09	101.03	111.90
3	F	400	ANP	N3-C2-N1	-7.01	123.52	128.89
3	G	400	ANP	N3-C2-N1	-6.98	123.55	128.89
3	A	3400	ANP	O1G-PG-N3B	-6.90	101.32	111.90
3	G	3400	ANP	O1G-PG-N3B	-6.88	101.34	111.90
3	E	3400	ANP	O1G-PG-N3B	-6.82	101.44	111.90
3	D	3400	ANP	O1G-PG-N3B	-6.63	101.72	111.90
3	H	3400	ANP	N3-C2-N1	-6.60	123.84	128.89
3	C	3400	ANP	O1G-PG-N3B	-6.40	102.08	111.90
3	G	3400	ANP	N3-C2-N1	-6.17	124.17	128.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3400	ANP	N3-C2-N1	-5.90	124.37	128.89
3	H	3400	ANP	C4-C5-N7	-5.89	104.06	109.48
3	D	3400	ANP	N3-C2-N1	-5.83	124.43	128.89
3	C	3400	ANP	N3-C2-N1	-5.81	124.44	128.89
3	B	3400	ANP	N3-C2-N1	-5.70	124.53	128.89
3	A	3400	ANP	C4-C5-N7	-5.61	104.32	109.48
3	B	3400	ANP	C4-C5-N7	-5.48	104.44	109.48
3	E	3400	ANP	C4-C5-N7	-5.44	104.48	109.48
3	G	3400	ANP	C4'-O4'-C1'	-5.19	104.02	109.72
3	D	3400	ANP	C4-C5-N7	-5.18	104.71	109.48
3	A	3400	ANP	N3-C2-N1	-5.09	125.00	128.89
3	C	3400	ANP	C4-C5-N7	-5.09	104.80	109.48
3	E	3400	ANP	N3-C2-N1	-5.01	125.06	128.89
3	D	3400	ANP	C4'-O4'-C1'	-4.85	104.39	109.72
3	H	3400	ANP	C4'-O4'-C1'	-4.84	104.40	109.72
3	C	3400	ANP	C4'-O4'-C1'	-4.81	104.44	109.72
3	A	2400	ANP	O1G-PG-N3B	-4.81	104.53	111.90
3	G	3400	ANP	C4-C5-N7	-4.79	105.07	109.48
3	B	2400	ANP	O1G-PG-N3B	-4.75	104.61	111.90
3	F	1400	ANP	O1G-PG-N3B	-4.71	104.67	111.90
3	F	3400	ANP	C4-C5-N7	-4.70	105.16	109.48
3	E	3400	ANP	C4'-O4'-C1'	-4.69	104.56	109.72
3	B	1400	ANP	O1G-PG-N3B	-4.69	104.71	111.90
3	H	2400	ANP	O1G-PG-N3B	-4.67	104.74	111.90
3	G	2400	ANP	O1G-PG-N3B	-4.66	104.75	111.90
3	G	3400	ANP	O1B-PB-N3B	-4.65	104.77	111.90
3	F	3400	ANP	C4'-O4'-C1'	-4.65	104.61	109.72
3	E	2400	ANP	O1G-PG-N3B	-4.64	104.78	111.90
3	D	2400	ANP	O1G-PG-N3B	-4.62	104.81	111.90
3	F	2400	ANP	O1G-PG-N3B	-4.62	104.81	111.90
3	C	2400	ANP	O1G-PG-N3B	-4.62	104.81	111.90
3	E	3400	ANP	O1B-PB-N3B	-4.62	104.81	111.90
3	B	3400	ANP	C4'-O4'-C1'	-4.59	104.68	109.72
3	D	3400	ANP	O1B-PB-N3B	-4.58	104.88	111.90
3	E	1400	ANP	O1G-PG-N3B	-4.56	104.91	111.90
3	C	1400	ANP	O1G-PG-N3B	-4.51	104.97	111.90
3	A	3400	ANP	C4'-O4'-C1'	-4.38	104.91	109.72
3	D	400	ANP	O1G-PG-N3B	-4.26	105.37	111.90
3	G	400	ANP	O1G-PG-N3B	-4.22	105.42	111.90
3	A	400	ANP	O1G-PG-N3B	-4.21	105.45	111.90
3	D	1400	ANP	O1G-PG-N3B	-4.20	105.45	111.90
3	A	3400	ANP	O1B-PB-N3B	-4.17	105.51	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3400	ANP	O1B-PB-N3B	-4.13	105.56	111.90
