Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:39 AM GMT

PDB ID	:	3FBV
Title	:	Crystal structure of the oligomer formed by the kinase-ribonuclease domain of Ire1
Authors	:	Korennykh, A.V.; Egea, P.F.; Korostelev, A.A.; Finer-Moore, J.; Zhang, C.; Shokat, K.M.; Stroud, R.M.; Walter, P.
Deposited on	:	2008-11-19
Resolution	:	3.20 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 (i) symbol.

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

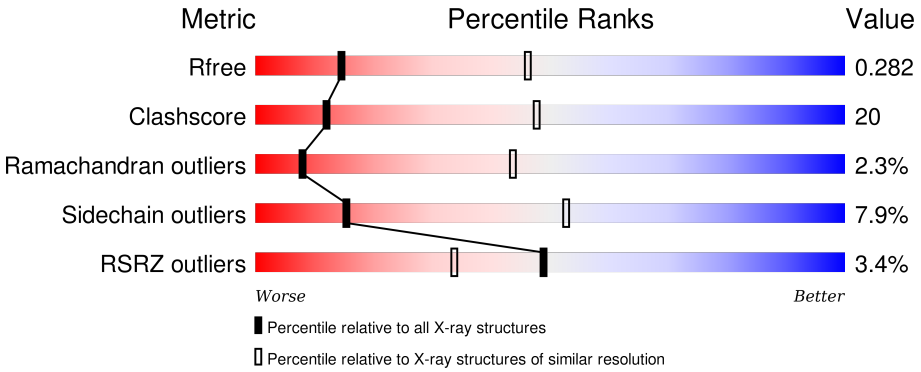
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	448	56% 32% 7%
1	B	448	58% 30% 5% 7%
1	C	448	54% 34% 5% 7%
1	D	448	55% 33% 6% 5%
1	E	448	57% 31% 5% 7%

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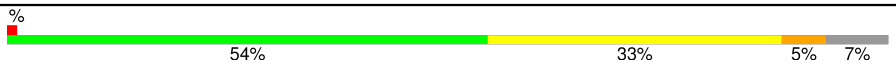
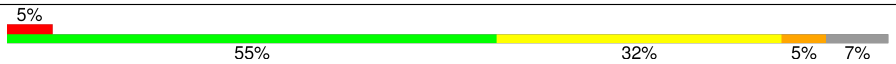
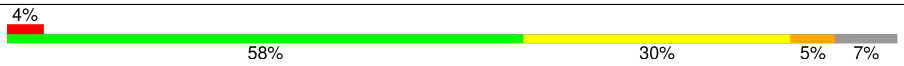
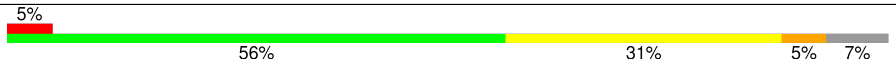
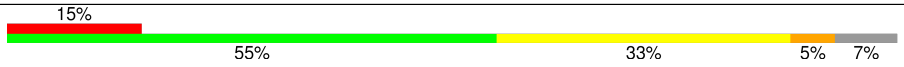
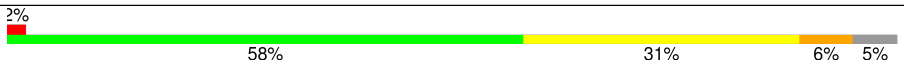
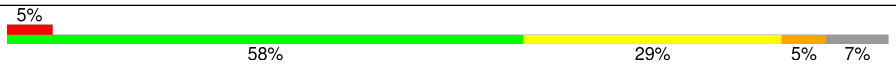
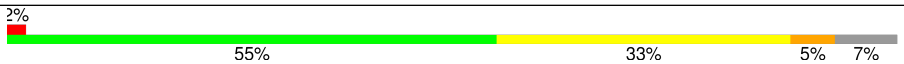
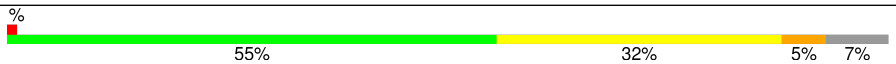
Mol	Chain	Length	Quality of chain
1	F	448	
1	G	448	
1	H	448	
1	I	448	
1	J	448	
1	K	448	
1	L	448	
1	M	448	
1	N	448	

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	APJ	H	1999	-	-	-	X
2	APJ	J	1999	-	-	-	X
2	APJ	K	1999	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 48018 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 Serine/threonine-protein kinase/endoribonuclease IRE1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	B	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	C	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	D	425	Total	C	N	O	P	S	0	0	0
			3457	2199	589	648	3	18			
1	E	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	F	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	G	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	H	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	I	416	Total	C	N	O	P	S	0	0	0
			3382	2150	577	634	3	18			
1	J	416	Total	C	N	O	P	S	0	0	0
			3382	2150	577	634	3	18			
1	K	425	Total	C	N	O	P	S	0	0	0
			3457	2199	589	648	3	18			
1	L	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	M	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			
1	N	418	Total	C	N	O	P	S	0	0	0
			3399	2162	580	636	3	18			