3	C	400	ANP	O1G-PG-N3B	-4.11	105.59	111.90
3	H	1400	ANP	O1G-PG-N3B	-4.05	105.69	111.90
3	G	1400	ANP	O1G-PG-N3B	-3.95	105.84	111.90
3	A	1400	ANP	O1G-PG-N3B	-3.93	105.86	111.90
3	F	3400	ANP	O1B-PB-N3B	-3.92	105.89	111.90
3	E	3400	ANP	PA-O3A-PB	-3.90	119.59	132.67
3	E	400	ANP	O1G-PG-N3B	-3.89	105.93	111.90
3	E	1400	ANP	C4-C5-N7	-3.85	105.94	109.48
3	H	3400	ANP	O1B-PB-N3B	-3.85	105.99	111.90
3	B	400	ANP	O1G-PG-N3B	-3.85	106.00	111.90
3	F	400	ANP	O1G-PG-N3B	-3.82	106.04	111.90
3	H	400	ANP	O1G-PG-N3B	-3.79	106.08	111.90
3	E	400	ANP	C4-C5-N7	-3.73	106.05	109.48
3	D	1400	ANP	C4-C5-N7	-3.70	106.08	109.48
3	F	1400	ANP	C4-C5-N7	-3.65	106.12	109.48
3	B	3400	ANP	PA-O3A-PB	-3.61	120.56	132.67
3	A	1400	ANP	C4-C5-N7	-3.59	106.18	109.48
3	H	2400	ANP	O1B-PB-N3B	-3.57	106.42	111.90
3	A	400	ANP	C4-C5-N7	-3.52	106.24	109.48
3	B	3400	ANP	O1B-PB-N3B	-3.52	106.50	111.90
3	G	3400	ANP	PA-O3A-PB	-3.51	120.89	132.67
3	H	3400	ANP	PA-O3A-PB	-3.48	120.98	132.67
3	C	3400	ANP	PA-O3A-PB	-3.48	121.00	132.67
3	C	1400	ANP	C4-C5-N7	-3.47	106.28	109.48
3	B	1400	ANP	C4-C5-N7	-3.46	106.30	109.48
3	C	1400	ANP	O1B-PB-N3B	-3.45	106.60	111.90
3	H	1400	ANP	C4-C5-N7	-3.44	106.31	109.48
3	D	3400	ANP	PA-O3A-PB	-3.44	121.13	132.67
3	G	400	ANP	C4-C5-N7	-3.44	106.31	109.48
3	H	400	ANP	C4-C5-N7	-3.42	106.33	109.48
3	E	2400	ANP	O1B-PB-N3B	-3.41	106.67	111.90
3	A	2400	ANP	O1B-PB-N3B	-3.39	106.69	111.90
3	B	1400	ANP	O1B-PB-N3B	-3.39	106.71	111.90
3	E	1400	ANP	O1B-PB-N3B	-3.38	106.71	111.90
3	F	3400	ANP	PA-O3A-PB	-3.37	121.37	132.67
3	D	2400	ANP	O1B-PB-N3B	-3.36	106.74	111.90
3	G	2400	ANP	O1B-PB-N3B	-3.36	106.75	111.90
3	B	2400	ANP	O1B-PB-N3B	-3.35	106.76	111.90
3	C	2400	ANP	O1B-PB-N3B	-3.34	106.77	111.90
3	G	1400	ANP	O1B-PB-N3B	-3.32	106.80	111.90
3	F	400	ANP	C4-C5-N7	-3.32	106.43	109.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1400	ANP	O1B-PB-N3B	-3.31	106.82	111.90
3	G	1400	ANP	C4-C5-N7	-3.31	106.43	109.48
3	C	400	ANP	C4-C5-N7	-3.27	106.47	109.48
3	A	1400	ANP	O1B-PB-N3B	-3.26	106.90	111.90
3	A	3400	ANP	PA-O3A-PB	-3.25	121.75	132.67
3	D	1400	ANP	O1B-PB-N3B	-3.22	106.96	111.90
3	F	2400	ANP	O1B-PB-N3B	-3.16	107.05	111.90
3	B	400	ANP	C4-C5-N7	-3.15	106.58	109.48
3	D	2400	ANP	C4-C5-N7	-3.08	106.64	109.48
3	H	1400	ANP	O1B-PB-N3B	-3.03	107.25	111.90
3	D	400	ANP	C4-C5-N7	-3.00	106.72	109.48