There are 406 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	640	PRO	-	EXPRESSION TAG	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	DELETION	UNP P32361
A	?	-	ASN	DELETION	UNP P32361
A	?	-	LEU	DELETION	UNP P32361
A	?	-	GLN	DELETION	UNP P32361
A	?	-	CYS	DELETION	UNP P32361
A	?	-	GLN	DELETION	UNP P32361
A	?	-	VAL	DELETION	UNP P32361
A	?	-	GLU	DELETION	UNP P32361
A	?	-	THR	DELETION	UNP P32361
A	?	-	GLU	DELETION	UNP P32361
A	?	-	HIS	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	ARG	DELETION	UNP P32361
A	?	-	HIS	DELETION	UNP P32361
A	?	-	THR	DELETION	UNP P32361
A	?	-	VAL	DELETION	UNP P32361
A	?	-	VAL	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	ASP	DELETION	UNP P32361
A	?	-	SER	DELETION	UNP P32361
A	?	-	PHE	DELETION	UNP P32361
A	?	-	TYR	DELETION	UNP P32361
A	?	-	ASP	DELETION	UNP P32361
A	?	-	PRO	DELETION	UNP P32361
A	?	-	PHE	DELETION	UNP P32361
B	640	PRO	-	EXPRESSION TAG	UNP P32361
B	?	-	ASN	DELETION	UNP P32361
B	?	-	ASN	DELETION	UNP P32361
B	?	-	LEU	DELETION	UNP P32361
B	?	-	GLN	DELETION	UNP P32361
B	?	-	CYS	DELETION	UNP P32361
B	?	-	GLN	DELETION	UNP P32361
B	?	-	VAL	DELETION	UNP P32361
B	?	-	GLU	DELETION	UNP P32361
B	?	-	THR	DELETION	UNP P32361
B	?	-	GLU	DELETION	UNP P32361
B	?	-	HIS	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	DELETION	UNP P32361
B	?	-	ARG	DELETION	UNP P32361
B	?	-	HIS	DELETION	UNP P32361
B	?	-	THR	DELETION	UNP P32361
B	?	-	VAL	DELETION	UNP P32361
B	?	-	VAL	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361
B	?	-	ASP	DELETION	UNP P32361
B	?	-	SER	DELETION	UNP P32361
B	?	-	PHE	DELETION	UNP P32361
B	?	-	TYR	DELETION	UNP P32361
B	?	-	ASP	DELETION	UNP P32361
B	?	-	PRO	DELETION	UNP P32361
B	?	-	PHE	DELETION	UNP P32361
C	640	PRO	-	EXPRESSION TAG	UNP P32361
C	?	-	ASN	DELETION	UNP P32361
C	?	-	ASN	DELETION	UNP P32361
C	?	-	LEU	DELETION	UNP P32361
C	?	-	GLN	DELETION	UNP P32361
C	?	-	CYS	DELETION	UNP P32361
C	?	-	GLN	DELETION	UNP P32361
C	?	-	VAL	DELETION	UNP P32361
C	?	-	GLU	DELETION	UNP P32361
C	?	-	THR	DELETION	UNP P32361
C	?	-	GLU	DELETION	UNP P32361
C	?	-	HIS	DELETION	UNP P32361
C	?	-	SER	DELETION	UNP P32361
C	?	-	SER	DELETION	UNP P32361
C	?	-	SER	DELETION	UNP P32361
C	?	-	ARG	DELETION	UNP P32361
C	?	-	HIS	DELETION	UNP P32361
C	?	-	THR	DELETION	UNP P32361
C	?	-	VAL	DELETION	UNP P32361
C	?	-	VAL	DELETION	UNP P32361
C	?	-	SER	DELETION	UNP P32361
C	?	-	SER	DELETION	UNP P32361
C	?	-	ASP	DELETION	UNP P32361
C	?	-	SER	DELETION	UNP P32361
C	?	-	PHE	DELETION	UNP P32361
C	?	-	TYR	DELETION	UNP P32361
C	?	-	ASP	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	PRO	DELETION	UNP P32361
C	?	-	PHE	DELETION	UNP P32361
D	640	PRO	-	EXPRESSION TAG	UNP P32361
D	?	-	ASN	DELETION	UNP P32361
D	?	-	ASN	DELETION	UNP P32361
D	?	-	LEU	DELETION	UNP P32361
D	?	-	GLN	DELETION	UNP P32361
D	?	-	CYS	DELETION	UNP P32361
D	?	-	GLN	DELETION	UNP P32361
D	?	-	VAL	DELETION	UNP P32361
D	?	-	GLU	DELETION	UNP P32361
D	?	-	THR	DELETION	UNP P32361
D	?	-	GLU	DELETION	UNP P32361
D	?	-	HIS	DELETION	UNP P32361
D	?	-	SER	DELETION	UNP P32361
D	?	-	SER	DELETION	UNP P32361
D	?	-	SER	DELETION	UNP P32361
D	?	-	ARG	DELETION	UNP P32361
D	?	-	HIS	DELETION	UNP P32361
D	?	-	THR	DELETION	UNP P32361
D	?	-	VAL	DELETION	UNP P32361
D	?	-	VAL	DELETION	UNP P32361
D	?	-	SER	DELETION	UNP P32361
D	?	-	SER	DELETION	UNP P32361
D	?	-	ASP	DELETION	UNP P32361
D	?	-	SER	DELETION	UNP P32361
D	?	-	PHE	DELETION	UNP P32361
D	?	-	TYR	DELETION	UNP P32361
D	?	-	ASP	DELETION	UNP P32361
D	?	-	PRO	DELETION	UNP P32361
D	?	-	PHE	DELETION	UNP P32361
E	640	PRO	-	EXPRESSION TAG	UNP P32361
E	?	-	ASN	DELETION	UNP P32361
E	?	-	ASN	DELETION	UNP P32361
E	?	-	LEU	DELETION	UNP P32361
E	?	-	GLN	DELETION	UNP P32361
E	?	-	CYS	DELETION	UNP P32361
E	?	-	GLN	DELETION	UNP P32361
E	?	-	VAL	DELETION	UNP P32361
E	?	-	GLU	DELETION	UNP P32361
E	?	-	THR	DELETION	UNP P32361
E	?	-	GLU	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	HIS	DELETION	UNP P32361
E	?	-	SER	DELETION	UNP P32361
E	?	-	SER	DELETION	UNP P32361
E	?	-	SER	DELETION	UNP P32361
E	?	-	ARG	DELETION	UNP P32361
E	?	-	HIS	DELETION	UNP P32361
E	?	-	THR	DELETION	UNP P32361
E	?	-	VAL	DELETION	UNP P32361
E	?	-	VAL	DELETION	UNP P32361
E	?	-	SER	DELETION	UNP P32361
E	?	-	SER	DELETION	UNP P32361
E	?	-	ASP	DELETION	UNP P32361
E	?	-	SER	DELETION	UNP P32361
E	?	-	PHE	DELETION	UNP P32361
E	?	-	TYR	DELETION	UNP P32361
E	?	-	ASP	DELETION	UNP P32361
E	?	-	PRO	DELETION	UNP P32361
E	?	-	PHE	DELETION	UNP P32361
F	640	PRO	-	EXPRESSION TAG	UNP P32361
F	?	-	ASN	DELETION	UNP P32361
F	?	-	ASN	DELETION	UNP P32361
F	?	-	LEU	DELETION	UNP P32361
F	?	-	GLN	DELETION	UNP P32361
F	?	-	CYS	DELETION	UNP P32361
F	?	-	GLN	DELETION	UNP P32361
F	?	-	VAL	DELETION	UNP P32361
F	?	-	GLU	DELETION	UNP P32361
F	?	-	THR	DELETION	UNP P32361
F	?	-	GLU	DELETION	UNP P32361
F	?	-	HIS	DELETION	UNP P32361
F	?	-	SER	DELETION	UNP P32361
F	?	-	SER	DELETION	UNP P32361
F	?	-	SER	DELETION	UNP P32361
F	?	-	ARG	DELETION	UNP P32361
F	?	-	HIS	DELETION	UNP P32361
F	?	-	THR	DELETION	UNP P32361
F	?	-	VAL	DELETION	UNP P32361
F	?	-	VAL	DELETION	UNP P32361
F	?	-	SER	DELETION	UNP P32361
F	?	-	SER	DELETION	UNP P32361
F	?	-	ASP	DELETION	UNP P32361
F	?	-	SER	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	PHE	DELETION	UNP P32361
F	?	-	TYR	DELETION	UNP P32361
F	?	-	ASP	DELETION	UNP P32361
F	?	-	PRO	DELETION	UNP P32361
F	?	-	PHE	DELETION	UNP P32361
G	640	PRO	-	EXPRESSION TAG	UNP P32361
G	?	-	ASN	DELETION	UNP P32361
G	?	-	ASN	DELETION	UNP P32361
G	?	-	LEU	DELETION	UNP P32361
G	?	-	GLN	DELETION	UNP P32361
G	?	-	CYS	DELETION	UNP P32361
G	?	-	GLN	DELETION	UNP P32361
G	?	-	VAL	DELETION	UNP P32361
G	?	-	GLU	DELETION	UNP P32361
G	?	-	THR	DELETION	UNP P32361
G	?	-	GLU	DELETION	UNP P32361
G	?	-	HIS	DELETION	UNP P32361
G	?	-	SER	DELETION	UNP P32361
G	?	-	SER	DELETION	UNP P32361
G	?	-	SER	DELETION	UNP P32361
G	?	-	ARG	DELETION	UNP P32361
G	?	-	HIS	DELETION	UNP P32361
G	?	-	THR	DELETION	UNP P32361
G	?	-	VAL	DELETION	UNP P32361
G	?	-	VAL	DELETION	UNP P32361
G	?	-	SER	DELETION	UNP P32361
G	?	-	SER	DELETION	UNP P32361
G	?	-	ASP	DELETION	UNP P32361
G	?	-	SER	DELETION	UNP P32361
G	?	-	PHE	DELETION	UNP P32361
G	?	-	TYR	DELETION	UNP P32361
G	?	-	ASP	DELETION	UNP P32361
G	?	-	PRO	DELETION	UNP P32361
G	?	-	PHE	DELETION	UNP P32361
H	640	PRO	-	EXPRESSION TAG	UNP P32361
H	?	-	ASN	DELETION	UNP P32361
H	?	-	ASN	DELETION	UNP P32361
H	?	-	LEU	DELETION	UNP P32361
H	?	-	GLN	DELETION	UNP P32361
H	?	-	CYS	DELETION	UNP P32361
H	?	-	GLN	DELETION	UNP P32361
H	?	-	VAL	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	GLU	DELETION	UNP P32361
H	?	-	THR	DELETION	UNP P32361
H	?	-	GLU	DELETION	UNP P32361
H	?	-	HIS	DELETION	UNP P32361
H	?	-	SER	DELETION	UNP P32361
H	?	-	SER	DELETION	UNP P32361
H	?	-	SER	DELETION	UNP P32361
H	?	-	ARG	DELETION	UNP P32361
H	?	-	HIS	DELETION	UNP P32361
H	?	-	THR	DELETION	UNP P32361
H	?	-	VAL	DELETION	UNP P32361
H	?	-	VAL	DELETION	UNP P32361
H	?	-	SER	DELETION	UNP P32361
H	?	-	SER	DELETION	UNP P32361
H	?	-	ASP	DELETION	UNP P32361
H	?	-	SER	DELETION	UNP P32361
H	?	-	PHE	DELETION	UNP P32361
H	?	-	TYR	DELETION	UNP P32361
H	?	-	ASP	DELETION	UNP P32361
H	?	-	PRO	DELETION	UNP P32361
H	?	-	PHE	DELETION	UNP P32361
I	640	PRO	-	EXPRESSION TAG	UNP P32361
I	?	-	ASN	DELETION	UNP P32361
I	?	-	ASN	DELETION	UNP P32361
I	?	-	LEU	DELETION	UNP P32361
I	?	-	GLN	DELETION	UNP P32361
I	?	-	CYS	DELETION	UNP P32361
I	?	-	GLN	DELETION	UNP P32361
I	?	-	VAL	DELETION	UNP P32361
I	?	-	GLU	DELETION	UNP P32361
I	?	-	THR	DELETION	UNP P32361
I	?	-	GLU	DELETION	UNP P32361
I	?	-	HIS	DELETION	UNP P32361
I	?	-	SER	DELETION	UNP P32361
I	?	-	SER	DELETION	UNP P32361
I	?	-	SER	DELETION	UNP P32361
I	?	-	ARG	DELETION	UNP P32361
I	?	-	HIS	DELETION	UNP P32361
I	?	-	THR	DELETION	UNP P32361
I	?	-	VAL	DELETION	UNP P32361
I	?	-	VAL	DELETION	UNP P32361
I	?	-	SER	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
I	?	-	SER	DELETION	UNP P32361
I	?	-	ASP	DELETION	UNP P32361
I	?	-	SER	DELETION	UNP P32361
I	?	-	PHE	DELETION	UNP P32361
I	?	-	TYR	DELETION	UNP P32361
I	?	-	ASP	DELETION	UNP P32361
I	?	-	PRO	DELETION	UNP P32361
I	?	-	PHE	DELETION	UNP P32361
J	640	PRO	-	EXPRESSION TAG	UNP P32361
J	?	-	ASN	DELETION	UNP P32361
J	?	-	ASN	DELETION	UNP P32361
J	?	-	LEU	DELETION	UNP P32361
J	?	-	GLN	DELETION	UNP P32361
J	?	-	CYS	DELETION	UNP P32361
J	?	-	GLN	DELETION	UNP P32361
J	?	-	VAL	DELETION	UNP P32361
J	?	-	GLU	DELETION	UNP P32361
J	?	-	THR	DELETION	UNP P32361
J	?	-	GLU	DELETION	UNP P32361
J	?	-	HIS	DELETION	UNP P32361
J	?	-	SER	DELETION	UNP P32361
J	?	-	SER	DELETION	UNP P32361
J	?	-	SER	DELETION	UNP P32361
J	?	-	ARG	DELETION	UNP P32361
J	?	-	HIS	DELETION	UNP P32361
J	?	-	THR	DELETION	UNP P32361
J	?	-	VAL	DELETION	UNP P32361
J	?	-	VAL	DELETION	UNP P32361
J	?	-	SER	DELETION	UNP P32361
J	?	-	SER	DELETION	UNP P32361
J	?	-	ASP	DELETION	UNP P32361
J	?	-	SER	DELETION	UNP P32361
J	?	-	PHE	DELETION	UNP P32361
J	?	-	TYR	DELETION	UNP P32361
J	?	-	ASP	DELETION	UNP P32361
J	?	-	PRO	DELETION	UNP P32361
J	?	-	PHE	DELETION	UNP P32361
K	640	PRO	-	EXPRESSION TAG	UNP P32361
K	?	-	ASN	DELETION	UNP P32361
K	?	-	ASN	DELETION	UNP P32361
K	?	-	LEU	DELETION	UNP P32361
K	?	-	GLN	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
K	?	-	CYS	DELETION	UNP P32361
K	?	-	GLN	DELETION	UNP P32361
K	?	-	VAL	DELETION	UNP P32361
K	?	-	GLU	DELETION	UNP P32361
K	?	-	THR	DELETION	UNP P32361
K	?	-	GLU	DELETION	UNP P32361
K	?	-	HIS	DELETION	UNP P32361
K	?	-	SER	DELETION	UNP P32361
K	?	-	SER	DELETION	UNP P32361
K	?	-	SER	DELETION	UNP P32361
K	?	-	ARG	DELETION	UNP P32361
K	?	-	HIS	DELETION	UNP P32361
K	?	-	THR	DELETION	UNP P32361
K	?	-	VAL	DELETION	UNP P32361
K	?	-	VAL	DELETION	UNP P32361
K	?	-	SER	DELETION	UNP P32361
K	?	-	SER	DELETION	UNP P32361
K	?	-	ASP	DELETION	UNP P32361
K	?	-	SER	DELETION	UNP P32361
K	?	-	PHE	DELETION	UNP P32361
K	?	-	TYR	DELETION	UNP P32361
K	?	-	ASP	DELETION	UNP P32361
K	?	-	PRO	DELETION	UNP P32361
K	?	-	PHE	DELETION	UNP P32361
L	640	PRO	-	EXPRESSION TAG	UNP P32361
L	?	-	ASN	DELETION	UNP P32361
L	?	-	ASN	DELETION	UNP P32361
L	?	-	LEU	DELETION	UNP P32361
L	?	-	GLN	DELETION	UNP P32361
L	?	-	CYS	DELETION	UNP P32361
L	?	-	GLN	DELETION	UNP P32361
L	?	-	VAL	DELETION	UNP P32361
L	?	-	GLU	DELETION	UNP P32361
L	?	-	THR	DELETION	UNP P32361
L	?	-	GLU	DELETION	UNP P32361
L	?	-	HIS	DELETION	UNP P32361
L	?	-	SER	DELETION	UNP P32361
L	?	-	SER	DELETION	UNP P32361
L	?	-	SER	DELETION	UNP P32361
L	?	-	ARG	DELETION	UNP P32361
L	?	-	HIS	DELETION	UNP P32361
L	?	-	THR	DELETION	UNP P32361

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Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	VAL	DELETION	UNP P32361
L	?	-	VAL	DELETION	UNP P32361
L	?	-	SER	DELETION	UNP P32361
L	?	-	SER	DELETION	UNP P32361
L	?	-	ASP	DELETION	UNP P32361
L	?	-	SER	DELETION	UNP P32361
L	?	-	PHE	DELETION	UNP P32361
L	?	-	TYR	DELETION	UNP P32361
L	?	-	ASP	DELETION	UNP P32361
L	?	-	PRO	DELETION	UNP P32361
L	?	-	PHE	DELETION	UNP P32361
M	640	PRO	-	EXPRESSION TAG	UNP P32361
M	?	-	ASN	DELETION	UNP P32361
M	?	-	ASN	DELETION	UNP P32361
M	?	-	LEU	DELETION	UNP P32361
M	?	-	GLN	DELETION	UNP P32361
M	?	-	CYS	DELETION	UNP P32361
M	?	-	GLN	DELETION	UNP P32361
M	?	-	VAL	DELETION	UNP P32361
M	?	-	GLU	DELETION	UNP P32361
M	?	-	THR	DELETION	UNP P32361
M	?	-	GLU	DELETION	UNP P32361
M	?	-	HIS	DELETION	UNP P32361
M	?	-	SER	DELETION	UNP P32361
M	?	-	SER	DELETION	UNP P32361
M	?	-	SER	DELETION	UNP P32361
M	?	-	ARG	DELETION	UNP P32361
M	?	-	HIS	DELETION	UNP P32361
M	?	-	THR	DELETION	UNP P32361
M	?	-	VAL	DELETION	UNP P32361
M	?	-	VAL	DELETION	UNP P32361
M	?	-	SER	DELETION	UNP P32361
M	?	-	SER	DELETION	UNP P32361
M	?	-	ASP	DELETION	UNP P32361
M	?	-	SER	DELETION	UNP P32361
M	?	-	PHE	DELETION	UNP P32361
M	?	-	TYR	DELETION	UNP P32361
M	?	-	ASP	DELETION	UNP P32361
M	?	-	PRO	DELETION	UNP P32361
M	?	-	PHE	DELETION	UNP P32361
N	640	PRO	-	EXPRESSION TAG	UNP P32361
N	?	-	ASN	DELETION	UNP P32361