3	C	2400	ANP	C4-C5-N7	-3.00	106.72	109.48
3	B	2400	ANP	C4-C5-N7	-3.00	106.72	109.48
3	G	2400	ANP	C4-C5-N7	-2.97	106.74	109.48
3	A	2400	ANP	C4-C5-N7	-2.95	106.77	109.48
3	E	2400	ANP	C4-C5-N7	-2.87	106.84	109.48
3	F	2400	ANP	C4-C5-N7	-2.81	106.89	109.48
3	H	2400	ANP	C4-C5-N7	-2.81	106.90	109.48
3	C	3400	ANP	C2'-C1'-N9	-2.55	110.39	114.29
3	A	3400	ANP	C2'-C1'-N9	-2.47	110.52	114.29
3	G	3400	ANP	C2'-C1'-N9	-2.36	110.68	114.29
3	D	3400	ANP	C2'-C1'-N9	-2.29	110.80	114.29
3	G	2400	ANP	PA-O3A-PB	-2.09	125.65	132.67
3	B	3400	ANP	C2'-C1'-N9	-2.08	111.11	114.29
3	B	400	ANP	O1B-PB-N3B	-2.05	108.75	111.90
3	C	2400	ANP	PA-O3A-PB	-2.04	125.83	132.67
3	H	2400	ANP	PA-O3A-PB	-2.04	125.83	132.67
3	F	3400	ANP	C2'-C1'-N9	-2.04	111.18	114.29
3	H	1400	ANP	C2'-C1'-N9	2.01	117.36	114.29
3	C	400	ANP	O3'-C3'-C4'	2.01	117.09	111.05
3	H	3400	ANP	O2A-PA-O3A	2.03	114.28	105.09
3	C	1400	ANP	C2'-C1'-N9	2.03	117.40	114.29
3	G	400	ANP	O3G-PG-O2G	2.07	113.70	107.58
3	B	1400	ANP	C2'-C1'-N9	2.07	117.46	114.29
3	F	400	ANP	O3G-PG-O2G	2.09	113.76	107.58
3	D	400	ANP	O3G-PG-O2G	2.13	113.88	107.58
3	G	3400	ANP	O3A-PB-N3B	2.20	112.48	106.44
3	E	3400	ANP	O3A-PB-N3B	2.23	112.57	106.44
3	E	3400	ANP	O3G-PG-O2G	2.53	115.09	107.58
3	G	3400	ANP	O3G-PG-O2G	2.66	115.45	107.58
3	B	3400	ANP	O3G-PG-O2G	2.66	115.46	107.58
3	D	3400	ANP	O3G-PG-O2G	2.66	115.47	107.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	ANP	O3A-PB-N3B	2.68	113.82	106.44
3	B	400	ANP	O3A-PB-N3B	2.73	113.94	106.44
3	F	3400	ANP	O3G-PG-O2G	2.74	115.69	107.58
3	C	3400	ANP	O3G-PG-O2G	2.80	115.89	107.58
3	H	3400	ANP	O3G-PG-O2G	2.87	116.08	107.58
3	F	400	ANP	O3A-PB-N3B	2.89	114.38	106.44
3	H	400	ANP	O3A-PB-N3B	2.90	114.41	106.44
3	D	400	ANP	O3A-PB-N3B	2.90	114.42	106.44
3	E	400	ANP	O3A-PB-N3B	2.94	114.52	106.44
3	G	400	ANP	O3A-PB-N3B	3.03	114.78	106.44
3	A	3400	ANP	O3G-PG-O2G	3.11	116.80	107.58
3	C	400	ANP	O3A-PB-N3B	3.15	115.10	106.44
3	D	2400	ANP	O3A-PB-N3B	3.58	116.29	106.44
3	E	1400	ANP	O3A-PB-N3B	3.60	116.33	106.44
3	E	2400	ANP	O3A-PB-N3B	3.66	116.50	106.44
3	B	2400	ANP	O3A-PB-N3B	3.66	116.50	106.44
3	A	2400	ANP	O3A-PB-N3B	3.68	116.56	106.44
3	A	3400	ANP	O2B-PB-O1B	3.70	117.73	110.00
3	A	400	ANP	O2B-PB-O1B	3.71	117.75	110.00
3	H	2400	ANP	O3A-PB-N3B	3.73	116.70	106.44
3	F	2400	ANP	O3A-PB-N3B	3.73	116.70	106.44
3	C	2400	ANP	O3A-PB-N3B	3.76	116.77	106.44
3	D	400	ANP	O2B-PB-O1B	3.77	117.86	110.00