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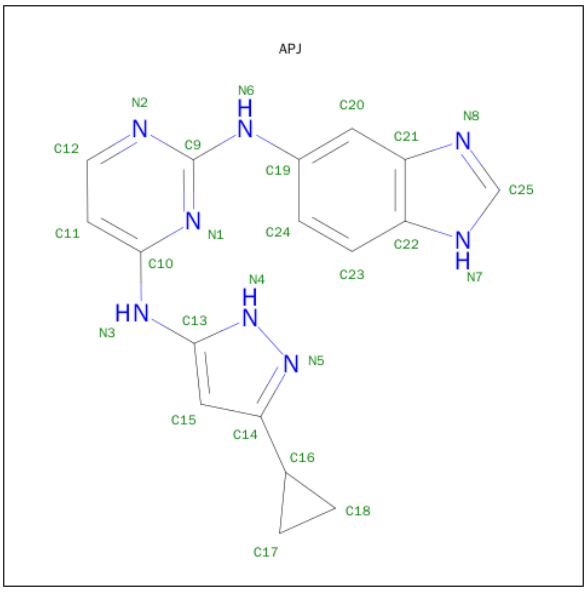
Chain	Residue	Modelled	Actual	Comment	Reference
N	?	-	ASN	DELETION	UNP P32361
N	?	-	LEU	DELETION	UNP P32361
N	?	-	GLN	DELETION	UNP P32361
N	?	-	CYS	DELETION	UNP P32361
N	?	-	GLN	DELETION	UNP P32361
N	?	-	VAL	DELETION	UNP P32361
N	?	-	GLU	DELETION	UNP P32361
N	?	-	THR	DELETION	UNP P32361
N	?	-	GLU	DELETION	UNP P32361
N	?	-	HIS	DELETION	UNP P32361
N	?	-	SER	DELETION	UNP P32361
N	?	-	SER	DELETION	UNP P32361
N	?	-	SER	DELETION	UNP P32361
N	?	-	ARG	DELETION	UNP P32361
N	?	-	HIS	DELETION	UNP P32361
N	?	-	THR	DELETION	UNP P32361
N	?	-	VAL	DELETION	UNP P32361
N	?	-	VAL	DELETION	UNP P32361
N	?	-	SER	DELETION	UNP P32361
N	?	-	SER	DELETION	UNP P32361
N	?	-	ASP	DELETION	UNP P32361
N	?	-	SER	DELETION	UNP P32361
N	?	-	PHE	DELETION	UNP P32361
N	?	-	TYR	DELETION	UNP P32361
N	?	-	ASP	DELETION	UNP P32361
N	?	-	PRO	DELETION	UNP P32361
N	?	-	PHE	DELETION	UNP P32361

- Molecule 2 is N 2 -1H-BENZIMIDAZOL-5-YL-N 4 -(3-CYCLOPROPYL-1H-PYRAZOL-5-YL)PYRIMIDINE-2,4-DIAMINE (three-letter code: APJ) (formula: $C_{17}H_{16}N_8$).



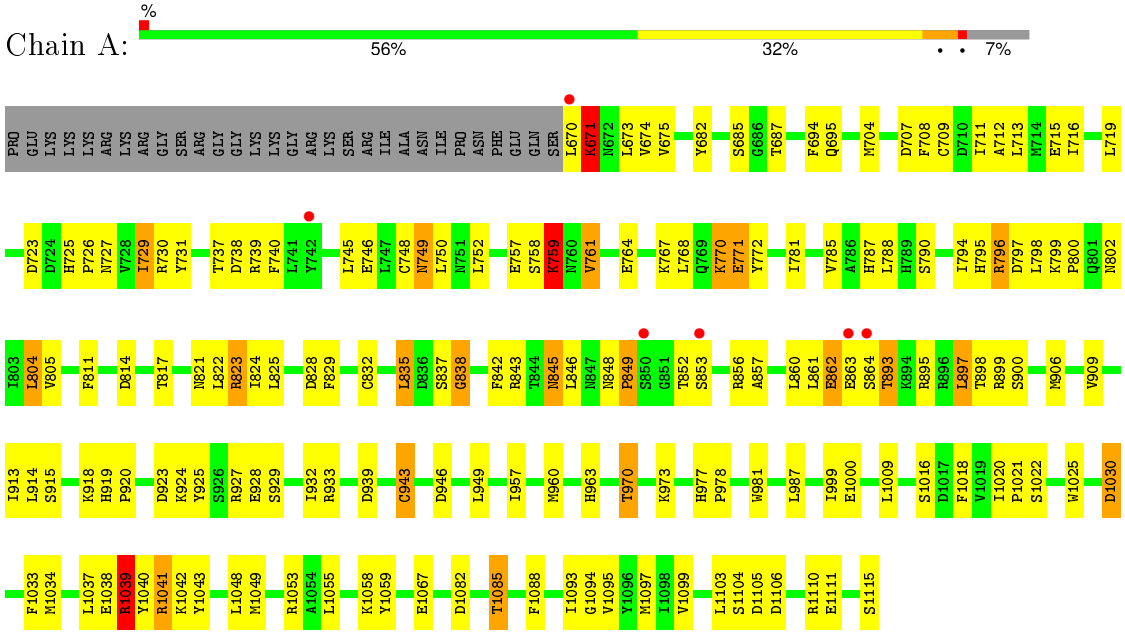
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N 25 17 8	0	0
2	B	1	Total C N 25 17 8	0	0
2	C	1	Total C N 25 17 8	0	0
2	D	1	Total C N 25 17 8	0	0
2	E	1	Total C N 25 17 8	0	0
2	F	1	Total C N 25 17 8	0	0
2	G	1	Total C N 25 17 8	0	0
2	H	1	Total C N 25 17 8	0	0
2	I	1	Total C N 25 17 8	0	0
2	J	1	Total C N 25 17 8	0	0
2	K	1	Total C N 25 17 8	0	0
2	L	1	Total C N 25 17 8	0	0
2	M	1	Total C N 25 17 8	0	0
2	N	1	Total C N 25 17 8	0	0

3 Residue-property plots (i)

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

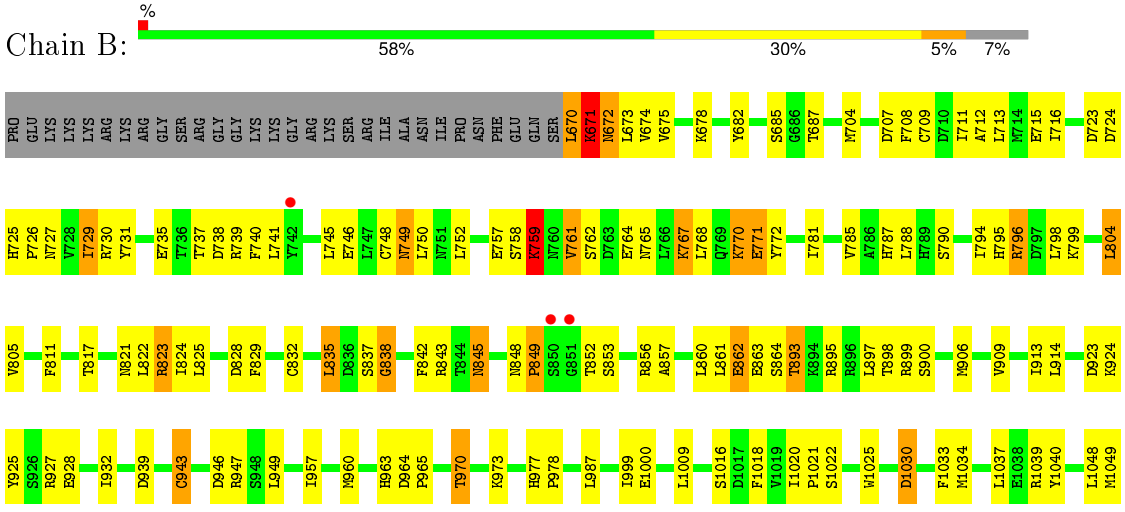
- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain A:



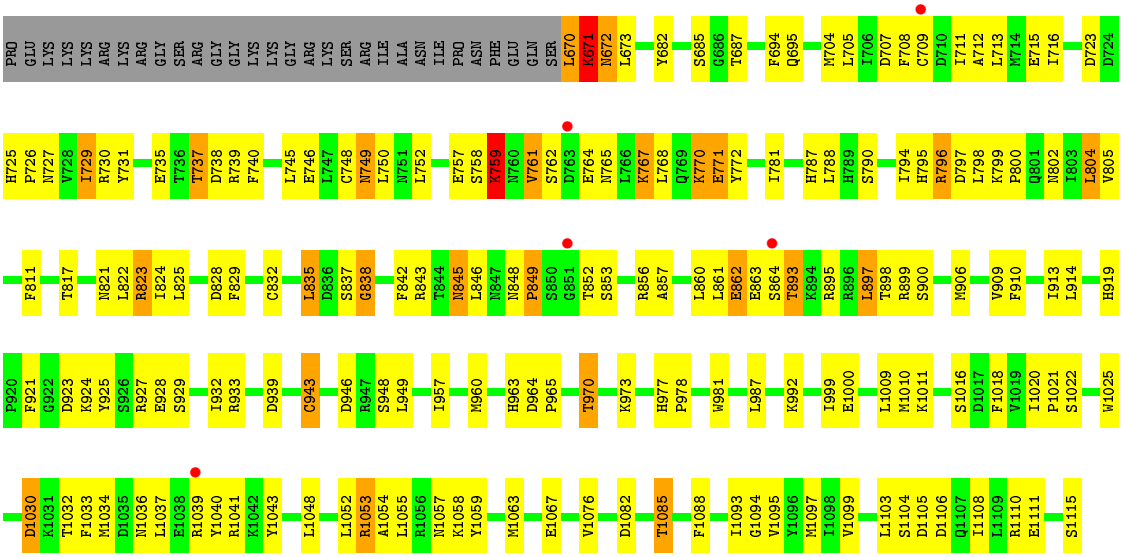
- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain B:



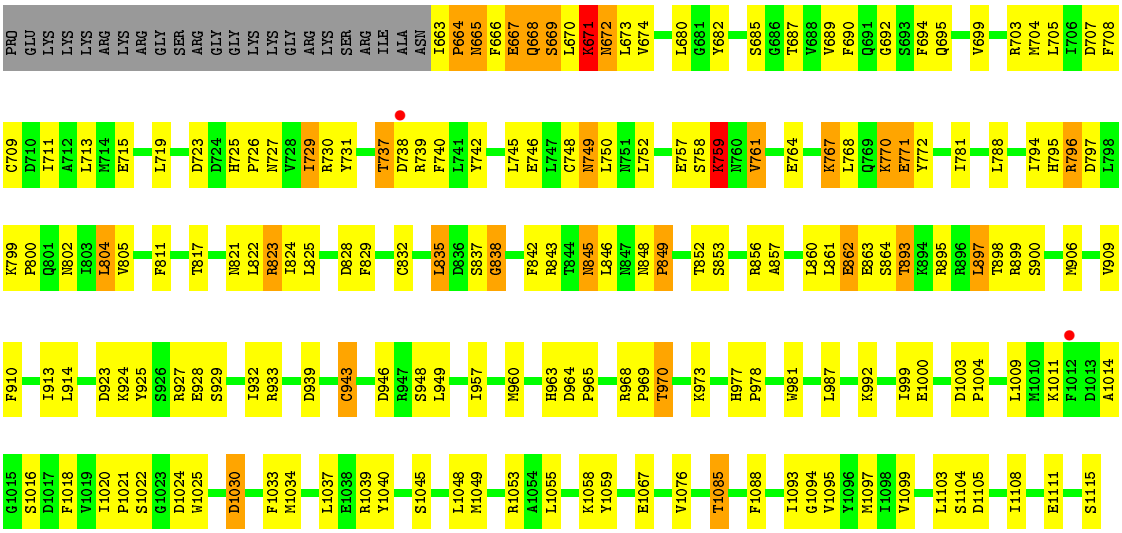
• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain C:



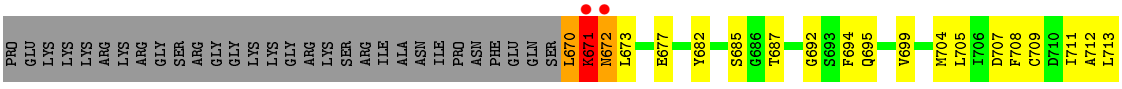
• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