3	H	400	ANP	O2B-PB-O1B	3.77	117.86	110.00
3	G	3400	ANP	O2B-PB-O1B	3.77	117.87	110.00
3	D	1400	ANP	O3A-PB-N3B	3.78	116.83	106.44
3	B	400	ANP	O2B-PB-O1B	3.78	117.89	110.00
3	E	400	ANP	O2B-PB-O1B	3.84	118.02	110.00
3	H	1400	ANP	O3A-PB-N3B	3.85	117.03	106.44
3	F	1400	ANP	O3A-PB-N3B	3.89	117.13	106.44
3	G	2400	ANP	O3A-PB-N3B	3.90	117.16	106.44
3	C	1400	ANP	O2B-PB-O1B	3.92	118.18	110.00
3	A	1400	ANP	O3A-PB-N3B	3.92	117.22	106.44
3	B	1400	ANP	O3A-PB-N3B	3.94	117.28	106.44
3	B	3400	ANP	O2B-PB-O1B	3.98	118.32	110.00
3	G	1400	ANP	O3A-PB-N3B	4.00	117.44	106.44
3	C	1400	ANP	O3A-PB-N3B	4.04	117.54	106.44
3	H	1400	ANP	O2B-PB-O1B	4.04	118.44	110.00
3	G	1400	ANP	O2B-PB-O1B	4.05	118.45	110.00
3	F	3400	ANP	O2B-PB-O1B	4.06	118.46	110.00
3	F	1400	ANP	O2B-PB-O1B	4.12	118.60	110.00
3	G	400	ANP	O2B-PB-O1B	4.13	118.63	110.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1400	ANP	O2B-PB-O1B	4.15	118.67	110.00
3	D	3400	ANP	O2B-PB-O1B	4.19	118.74	110.00
3	D	1400	ANP	O2B-PB-O1B	4.20	118.76	110.00
3	F	400	ANP	O2B-PB-O1B	4.20	118.77	110.00
3	E	1400	ANP	O2B-PB-O1B	4.21	118.79	110.00
3	H	2400	ANP	O2B-PB-O1B	4.22	118.81	110.00
3	A	1400	ANP	O2B-PB-O1B	4.24	118.84	110.00
3	G	2400	ANP	O2B-PB-O1B	4.27	118.92	110.00
3	C	400	ANP	O2B-PB-O1B	4.30	118.97	110.00
3	A	2400	ANP	O2B-PB-O1B	4.33	119.03	110.00
3	B	2400	ANP	O2B-PB-O1B	4.39	119.15	110.00
3	D	2400	ANP	O2B-PB-O1B	4.39	119.17	110.00
3	C	2400	ANP	O2B-PB-O1B	4.42	119.22	110.00
3	E	2400	ANP	O2B-PB-O1B	4.42	119.23	110.00
3	C	3400	ANP	O2B-PB-O1B	4.44	119.27	110.00
3	F	2400	ANP	O2B-PB-O1B	4.48	119.34	110.00
3	E	3400	ANP	O2B-PB-O1B	4.56	119.51	110.00
3	H	3400	ANP	O2B-PB-O1B	4.61	119.62	110.00

All (32) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	3400	ANP	C4'
3	D	3400	ANP	C4'
3	E	400	ANP	C4'
3	F	3400	ANP	C4'
3	E	2400	ANP	C4'
3	H	2400	ANP	C4'
3	H	1400	ANP	C4'
3	D	400	ANP	C4'
3	E	3400	ANP	C4'
3	B	3400	ANP	C4'
3	C	3400	ANP	C4'
3	C	1400	ANP	C4'
3	A	2400	ANP	C4'
3	B	2400	ANP	C4'
3	C	2400	ANP	C4'
3	D	2400	ANP	C4'
3	G	1400	ANP	C4'
3	A	400	ANP	C4'
3	G	400	ANP	C4'
3	D	1400	ANP	C4'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
3	F	1400	ANP	C4'
3	F	2400	ANP	C4'
3	G	2400	ANP	C4'
3	A	1400	ANP	C4'
3	F	400	ANP	C4'
3	A	3400	ANP	C4'
3	H	400	ANP	C4'
3	C	400	ANP	C4'
3	B	1400	ANP	C4'
3	H	3400	ANP	C4'
3	E	1400	ANP	C4'
3	B	400	ANP	C4'

There are no torsion outliers.