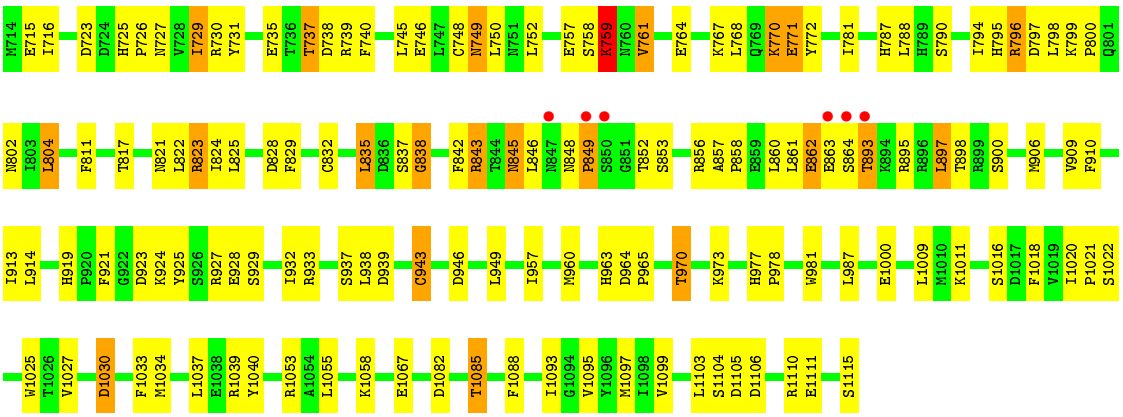
Chain D:



• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

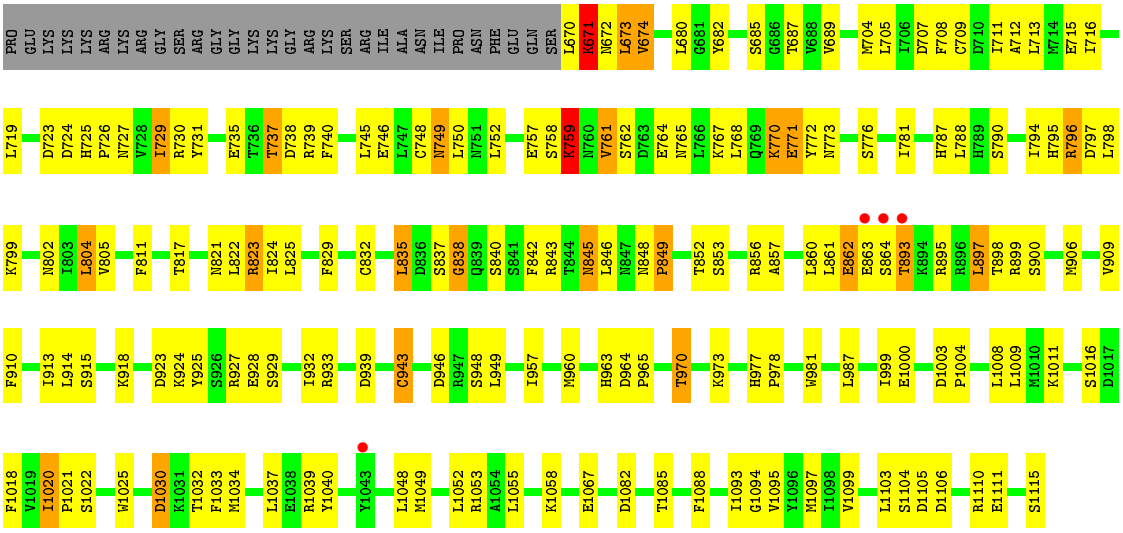
Chain E:





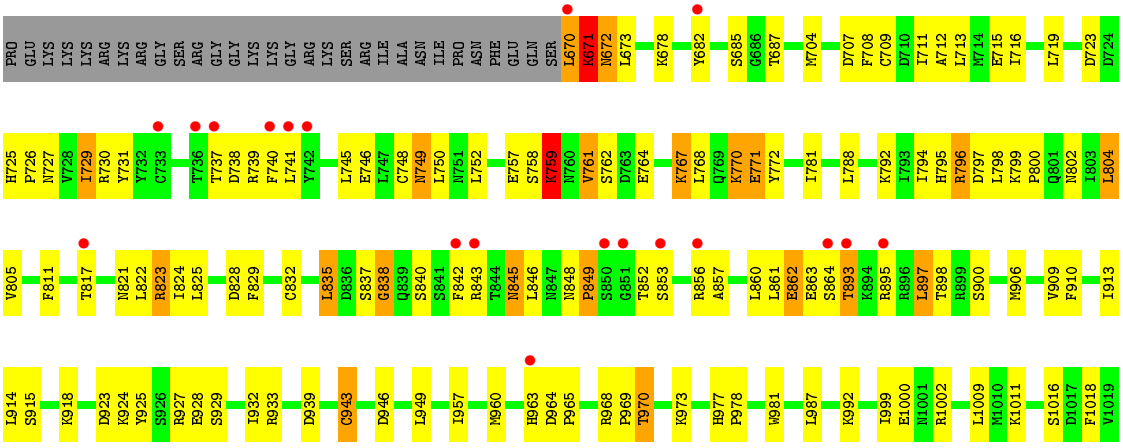
• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

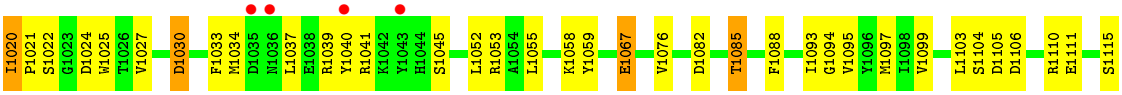
Chain F:



• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

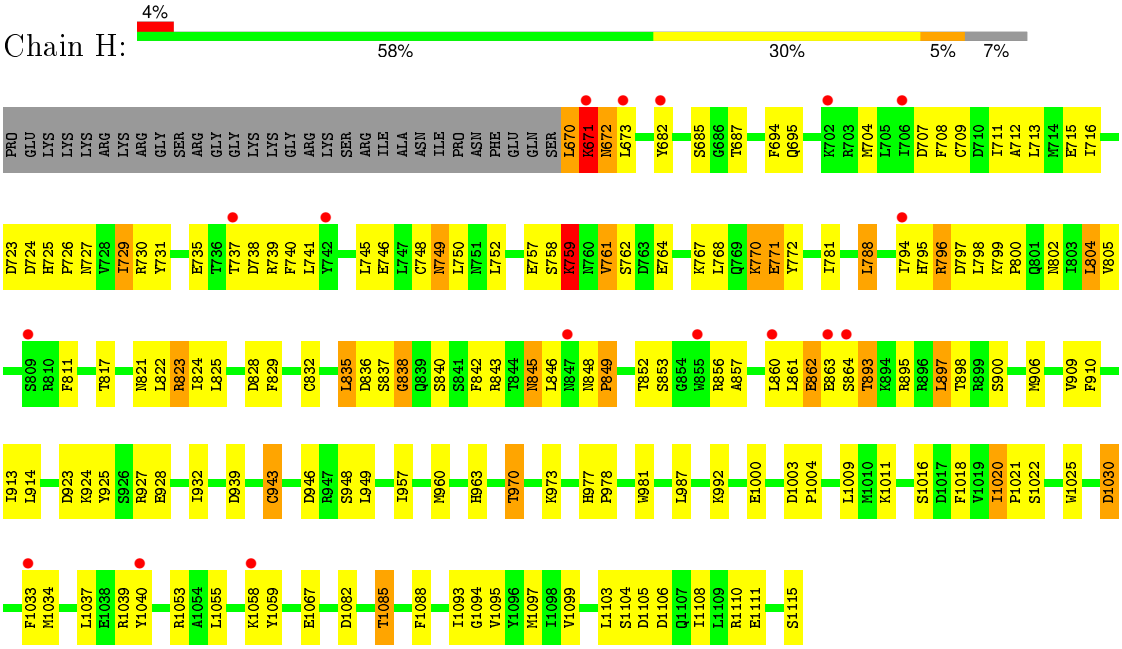
Chain G:





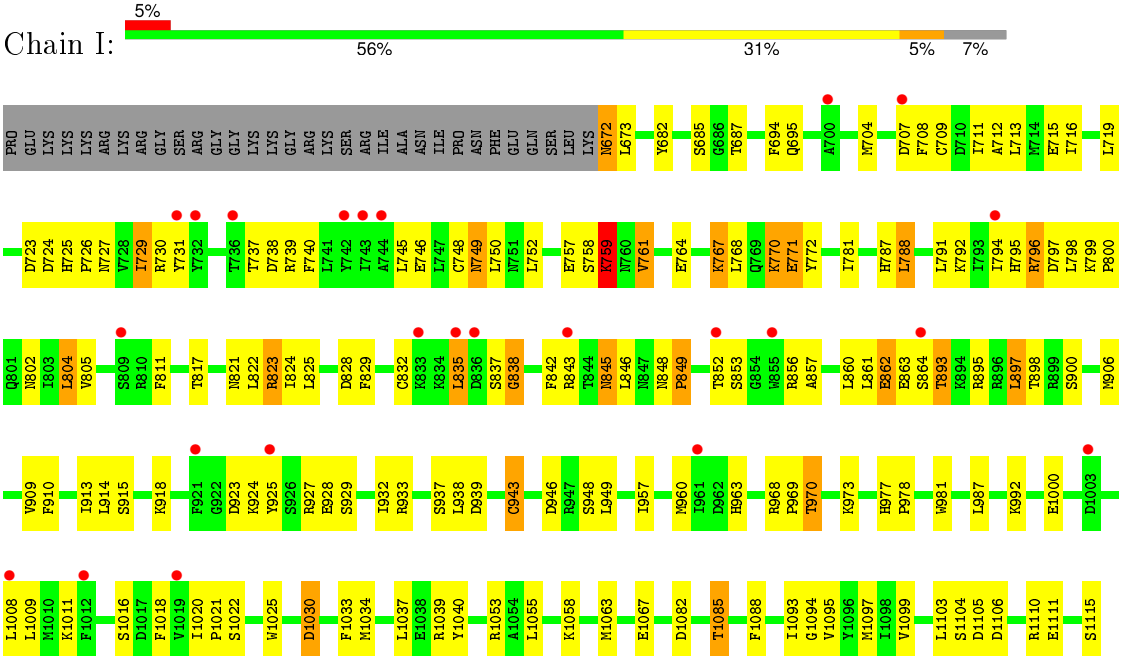
• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain H:



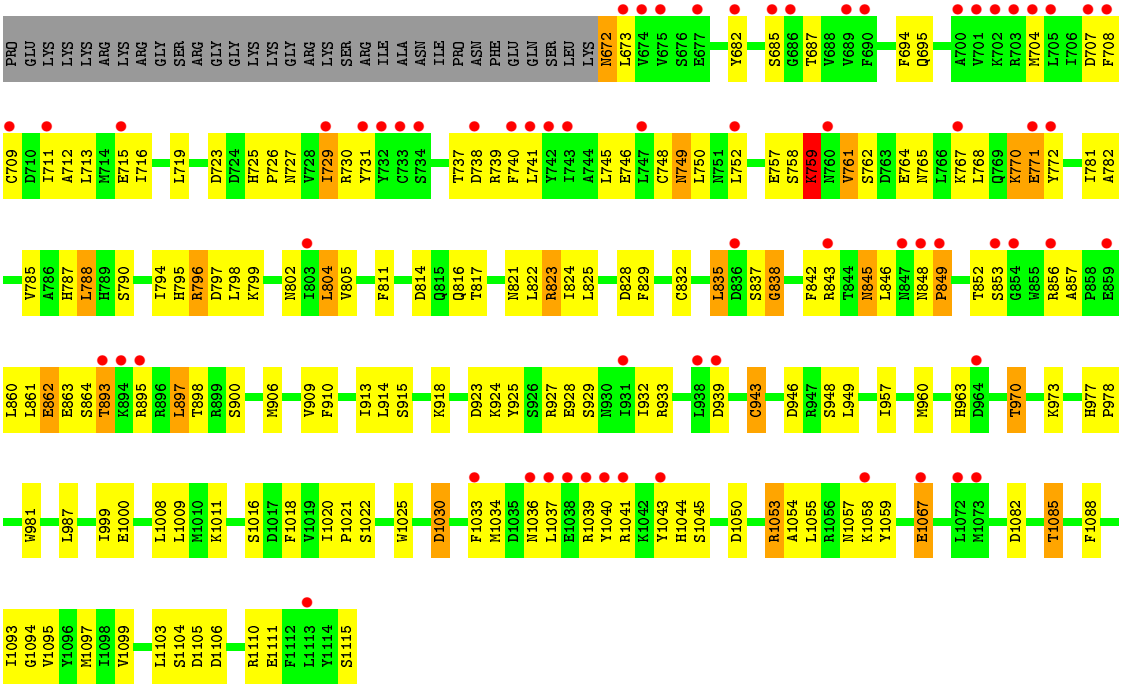
• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain I:



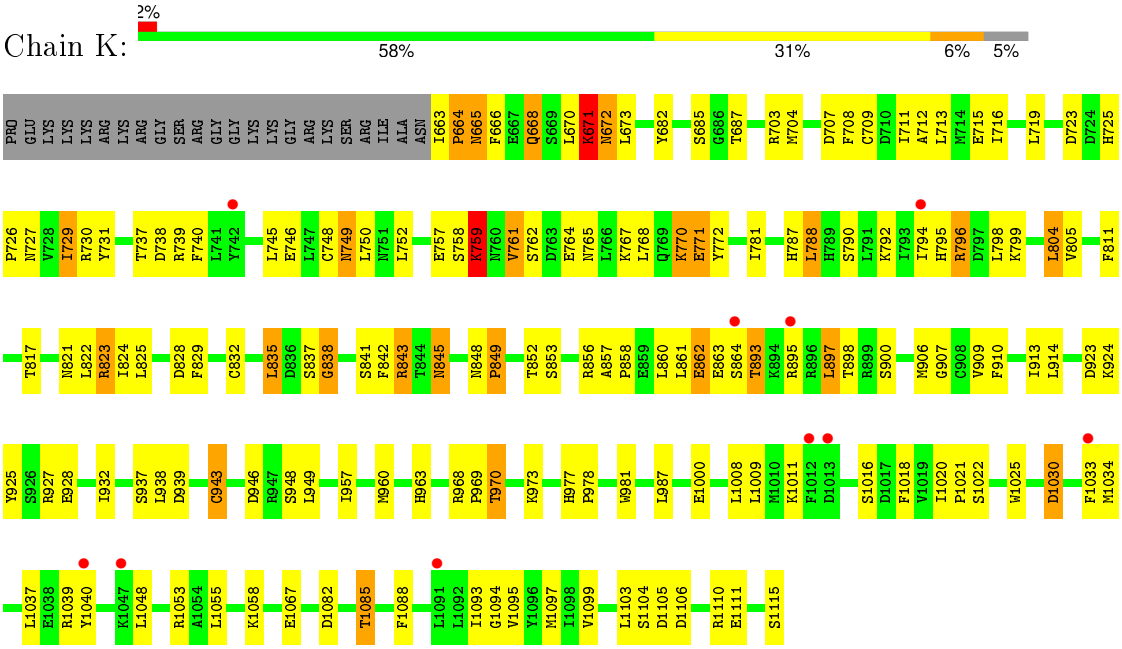
• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain J:



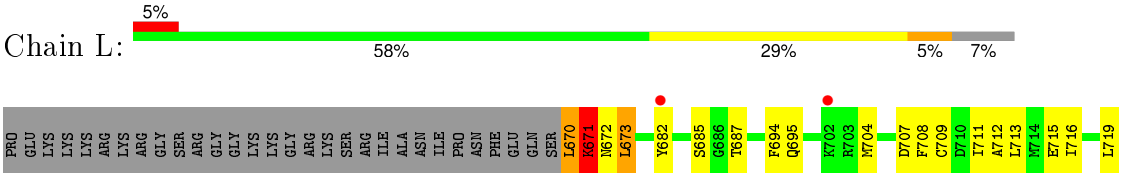
• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

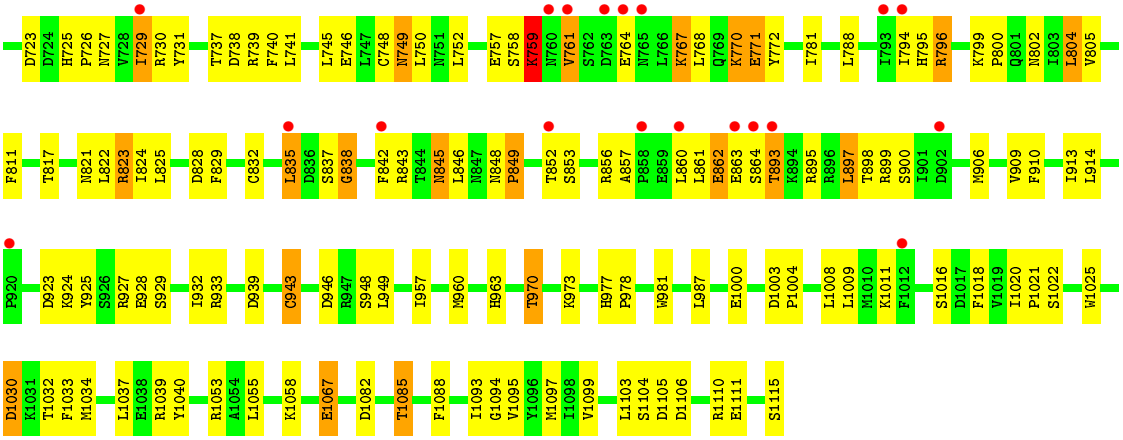
Chain K:



• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

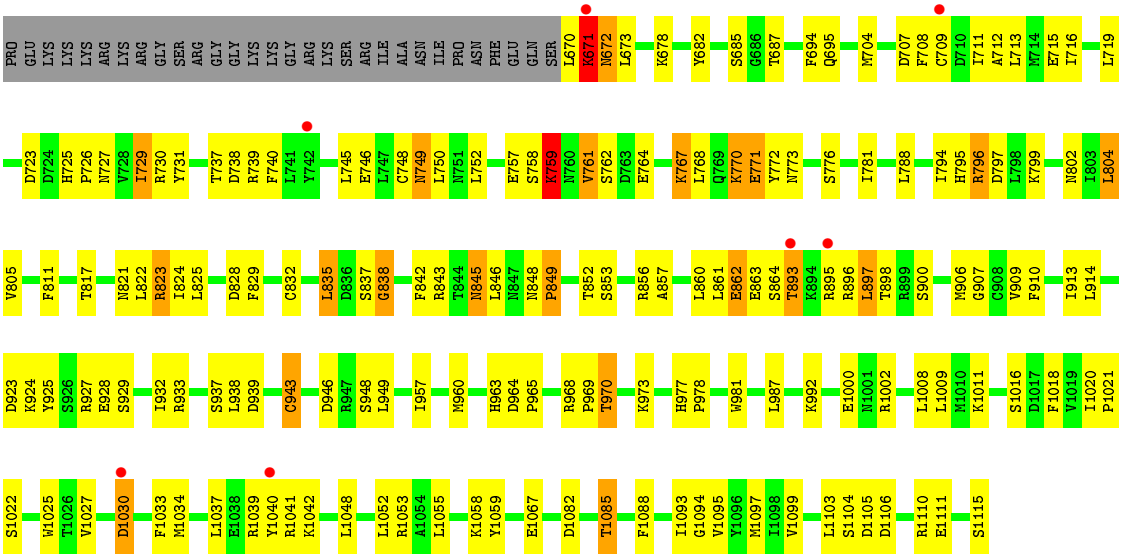
Chain L:





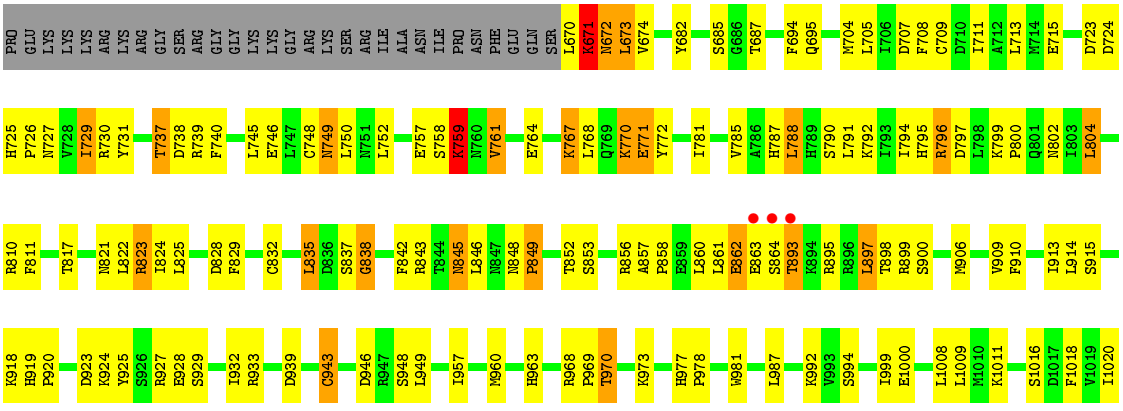
• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

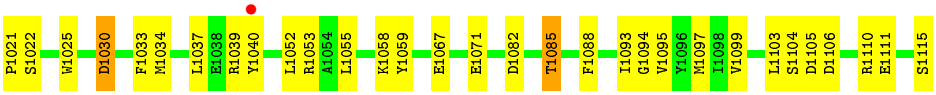
Chain M:



• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

Chain N:




P1021
S1022
W1025
D1030
F1033
M1034
L1037
E1038
R1039
Y1040
L1052
R1053
A1054
L1055
K1058
Y1059
E1067
E1071
D1082
T1085
F1088
I1093
G1094
V1095
Y1096
M1097
I1098
V1099
L1103
S1104
D1105
D1106
R1110
E1111
S1115

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	156.82Å 163.47Å 292.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 3.20 48.95 – 3.11	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-3.20) 99.0 (48.95-3.11)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 3.12Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.235 , 0.283 0.235 , 0.282	Depositor DCC
R_{free} test set	6727 reflections (5.74%)	DCC
Wilson B-factor (Å^2)	82.4	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 82.0	EDS
Estimated twinning fraction	0.075 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Outliers	0 of 134393 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	48018	wwPDB-VP
Average B, all atoms (Å^2)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, APJ, SEP

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	0.35	0/3437	0.51	1/4629 (0.0%)
1	B	0.35	0/3437	0.49	0/4629
1	C	0.37	0/3437	0.51	0/4629
1	D	0.37	0/3497	0.51	0/4711
1	E	0.33	0/3437	0.48	0/4629
1	F	0.34	0/3437	0.49	0/4629
1	G	0.29	0/3437	0.47	0/4629
1	H	0.28	0/3437	0.47	0/4629
1	I	0.27	0/3420	0.45	0/4607
1	J	0.27	0/3420	0.45	0/4607
1	K	0.28	0/3497	0.47	0/4711
1	L	0.28	0/3437	0.47	0/4629
1	M	0.32	0/3437	0.48	0/4629
1	N	0.34	0/3437	0.50	0/4629
All	All	0.32	0/48204	0.48	1/64926 (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	1
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	1
1	G	0	2
1	H	0	1
1	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
1	M	0	2
1	N	0	1
All	All	0	17

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1039	ARG	N-CA-C	-5.47	96.22	111.00

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	671	LYS	Peptide
1	B	671	LYS	Peptide
1	C	671	LYS	Peptide
1	D	670	LEU	Peptide
1	D	671	LYS	Peptide
1	E	671	LYS	Peptide
1	F	671	LYS	Peptide
1	G	670	LEU	Peptide
1	G	671	LYS	Peptide
1	H	671	LYS	Peptide
1	K	670	LEU	Peptide
1	K	671	LYS	Peptide
1	L	670	LEU	Peptide
1	L	671	LYS	Peptide
1	M	670	LEU	Peptide
1	M	671	LYS	Peptide
1	N	671	LYS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3399	0	3409	136	1
1	B	3399	0	3409	132	0
1	C	3399	0	3409	151	1
1	D	3457	0	3461	158	0
1	E	3399	0	3409	135	0
1	F	3399	0	3409	141	0
1	G	3399	0	3409	145	0
1	H	3399	0	3409	130	0
1	I	3382	0	3385	136	2
1	J	3382	0	3385	148	2
1	K	3457	0	3461	141	0
1	L	3399	0	3409	123	0
1	M	3399	0	3409	147	0
1	N	3399	0	3409	138	0
2	A	25	0	16	7	0
2	B	25	0	16	8	0
2	C	25	0	16	7	0
2	D	25	0	16	8	0
2	E	25	0	16	7	0
2	F	25	0	16	7	0
2	G	25	0	16	7	0
2	H	25	0	16	7	0
2	I	25	0	16	7	0
2	J	25	0	16	7	0
2	K	25	0	16	8	0
2	L	25	0	16	7	0
2	M	25	0	16	7	0
2	N	25	0	16	7	0
All	All	48018	0	48006	1914	3

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 20.