There are no ring outliers.

17 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1400	ANP	3	0
3	A	3400	ANP	3	0
3	A	400	ANP	1	0
3	B	3400	ANP	1	0
3	B	400	ANP	1	0
3	C	3400	ANP	2	0
3	C	400	ANP	1	0
3	D	3400	ANP	2	0
3	E	1400	ANP	1	0
3	E	3400	ANP	1	0
3	E	400	ANP	1	0
3	F	3400	ANP	3	0
3	F	400	ANP	6	0
3	G	3400	ANP	2	0
3	G	400	ANP	2	0
3	H	3400	ANP	3	0
3	H	400	ANP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	1190/1357 (87%)	-0.13	16 (1%) 79 71	181, 217, 253, 285	0
1	B	1163/1357 (85%)	-0.28	12 (1%) 84 77	175, 217, 254, 286	0
1	C	1175/1357 (86%)	-0.20	13 (1%) 82 76	187, 216, 253, 284	0
1	D	1175/1357 (86%)	-0.11	31 (2%) 59 49	181, 218, 256, 286	0
1	E	1165/1357 (85%)	-0.14	21 (1%) 71 62	186, 218, 255, 288	0
1	F	1175/1357 (86%)	-0.16	13 (1%) 82 76	185, 217, 255, 285	0
1	G	1167/1357 (85%)	-0.18	12 (1%) 84 77	185, 216, 254, 291	0
1	H	1173/1357 (86%)	-0.17	26 (2%) 65 56	186, 218, 255, 288	0
All	All	9383/10856 (86%)	-0.17	144 (1%) 76 67	175, 217, 255, 291	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	3151	PRO	6.6
1	A	3151	PRO	5.9
1	C	3151	PRO	5.1
1	C	2137	ALA	4.8
1	D	211	GLY	4.7
1	G	161	ASP	4.7
1	D	38	GLU	4.7
1	E	3151	PRO	4.5
1	D	39	THR	4.4
1	A	3211	GLY	4.4
1	H	1325	GLU	4.3
1	A	1053	ALA	4.0
1	F	3211	GLY	4.0
1	D	3151	PRO	4.0
1	C	211	GLY	4.0
1	B	3151	PRO	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	3211	GLY	3.9
1	H	309	LEU	3.8
1	B	2237	VAL	3.7
1	G	3151	PRO	3.7
1	E	120	ASP	3.5
1	H	293	TYR	3.5
1	D	1300	GLN	3.5
1	C	3211	GLY	3.5
1	D	295	GLY	3.5
1	B	57	PRO	3.5
1	D	212	GLY	3.4
1	E	3136	GLY	3.3
1	G	3167	ALA	3.3
1	B	1137	ALA	3.3
1	H	291	TYR	3.3
1	D	137	ALA	3.2
1	A	3167	ALA	3.2
1	H	3151	PRO	3.1
1	F	294	LYS	3.1
1	D	57	PRO	3.1
1	E	37	VAL	3.1
1	D	1299	GLY	3.1
1	E	3135	SER	3.1
1	A	1023	LYS	3.1
1	H	298	ILE	3.1
1	H	310	LYS	3.1
1	E	3167	ALA	3.0
1	F	1150	THR	3.0
1	H	308	TRP	3.0
1	D	253	ALA	3.0
1	C	2165	GLY	2.9
1	D	1211	GLY	2.9
1	E	137	ALA	2.9
1	A	1197	MET	2.9
1	D	150	THR	2.9
1	C	3288	GLY	2.9
1	G	60	ARG	2.8
1	B	37	VAL	2.8
1	E	2138	VAL	2.8
1	F	295	GLY	2.8
1	G	2054	GLY	2.7
1	H	305	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	53	ALA	2.7
1	F	162	SER	2.7
1	C	1163	HIS	2.7
1	A	3291	TYR	2.6
1	F	2298	ILE	2.6
1	H	301	GLY	2.6
1	D	1298	ILE	2.6
1	H	1137	ALA	2.5
1	H	1237	VAL	2.5
1	A	53	ALA	2.5
1	H	2213	ASN	2.5
1	B	60	ARG	2.5
1	C	3117	SER	2.5
1	A	1054	GLY	2.5
1	D	285	GLU	2.4
1	F	3290	TRP	2.4