All (1914) 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:D:668:GLN:HG3	1:D:739:ARG:HE	0.93	1.07
1:K:668:GLN:HG3	1:K:739:ARG:HE	1.19	1.02
1:F:848:ASN:HB3	1:F:849:PRO:HA	1.42	1.02
1:I:848:ASN:HB3	1:I:849:PRO:HA	1.42	1.01
1:A:848:ASN:HB3	1:A:849:PRO:HA	1.43	1.01
1:C:848:ASN:HB3	1:C:849:PRO:HA	1.42	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:848:ASN:HB3	1:J:849:PRO:HA	1.43	1.00
1:H:848:ASN:HB3	1:H:849:PRO:HA	1.42	1.00
1:L:848:ASN:HB3	1:L:849:PRO:HA	1.42	0.99
1:G:848:ASN:HB3	1:G:849:PRO:HA	1.42	0.99
1:D:668:GLN:HG3	1:D:739:ARG:NE	1.77	0.99
1:B:848:ASN:HB3	1:B:849:PRO:HA	1.42	0.98
1:M:848:ASN:HB3	1:M:849:PRO:HA	1.43	0.98
1:D:848:ASN:HB3	1:D:849:PRO:HA	1.43	0.98
1:N:848:ASN:HB3	1:N:849:PRO:HA	1.42	0.97
1:E:848:ASN:HB3	1:E:849:PRO:HA	1.42	0.97
1:K:848:ASN:HB3	1:K:849:PRO:HA	1.42	0.96
1:D:668:GLN:CG	1:D:739:ARG:HE	1.78	0.96
1:E:970:THR:CB	1:G:762:SER:HB2	1.97	0.94
1:C:761:VAL:HG12	1:F:840:SEP:O2P	1.68	0.91
1:D:668:GLN:CD	1:D:739:ARG:HH21	1.76	0.87
1:A:862:GLU:HG3	1:A:863:GLU:H	1.42	0.85
1:D:862:GLU:HG3	1:D:863:GLU:H	1.41	0.84
1:H:862:GLU:HG3	1:H:863:GLU:H	1.43	0.83
1:J:862:GLU:HG3	1:J:863:GLU:H	1.43	0.83
1:K:843:ARG:HH22	1:M:678:LYS:HD3	1.41	0.83
1:I:862:GLU:HG3	1:I:863:GLU:H	1.43	0.83
1:L:862:GLU:HG3	1:L:863:GLU:H	1.43	0.83
1:F:862:GLU:HG3	1:F:863:GLU:H	1.43	0.83
1:G:862:GLU:HG3	1:G:863:GLU:H	1.44	0.82
1:C:862:GLU:HG3	1:C:863:GLU:H	1.43	0.82
1:M:862:GLU:HG3	1:M:863:GLU:H	1.42	0.82
1:K:668:GLN:CG	1:K:739:ARG:HE	1.91	0.82
1:B:862:GLU:HG3	1:B:863:GLU:H	1.42	0.82
1:E:862:GLU:HG3	1:E:863:GLU:H	1.43	0.82
1:K:862:GLU:HG3	1:K:863:GLU:H	1.44	0.81
1:N:862:GLU:HG3	1:N:863:GLU:H	1.43	0.81
1:I:787:HIS:HD2	1:J:814:ASP:CG	1.87	0.77
1:D:668:GLN:NE2	1:D:739:ARG:HH21	1.82	0.77
1:I:724:ASP:OD2	1:J:823:ARG:NH2	2.19	0.76
1:I:787:HIS:HD2	1:J:814:ASP:OD2	1.69	0.76
1:E:970:THR:HB	1:G:762:SER:HB2	1.68	0.76
1:A:725:HIS:CD2	1:A:727:ASN:H	2.05	0.75
1:C:725:HIS:CD2	1:C:727:ASN:H	2.05	0.74
1:E:715:GLU:HG3	1:E:829:PHE:HB2	1.70	0.74
1:D:715:GLU:HG3	1:D:829:PHE:HB2	1.70	0.74
1:D:665:ASN:HD22	1:D:665:ASN:N	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1034:MET:HE2	1:B:1037:LEU:HD23	1.68	0.73
1:M:715:GLU:HG3	1:M:829:PHE:HB2	1.71	0.73
1:L:715:GLU:HG3	1:L:829:PHE:HB2	1.71	0.73
1:B:715:GLU:HG3	1:B:829:PHE:HB2	1.71	0.73
1:K:715:GLU:HG3	1:K:829:PHE:HB2	1.71	0.72
1:N:715:GLU:HG3	1:N:829:PHE:HB2	1.71	0.72
1:K:668:GLN:HG3	1:K:739:ARG:NE	2.01	0.72
1:B:762:SER:HB2	1:M:970:THR:HG21	1.70	0.72
1:A:715:GLU:HG3	1:A:829:PHE:HB2	1.71	0.72
1:G:715:GLU:HG3	1:G:829:PHE:HB2	1.70	0.72
1:A:1020:ILE:HG22	1:A:1022:SER:N	2.04	0.72
1:B:957:ILE:HA	1:B:960:MET:HE3	1.71	0.71
1:F:715:GLU:HG3	1:F:829:PHE:HB2	1.72	0.71
1:K:957:ILE:HA	1:K:960:MET:HE3	1.73	0.70
1:C:715:GLU:HG3	1:C:829:PHE:HB2	1.72	0.70
1:N:795:HIS:HA	1:N:832:CYS:HB3	1.73	0.70
1:L:848:ASN:HB3	1:L:849:PRO:CA	2.21	0.70
1:F:730:ARG:HB3	1:F:746:GLU:HG2	1.74	0.70
1:M:725:HIS:CD2	1:M:727:ASN:H	2.09	0.70
1:E:862:GLU:HG3	1:E:863:GLU:N	2.07	0.70
1:B:762:SER:HB2	1:M:970:THR:CB	2.22	0.70
1:L:1032:THR:HG23	1:M:1027:VAL:HB	1.72	0.70
1:B:862:GLU:HG3	1:B:863:GLU:N	2.07	0.70
1:J:715:GLU:HG3	1:J:829:PHE:HB2	1.72	0.70
1:B:730:ARG:HB3	1:B:746:GLU:HG2	1.74	0.70
1:I:715:GLU:HG3	1:I:829:PHE:HB2	1.72	0.70
1:M:862:GLU:HG3	1:M:863:GLU:N	2.07	0.70
1:D:725:HIS:CD2	1:D:727:ASN:H	2.09	0.70
1:D:862:GLU:HG3	1:D:863:GLU:N	2.06	0.69
1:H:715:GLU:HG3	1:H:829:PHE:HB2	1.72	0.69
1:J:848:ASN:HB3	1:J:849:PRO:CA	2.22	0.69
1:A:862:GLU:HG3	1:A:863:GLU:N	2.06	0.69
1:K:730:ARG:HB3	1:K:746:GLU:HG2	1.73	0.69
1:K:862:GLU:HG3	1:K:863:GLU:N	2.08	0.69
1:D:957:ILE:HA	1:D:960:MET:HE3	1.75	0.69
1:H:730:ARG:HB3	1:H:746:GLU:HG2	1.74	0.69
1:L:862:GLU:HG3	1:L:863:GLU:N	2.08	0.69
1:G:848:ASN:HB3	1:G:849:PRO:CA	2.21	0.69
1:N:862:GLU:HG3	1:N:863:GLU:N	2.08	0.69
1:M:795:HIS:HA	1:M:832:CYS:HB3	1.75	0.69
1:B:848:ASN:HB3	1:B:849:PRO:CA	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:862:GLU:HG3	1:F:863:GLU:N	2.07	0.69
1:B:725:HIS:CD2	1:B:727:ASN:H	2.10	0.69
1:H:862:GLU:HG3	1:H:863:GLU:N	2.07	0.69
1:F:795:HIS:HA	1:F:832:CYS:HB3	1.75	0.69
1:I:730:ARG:HB3	1:I:746:GLU:HG2	1.74	0.68
1:J:862:GLU:HG3	1:J:863:GLU:N	2.07	0.68
1:C:862:GLU:HG3	1:C:863:GLU:N	2.08	0.68
1:H:762:SER:HB2	1:J:970:THR:HG21	1.75	0.68
1:E:957:ILE:HA	1:E:960:MET:HE3	1.74	0.68
1:D:795:HIS:HA	1:D:832:CYS:HB3	1.73	0.68
1:E:730:ARG:HB3	1:E:746:GLU:HG2	1.75	0.68
1:F:725:HIS:CD2	1:F:727:ASN:H	2.12	0.68
1:E:795:HIS:HA	1:E:832:CYS:HB3	1.74	0.68
1:D:848:ASN:HB3	1:D:849:PRO:CA	2.22	0.68
1:F:848:ASN:HB3	1:F:849:PRO:CA	2.21	0.68
1:H:957:ILE:HA	1:H:960:MET:HE3	1.74	0.68
1:J:781:ILE:HG22	1:J:906:MET:HE2	1.75	0.68
1:A:730:ARG:HB3	1:A:746:GLU:HG2	1.75	0.68
1:N:730:ARG:HB3	1:N:746:GLU:HG2	1.74	0.68
1:C:957:ILE:HA	1:C:960:MET:HE3	1.73	0.68
1:I:848:ASN:HB3	1:I:849:PRO:CA	2.21	0.68
1:L:795:HIS:HA	1:L:832:CYS:HB3	1.76	0.68
1:G:730:ARG:HB3	1:G:746:GLU:HG2	1.76	0.68
1:M:897:LEU:HD12	1:M:897:LEU:H	1.59	0.68
1:L:730:ARG:HB3	1:L:746:GLU:HG2	1.75	0.68
1:A:1034:MET:CE	1:A:1037:LEU:HD23	2.24	0.67
1:C:848:ASN:HB3	1:C:849:PRO:CA	2.20	0.67
1:I:957:ILE:HA	1:I:960:MET:HE3	1.76	0.67
1:G:862:GLU:HG3	1:G:863:GLU:N	2.08	0.67
1:K:795:HIS:HA	1:K:832:CYS:HB3	1.76	0.67
1:J:730:ARG:HB3	1:J:746:GLU:HG2	1.76	0.67
1:C:730:ARG:HB3	1:C:746:GLU:HG2	1.76	0.67
1:B:795:HIS:HA	1:B:832:CYS:HB3	1.76	0.67
1:A:848:ASN:HB3	1:A:849:PRO:CA	2.22	0.67
1:C:781:ILE:HG22	1:C:906:MET:HE2	1.76	0.67
1:M:730:ARG:HB3	1:M:746:GLU:HG2	1.76	0.67
1:D:748:CYS:H	2:D:1999:APJ:HN4	1.43	0.67
1:I:862:GLU:HG3	1:I:863:GLU:N	2.07	0.67
1:M:957:ILE:HA	1:M:960:MET:HE3	1.77	0.67
1:N:748:CYS:H	2:N:1999:APJ:HN4	1.42	0.67
1:H:1020:ILE:HG22	1:H:1022:SER:N	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:848:ASN:HB3	1:M:849:PRO:CA	2.22	0.67
1:G:725:HIS:CD2	1:G:727:ASN:H	2.12	0.66
1:E:725:HIS:CD2	1:E:727:ASN:H	2.13	0.66
1:L:725:HIS:CD2	1:L:727:ASN:H	2.12	0.66
1:N:725:HIS:CD2	1:N:727:ASN:H	2.12	0.66
1:G:957:ILE:HA	1:G:960:MET:HE3	1.77	0.66
1:E:970:THR:CG2	1:G:762:SER:HB2	2.25	0.66
1:G:864:SER:HB3	1:G:963:HIS:NE2	2.11	0.66
1:I:725:HIS:CD2	1:I:727:ASN:H	2.13	0.66
1:D:665:ASN:O	1:D:666:PHE:HB2	1.96	0.66
1:C:795:HIS:HA	1:C:832:CYS:HB3	1.78	0.66
1:D:730:ARG:HB3	1:D:746:GLU:HG2	1.77	0.66
1:A:795:HIS:HA	1:A:832:CYS:HB3	1.78	0.66
1:H:795:HIS:HA	1:H:832:CYS:HB3	1.77	0.66
1:K:848:ASN:HB3	1:K:849:PRO:CA	2.21	0.66
1:D:666:PHE:HE1	1:D:703:ARG:HD3	1.61	0.66
1:C:1020:ILE:HG22	1:C:1022:SER:N	2.11	0.66
1:M:781:ILE:HG22	1:M:906:MET:HE2	1.78	0.66
1:M:923:ASP:O	1:M:927:ARG:HB2	1.96	0.66
1:B:897:LEU:H	1:B:897:LEU:HD12	1.61	0.66
1:E:794:ILE:HD11	1:E:835:LEU:HD12	1.78	0.66
1:K:748:CYS:H	2:K:1999:APJ:HN4	1.44	0.66
1:L:957:ILE:HA	1:L:960:MET:HE3	1.77	0.66
1:A:897:LEU:HD12	1:A:897:LEU:H	1.61	0.66
1:I:795:HIS:HA	1:I:832:CYS:HB3	1.77	0.65
1:H:725:HIS:CD2	1:H:727:ASN:H	2.14	0.65
1:F:673:LEU:HD23	1:F:673:LEU:C	2.16	0.65
1:H:864:SER:HB3	1:H:963:HIS:NE2	2.12	0.65
1:J:795:HIS:HA	1:J:832:CYS:HB3	1.77	0.65
1:L:1020:ILE:HG22	1:L:1022:SER:N	2.10	0.65
1:A:673:LEU:O	1:A:673:LEU:HD23	1.95	0.65
1:K:794:ILE:HD11	1:K:835:LEU:HD12	1.78	0.65
1:A:923:ASP:O	1:A:927:ARG:HB2	1.97	0.65
1:E:897:LEU:H	1:E:897:LEU:HD12	1.61	0.65
1:N:897:LEU:HD12	1:N:897:LEU:H	1.61	0.65
1:E:672:ASN:ND2	1:E:672:ASN:H	1.93	0.65
1:I:1034:MET:HE2	1:I:1037:LEU:HD23	1.78	0.65
1:F:1020:ILE:HG22	1:F:1022:SER:N	2.11	0.65
1:G:923:ASP:O	1:G:927:ARG:HB2	1.96	0.65
1:C:897:LEU:HD12	1:C:897:LEU:H	1.61	0.65
1:I:1020:ILE:HG22	1:I:1022:SER:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1020:ILE:HG22	1:K:1022:SER:N	2.12	0.65
1:J:725:HIS:CD2	1:J:727:ASN:H	2.14	0.65
1:M:1020:ILE:HG22	1:M:1022:SER:N	2.12	0.65
1:B:1020:ILE:HG22	1:B:1022:SER:N	2.11	0.65
1:H:848:ASN:HB3	1:H:849:PRO:CA	2.21	0.65
1:L:748:CYS:H	2:L:1999:APJ:HN4	1.45	0.65
1:E:1020:ILE:HG22	1:E:1022:SER:N	2.12	0.65
1:N:794:ILE:HD11	1:N:835:LEU:HD12	1.78	0.65
1:D:794:ILE:HD11	1:D:835:LEU:HD12	1.79	0.65
1:I:725:HIS:CE1	1:J:816:GLN:NE2	2.64	0.65
1:N:957:ILE:HA	1:N:960:MET:HE3	1.77	0.65
1:D:1034:MET:HE2	1:D:1037:LEU:HD23	1.78	0.65
1:C:923:ASP:O	1:C:927:ARG:HB2	1.97	0.65
1:I:923:ASP:O	1:I:927:ARG:HB2	1.97	0.65
1:I:748:CYS:H	2:I:1999:APJ:HN4	1.45	0.65
1:G:1020:ILE:HG22	1:G:1022:SER:N	2.11	0.65
1:N:864:SER:HB3	1:N:963:HIS:NE2	2.12	0.65
1:K:725:HIS:CD2	1:K:727:ASN:H	2.14	0.65
1:B:864:SER:HB3	1:B:963:HIS:NE2	2.12	0.65
1:J:864:SER:HB3	1:J:963:HIS:NE2	2.12	0.65
1:L:923:ASP:O	1:L:927:ARG:HB2	1.97	0.65
1:G:897:LEU:H	1:G:897:LEU:HD12	1.62	0.65
1:G:781:ILE:HG22	1:G:906:MET:HE2	1.79	0.64
1:D:781:ILE:HG22	1:D:906:MET:HE2	1.78	0.64
1:J:1020:ILE:HG22	1:J:1022:SER:N	2.11	0.64
1:J:957:ILE:HA	1:J:960:MET:HE3	1.77	0.64
1:N:1020:ILE:HG22	1:N:1022:SER:N	2.12	0.64
1:I:794:ILE:HD11	1:I:835:LEU:HD12	1.80	0.64
1:F:748:CYS:H	2:F:1999:APJ:HN4	1.44	0.64
1:H:794:ILE:HD11	1:H:835:LEU:HD12	1.78	0.64
1:H:781:ILE:HG22	1:H:906:MET:HE2	1.78	0.64
1:L:864:SER:HB3	1:L:963:HIS:NE2	2.12	0.64
1:B:762:SER:HB2	1:M:970:THR:CG2	2.28	0.64
1:E:677:GLU:CD	1:E:677:GLU:H	2.01	0.64
1:K:897:LEU:H	1:K:897:LEU:HD12	1.62	0.64
1:I:864:SER:HB3	1:I:963:HIS:NE2	2.13	0.64
1:B:1034:MET:CE	1:B:1037:LEU:HD23	2.28	0.64
1:J:794:ILE:HD11	1:J:835:LEU:HD12	1.80	0.64
1:F:864:SER:HB3	1:F:963:HIS:NE2	2.12	0.64
1:C:748:CYS:H	2:C:1999:APJ:HN4	1.46	0.64
1:M:748:CYS:H	2:M:1999:APJ:HN4	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:864:SER:HB3	1:E:963:HIS:NE2	2.13	0.64
1:A:796:ARG:HD3	1:A:832:CYS:HA	1.80	0.64
1:D:1034:MET:CE	1:D:1037:LEU:HD23	2.28	0.64
1:J:923:ASP:O	1:J:927:ARG:HB2	1.97	0.64
1:J:748:CYS:H	2:J:1999:APJ:HN4	1.46	0.64
1:G:795:HIS:HA	1:G:832:CYS:HB3	1.79	0.64
1:M:864:SER:HB3	1:M:963:HIS:NE2	2.12	0.63
1:E:923:ASP:O	1:E:927:ARG:HB2	1.98	0.63
1:I:897:LEU:HD12	1:I:897:LEU:H	1.64	0.63
1:F:897:LEU:HD12	1:F:897:LEU:H	1.63	0.63
1:C:864:SER:HB3	1:C:963:HIS:NE2	2.13	0.63
1:K:864:SER:HB3	1:K:963:HIS:NE2	2.12	0.63
1:B:923:ASP:O	1:B:927:ARG:HB2	1.99	0.63
1:H:897:LEU:H	1:H:897:LEU:HD12	1.63	0.63
1:E:796:ARG:HD3	1:E:832:CYS:HA	1.78	0.63
1:K:923:ASP:O	1:K:927:ARG:HB2	1.98	0.63
1:D:1020:ILE:HG22	1:D:1022:SER:N	2.14	0.63
1:B:748:CYS:H	2:B:1999:APJ:HN4	1.45	0.63
1:D:864:SER:HB3	1:D:963:HIS:NE2	2.13	0.63
1:C:992:LYS:HE3	1:D:1059:TYR:OH	1.98	0.63
1:H:923:ASP:O	1:H:927:ARG:HB2	1.97	0.63
1:A:864:SER:HB3	1:A:963:HIS:NE2	2.12	0.63
1:F:794:ILE:HD11	1:F:835:LEU:HD12	1.79	0.63
1:A:673:LEU:C	1:A:673:LEU:HD23	2.19	0.63
1:D:923:ASP:O	1:D:927:ARG:HB2	1.98	0.63
1:H:748:CYS:H	2:H:1999:APJ:HN4	1.46	0.63
1:D:795:HIS:HA	1:D:832:CYS:CB	2.29	0.63
1:N:1034:MET:HE1	1:N:1037:LEU:HD23	1.81	0.63
1:K:781:ILE:HG22	1:K:906:MET:HE2	1.79	0.63
1:G:794:ILE:HD11	1:G:835:LEU:HD12	1.81	0.62
1:A:823:ARG:NH2	1:B:724:ASP:OD2	2.32	0.62
1:J:1034:MET:HE2	1:J:1034:MET:HA	1.80	0.62
1:I:1063:MET:HG2	1:J:999:ILE:HG12	1.81	0.62
1:N:848:ASN:HB3	1:N:849:PRO:CA	2.21	0.62
1:C:794:ILE:HD11	1:C:835:LEU:HD12	1.80	0.62
1:N:923:ASP:O	1:N:927:ARG:HB2	1.99	0.62
1:J:897:LEU:H	1:J:897:LEU:HD12	1.64	0.62
1:B:794:ILE:HD11	1:B:835:LEU:HD12	1.81	0.62
1:E:771:GLU:HB2	1:E:821:ASN:ND2	2.15	0.62
1:A:748:CYS:H	2:A:1999:APJ:HN4	1.47	0.62
1:F:923:ASP:O	1:F:927:ARG:HB2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:771:GLU:HB2	1:A:821:ASN:HD21	1.65	0.62
1:I:781:ILE:HG22	1:I:906:MET:HE2	1.82	0.62
1:G:748:CYS:H	2:G:1999:APJ:HN4	1.46	0.62
1:F:957:ILE:HA	1:F:960:MET:HE3	1.81	0.61
1:F:796:ARG:HD3	1:F:832:CYS:HA	1.82	0.61
1:A:957:ILE:HA	1:A:960:MET:HE3	1.81	0.61
1:L:897:LEU:HD12	1:L:897:LEU:H	1.64	0.61
1:E:970:THR:HG21	1:G:762:SER:HB2	1.81	0.61
1:D:666:PHE:HE1	1:D:703:ARG:CD	2.13	0.61
1:G:840:SEP:O2P	1:I:761:VAL:HG11	2.00	0.61
1:L:781:ILE:HG22	1:L:906:MET:HE2	1.81	0.61
1:D:897:LEU:HD12	1:D:897:LEU:H	1.65	0.61
1:M:796:ARG:HD3	1:M:832:CYS:HA	1.81	0.61
1:H:796:ARG:HD3	1:H:832:CYS:HA	1.83	0.61
1:J:1037:LEU:HB2	1:J:1058:LYS:NZ	2.15	0.61
1:D:771:GLU:HB2	1:D:821:ASN:ND2	2.16	0.61
1:C:970:THR:HG23	1:C:973:LYS:HB2	1.83	0.61
1:K:771:GLU:HB2	1:K:821:ASN:ND2	2.15	0.61
1:L:794:ILE:HD11	1:L:835:LEU:HD12	1.80	0.61
1:A:794:ILE:HD11	1:A:835:LEU:HD12	1.81	0.61
1:K:796:ARG:HD3	1:K:832:CYS:HA	1.83	0.61
1:G:796:ARG:HD3	1:G:832:CYS:HA	1.83	0.61
1:H:771:GLU:HB2	1:H:821:ASN:ND2	2.16	0.61
1:B:781:ILE:HG22	1:B:906:MET:HE2	1.82	0.61
1:E:748:CYS:H	2:E:1999:APJ:HN4	1.47	0.61
1:L:796:ARG:HD3	1:L:832:CYS:HA	1.81	0.60
1:J:796:ARG:HD3	1:J:832:CYS:HA	1.82	0.60
1:G:771:GLU:HB2	1:G:821:ASN:ND2	2.16	0.60
1:N:796:ARG:HD3	1:N:832:CYS:HA	1.82	0.60
1:J:771:GLU:HB2	1:J:821:ASN:ND2	2.17	0.60
1:E:761:VAL:HG21	1:E:764:GLU:HG3	1.83	0.60
1:B:771:GLU:HB2	1:B:821:ASN:ND2	2.16	0.60
1:I:796:ARG:HD3	1:I:832:CYS:HA	1.84	0.60
1:A:771:GLU:HB2	1:A:821:ASN:ND2	2.15	0.60
1:E:781:ILE:HG22	1:E:906:MET:HE2	1.82	0.60
1:F:709:CYS:O	1:F:713:LEU:HD13	2.02	0.60
1:I:771:GLU:HB2	1:I:821:ASN:ND2	2.16	0.60
1:M:970:THR:HG23	1:M:973:LYS:HB2	1.82	0.60
1:L:970:THR:HG23	1:L:973:LYS:HB2	1.84	0.60
1:J:1043:TYR:OH	1:J:1057:ASN:ND2	2.34	0.60
1:A:1038:GLU:O	1:A:1039:ARG:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:771:GLU:HB2	1:L:821:ASN:ND2	2.17	0.60
1:M:794:ILE:HD11	1:M:835:LEU:HD12	1.82	0.60