1	C	238	VAL	2.4
1	D	54	GLY	2.4
1	D	172	SER	2.4
1	E	2036	ASP	2.4
1	H	311	ASP	2.4
1	G	3176	ARG	2.4
1	D	1291	TYR	2.4
1	D	55	GLY	2.4
1	D	1090	CYS	2.4
1	C	239	GLY	2.4
1	D	297	LYS	2.3
1	B	3167	ALA	2.3
1	D	37	VAL	2.3
1	C	240	SER	2.3
1	H	162	SER	2.3
1	G	1008	LYS	2.3
1	B	53	ALA	2.3
1	H	306	THR	2.3
1	H	292	SER	2.3
1	C	3287	ALA	2.3
1	D	1009	ALA	2.3
1	E	295	GLY	2.3
1	B	38	GLU	2.3
1	G	1007	GLN	2.3
1	A	3300	GLN	2.3
1	A	284	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	2035	MET	2.3
1	A	1024	GLY	2.3
1	E	3134	ARG	2.2
1	G	2098	ALA	2.2
1	F	293	TYR	2.2
1	F	3287	ALA	2.2
1	H	307	ALA	2.2
1	E	2309	LEU	2.2
1	E	2316	ALA	2.2
1	D	1325	GLU	2.2
1	E	38	GLU	2.2
1	G	315	THR	2.2
1	E	2281	GLU	2.2
1	B	2238	VAL	2.2
1	H	2256	LYS	2.2
1	A	305	ALA	2.2
1	H	2098	ALA	2.2
1	F	2028	ARG	2.2
1	H	312	ASN	2.2
1	H	1090	CYS	2.2
1	D	1012	ALA	2.1
1	A	1022	GLY	2.1
1	B	1035	MET	2.1
1	E	296	GLU	2.1
1	H	304	ASN	2.1
1	E	3211	GLY	2.1
1	G	1283	LEU	2.1
1	A	3297	LYS	2.1
1	D	60	ARG	2.1
1	D	1089	THR	2.1
1	E	211	GLY	2.1
1	E	2137	ALA	2.1
1	D	87	GLY	2.1
1	E	2314	GLU	2.1
1	C	1164	MET	2.0
1	A	3299	GLY	2.0
1	F	161	ASP	2.0
1	F	302	LYS	2.0
1	G	113	ASN	2.0
1	H	165	GLY	2.0
1	D	1297	LYS	2.0
1	D	296	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	39	THR	2.0
1	E	3009	ALA	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MG	E	701	1/1	0.58	1.16	7.93	204,204,204,204	0
2	MG	F	701	1/1	0.94	0.55	4.64	189,189,189,189	0
2	MG	E	2701	1/1	0.87	0.34	1.08	228,228,228,228	0
3	ANP	G	2400	31/31	0.72	0.41	1.02	303,308,315,315	0
3	ANP	H	400	31/31	0.83	0.42	0.90	254,263,265,265	0
3	ANP	E	1400	31/31	0.79	0.32	0.83	287,293,296,296	0
3	ANP	D	400	31/31	0.84	0.29	0.78	263,273,274,274	0
3	ANP	B	1400	31/31	0.86	0.30	0.76	275,286,290,290	0
3	ANP	F	1400	31/31	0.82	0.34	0.70	271,280,286,286	0
2	MG	D	2701	1/1	0.67	0.41	0.69	237,237,237,237	0
3	ANP	F	2400	31/31	0.72	0.44	0.68	286,303,310,310	0
3	ANP	D	1400	31/31	0.75	0.38	0.66	287,290,294,294	0
3	ANP	A	2400	31/31	0.86	0.34	0.65	308,311,315,315	0
3	ANP	H	2400	31/31	0.73	0.38	0.59	298,312,316,316	0
3	ANP	B	2400	31/31	0.79	0.34	0.40	306,312,314,314	0
3	ANP	A	1400	31/31	0.75	0.36	0.40	267,280,283,283	0
3	ANP	B	400	31/31	0.80	0.33	0.32	242,255,259,260	0
3	ANP	H	1400	31/31	0.83	0.32	0.31	296,299,304,304	0
3	ANP	G	400	31/31	0.84	0.28	0.26	253,262,264,265	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ANP	C	1400	31/31	0.84	0.25	0.26	288,291,293,294	0
2	MG	G	2701	1/1	0.93	0.45	0.24	192,192,192,192	0
3	ANP	F	400	31/31	0.86	0.33	0.11	243,257,263,263	0
2	MG	F	2701	1/1	0.80	0.37	0.10	232,232,232,232	0
3	ANP	D	2400	31/31	0.85	0.30	0.07	305,310,315,315	0
2	MG	H	2701	1/1	0.83	0.36	0.01	271,271,271,271	0
3	ANP	E	2400	31/31	0.90	0.25	-0.05	307,317,320,320	0
2	MG	B	3701	1/1	0.96	0.18	-0.07	69,69,69,69	0
3	ANP	A	400	31/31	0.88	0.27	-0.09	246,250,255,256	0
3	ANP	E	400	31/31	0.89	0.26	-0.15	256,261,264,265	0
3	ANP	C	2400	31/31	0.89	0.28	-0.25	296,309,314,315	0
2	MG	E	3701	1/1	0.86	0.20	-0.29	131,131,131,131	0
3	ANP	C	400	31/31	0.84	0.29	-0.30	226,245,250,250	0
3	ANP	G	1400	31/31	0.81	0.25	-0.45	279,285,289,290	0
3	ANP	G	3400	31/31	0.91	0.19	-0.46	153,176,191,192	0
3	ANP	H	3400	31/31	0.90	0.18	-0.54	180,187,196,197	0
3	ANP	F	3400	31/31	0.92	0.20	-0.57	148,171,183,183	0
2	MG	B	2701	1/1	0.71	0.26	-0.71	238,238,238,238	0
2	MG	C	2701	1/1	0.93	0.26	-0.74	211,211,211,211	0
3	ANP	E	3400	31/31	0.94	0.19	-0.79	163,180,187,187	0
2	MG	C	3701	1/1	0.83	0.14	-0.83	140,140,140,140	0
3	ANP	B	3400	31/31	0.93	0.18	-0.86	143,159,176,178	0
3	ANP	C	3400	31/31	0.93	0.14	-0.87	176,190,200,200	0
2	MG	D	3701	1/1	0.95	0.14	-0.90	108,108,108,108	0
3	ANP	D	3400	31/31	0.92	0.16	-0.93	149,170,188,189	0
2	MG	G	3701	1/1	0.97	0.10	-1.30	100,100,100,100	0
2	MG	A	2701	1/1	0.89	0.15	-1.44	247,247,247,247	0
3	ANP	A	3400	31/31	0.94	0.17	-1.47	152,165,180,181	0
2	MG	H	3701	1/1	0.95	0.15	-1.55	121,121,121,121	0
2	MG	A	3701	1/1	0.97	0.09	-3.54	116,116,116,116	0
2	MG	F	3701	1/1	0.98	0.09	-4.18	77,77,77,77	0
2	MG	B	701	1/1	0.84	1.12	-	184,184,184,184	0
2	MG	E	1701	1/1	0.83	0.48	-	190,190,190,190	0
2	MG	D	701	1/1	0.76	0.65	-	261,261,261,261	0
2	MG	D	1701	1/1	0.75	1.11	-	212,212,212,212	0
2	MG	F	1701	1/1	0.86	0.59	-	175,175,175,175	0
2	MG	A	701	1/1	0.86	0.63	-	143,143,143,143	0
2	MG	C	1701	1/1	0.96	0.18	-	132,132,132,132	0
2	MG	C	701	1/1	0.58	0.61	-	177,177,177,177	0
2	MG	A	1701	1/1	0.87	0.86	-	181,181,181,181	0
2	MG	G	1701	1/1	0.89	0.53	-	191,191,191,191	0
2	MG	H	1701	1/1	0.83	0.67	-	188,188,188,188	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	H	701	1/1	0.92	0.17	-	200,200,200,200	0
2	MG	G	701	1/1	0.54	0.96	-	215,215,215,215	0
2	MG	B	1701	1/1	0.74	0.41	-	214,214,214,214	0

6.5 Other polymers [i](#)

There are no such residues in this entry.