1:B:796:ARG:HD3	1:B:832:CYS:HA	1.83	0.60
1:C:1059:TYR:OH	1:D:992:LYS:HE3	2.02	0.60
1:D:666:PHE:HZ	1:D:690:PHE:CE1	2.19	0.59
1:D:771:GLU:HB2	1:D:821:ASN:HD21	1.67	0.59
1:I:977:HIS:CG	1:I:978:PRO:HD2	2.37	0.59
1:M:761:VAL:HG21	1:M:764:GLU:HG3	1.85	0.59
1:C:781:ILE:HG12	1:C:824:ILE:HG21	1.85	0.59
1:L:1034:MET:HE2	1:L:1037:LEU:HD23	1.83	0.59
1:N:795:HIS:HA	1:N:832:CYS:CB	2.32	0.59
1:A:772:TYR:O	1:A:772:TYR:CG	2.54	0.59
1:K:771:GLU:HB2	1:K:821:ASN:HD21	1.67	0.59
1:C:670:LEU:O	1:C:735:GLU:OE2	2.21	0.59
1:B:970:THR:HG23	1:B:973:LYS:HB2	1.83	0.59
1:K:761:VAL:HG21	1:K:764:GLU:HG3	1.84	0.59
1:K:663:ILE:N	1:K:664:PRO:CD	2.66	0.59
1:N:781:ILE:HG22	1:N:906:MET:HE2	1.84	0.59
1:F:771:GLU:HB2	1:F:821:ASN:ND2	2.17	0.59
1:B:795:HIS:HA	1:B:832:CYS:CB	2.32	0.59
1:M:772:TYR:CG	1:M:772:TYR:O	2.55	0.59
1:E:772:TYR:CG	1:E:772:TYR:O	2.56	0.59
1:D:666:PHE:CE1	1:D:703:ARG:HD3	2.38	0.59
1:J:745:LEU:HD12	2:J:1999:APJ:H18A	1.85	0.59
1:C:752:LEU:HD21	1:C:913:ILE:HD11	1.85	0.59
1:K:970:THR:HG23	1:K:973:LYS:HB2	1.85	0.59
1:F:795:HIS:HA	1:F:832:CYS:CB	2.33	0.59
1:K:772:TYR:O	1:K:772:TYR:CG	2.56	0.59
1:M:795:HIS:HA	1:M:832:CYS:CB	2.33	0.58
1:N:673:LEU:HD23	1:N:673:LEU:C	2.22	0.58
1:K:795:HIS:HA	1:K:832:CYS:CB	2.33	0.58
1:M:771:GLU:HB2	1:M:821:ASN:ND2	2.17	0.58
1:A:761:VAL:HG21	1:A:764:GLU:HG3	1.85	0.58
1:C:761:VAL:HG21	1:C:764:GLU:HG3	1.85	0.58
1:D:796:ARG:HD3	1:D:832:CYS:HA	1.85	0.58
1:C:1037:LEU:HB2	1:C:1058:LYS:NZ	2.18	0.58
1:F:970:THR:HG23	1:F:973:LYS:HB2	1.86	0.58
1:K:668:GLN:CD	1:K:739:ARG:HH21	2.05	0.58
1:E:771:GLU:HB2	1:E:821:ASN:HD21	1.67	0.58
1:B:761:VAL:HG21	1:B:764:GLU:HG3	1.85	0.58
1:K:752:LEU:HD21	1:K:913:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:970:THR:HG23	1:A:973:LYS:HB2	1.86	0.58
1:N:771:GLU:HB2	1:N:821:ASN:ND2	2.18	0.58
1:F:1034:MET:HE2	1:F:1037:LEU:HD23	1.85	0.58
1:E:795:HIS:HA	1:E:832:CYS:CB	2.33	0.58
1:J:781:ILE:HG12	1:J:824:ILE:HG21	1.85	0.58
1:D:761:VAL:HG21	1:D:764:GLU:HG3	1.86	0.58
1:D:970:THR:HG23	1:D:973:LYS:HB2	1.83	0.58
1:N:761:VAL:HG21	1:N:764:GLU:HG3	1.86	0.58
1:D:772:TYR:O	1:D:772:TYR:CG	2.56	0.58
1:N:970:THR:HG23	1:N:973:LYS:HB2	1.85	0.58
1:B:1034:MET:HE3	1:B:1034:MET:HA	1.84	0.58
1:C:796:ARG:HD3	1:C:832:CYS:HA	1.85	0.58
1:H:781:ILE:HG12	1:H:824:ILE:HG21	1.85	0.58
1:I:761:VAL:HG21	1:I:764:GLU:HG3	1.85	0.58
1:E:781:ILE:HG12	1:E:824:ILE:HG21	1.86	0.58
1:D:663:ILE:N	1:D:664:PRO:HD3	2.18	0.58
1:C:977:HIS:CG	1:C:978:PRO:HD2	2.38	0.58
1:B:772:TYR:CG	1:B:772:TYR:O	2.56	0.58
1:H:761:VAL:HG21	1:H:764:GLU:HG3	1.86	0.58
1:C:795:HIS:HA	1:C:832:CYS:CB	2.33	0.58
1:F:771:GLU:HB2	1:F:821:ASN:HD21	1.69	0.58
1:C:771:GLU:HB2	1:C:821:ASN:ND2	2.18	0.58
1:F:761:VAL:HG11	1:H:840:SEP:O2P	2.03	0.58
1:G:781:ILE:HG12	1:G:824:ILE:HG21	1.85	0.58
1:L:771:GLU:HB2	1:L:821:ASN:HD21	1.69	0.58
1:G:970:THR:HG23	1:G:973:LYS:HB2	1.84	0.58
1:A:977:HIS:CG	1:A:978:PRO:HD2	2.39	0.58
1:K:1034:MET:HE2	1:K:1037:LEU:HD23	1.85	0.58
1:B:861:LEU:O	1:B:862:GLU:HB3	2.04	0.58
1:H:772:TYR:CG	1:H:772:TYR:O	2.56	0.58
1:I:772:TYR:O	1:I:772:TYR:CG	2.57	0.58
1:D:672:ASN:ND2	1:D:672:ASN:H	2.02	0.58
1:F:772:TYR:O	1:F:772:TYR:CG	2.57	0.58
1:I:725:HIS:CE1	1:J:816:GLN:HE22	2.22	0.57
1:L:781:ILE:HG12	1:L:824:ILE:HG21	1.86	0.57
1:N:781:ILE:HG12	1:N:824:ILE:HG21	1.86	0.57
1:M:1002:ARG:HH12	1:M:1041:ARG:CZ	2.17	0.57
1:K:665:ASN:HD22	1:K:665:ASN:N	2.00	0.57
1:J:771:GLU:HB2	1:J:821:ASN:HD21	1.69	0.57
1:I:781:ILE:HG12	1:I:824:ILE:HG21	1.86	0.57
1:H:771:GLU:HB2	1:H:821:ASN:HD21	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:970:THR:HG23	1:H:973:LYS:HB2	1.87	0.57
1:M:752:LEU:HD21	1:M:913:ILE:HD11	1.86	0.57
1:G:772:TYR:O	1:G:772:TYR:CG	2.57	0.57
1:N:772:TYR:O	1:N:772:TYR:CG	2.57	0.57
1:N:1034:MET:CE	1:N:1037:LEU:HD23	2.33	0.57
1:M:771:GLU:HB2	1:M:821:ASN:HD21	1.69	0.57
1:F:761:VAL:HG21	1:F:764:GLU:HG3	1.87	0.57
1:A:1093:ILE:O	1:A:1097:MET:HG3	2.04	0.57
1:G:761:VAL:HG21	1:G:764:GLU:HG3	1.87	0.57
1:D:663:ILE:N	1:D:664:PRO:CD	2.68	0.57
1:E:672:ASN:HD22	1:E:672:ASN:H	1.50	0.57
1:I:745:LEU:HD12	2:I:1999:APJ:H18A	1.87	0.57
1:B:771:GLU:HB2	1:B:821:ASN:HD21	1.68	0.57
1:J:772:TYR:CG	1:J:772:TYR:O	2.57	0.57
1:L:673:LEU:C	1:L:673:LEU:HD23	2.25	0.57
1:M:672:ASN:ND2	1:M:672:ASN:H	2.03	0.57
1:H:795:HIS:HA	1:H:832:CYS:CB	2.34	0.57
1:J:795:HIS:HA	1:J:832:CYS:CB	2.35	0.57
1:G:1034:MET:HE2	1:G:1037:LEU:HD23	1.86	0.57
1:L:761:VAL:HG21	1:L:764:GLU:HG3	1.86	0.57
1:L:795:HIS:HA	1:L:832:CYS:CB	2.34	0.57
1:I:795:HIS:HA	1:I:832:CYS:CB	2.35	0.57
1:B:781:ILE:HG12	1:B:824:ILE:HG21	1.87	0.57
1:C:771:GLU:HB2	1:C:821:ASN:HD21	1.70	0.57
1:H:752:LEU:HD21	1:H:913:ILE:HD11	1.86	0.57
1:L:772:TYR:CG	1:L:772:TYR:O	2.57	0.57
1:M:781:ILE:HG12	1:M:824:ILE:HG21	1.87	0.57
1:A:709:CYS:O	1:A:713:LEU:HD13	2.05	0.57
1:J:709:CYS:O	1:J:713:LEU:HD13	2.05	0.57
1:A:1038:GLU:OE2	1:A:1043:TYR:HB2	2.05	0.57
1:M:1002:ARG:HH12	1:M:1041:ARG:NH2	2.03	0.57
1:H:709:CYS:O	1:H:713:LEU:HD13	2.05	0.57
1:L:709:CYS:O	1:L:713:LEU:HD13	2.05	0.56
1:J:970:THR:HG23	1:J:973:LYS:HB2	1.86	0.56
1:D:861:LEU:O	1:D:862:GLU:HB3	2.06	0.56
1:M:897:LEU:N	1:M:897:LEU:HD12	2.20	0.56
1:N:745:LEU:HD12	2:N:1999:APJ:H18A	1.87	0.56
1:M:745:LEU:HD12	2:M:1999:APJ:H18A	1.87	0.56
1:C:1034:MET:HA	1:C:1034:MET:HE2	1.87	0.56
1:N:771:GLU:HB2	1:N:821:ASN:HD21	1.70	0.56
1:H:1034:MET:HE3	1:H:1034:MET:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1041:ARG:NH2	1:C:1053:ARG:HG2	2.20	0.56
1:C:709:CYS:O	1:C:713:LEU:HD13	2.05	0.56
1:G:672:ASN:H	1:G:672:ASN:ND2	2.03	0.56
1:J:761:VAL:HG21	1:J:764:GLU:HG3	1.86	0.56
1:A:752:LEU:HD21	1:A:913:ILE:HD11	1.88	0.56
1:N:737:THR:HG23	1:N:740:PHE:H	1.70	0.56
1:G:745:LEU:HD12	2:G:1999:APJ:H18A	1.87	0.56
1:J:1037:LEU:HD21	1:J:1054:ALA:HB1	1.86	0.56
1:K:663:ILE:N	1:K:664:PRO:HD3	2.20	0.56
1:I:709:CYS:O	1:I:713:LEU:HD13	2.06	0.56
1:C:673:LEU:HD23	1:C:673:LEU:C	2.26	0.56
1:E:848:ASN:HB3	1:E:849:PRO:CA	2.21	0.56
1:E:970:THR:HG23	1:E:973:LYS:HB2	1.86	0.56
1:G:795:HIS:HA	1:G:832:CYS:CB	2.36	0.56
1:J:752:LEU:HD21	1:J:913:ILE:HD11	1.86	0.56
1:G:709:CYS:O	1:G:713:LEU:HD13	2.05	0.56
1:G:672:ASN:N	1:G:672:ASN:HD22	2.03	0.56
1:E:752:LEU:HD21	1:E:913:ILE:HD11	1.86	0.56
1:D:811:PHE:HB3	1:D:823:ARG:NH1	2.20	0.56
1:B:897:LEU:HD12	1:B:897:LEU:N	2.20	0.56
1:F:731:TYR:HA	1:F:745:LEU:HD23	1.88	0.56
1:I:771:GLU:HB2	1:I:821:ASN:HD21	1.69	0.56
1:L:752:LEU:HD21	1:L:913:ILE:HD11	1.88	0.56
1:C:861:LEU:O	1:C:862:GLU:HB3	2.06	0.56
2:A:1999:APJ:H17	2:A:1999:APJ:N8	2.21	0.56
1:C:1036:ASN:O	1:C:1039:ARG:HB3	2.05	0.56
1:L:861:LEU:O	1:L:862:GLU:HB3	2.06	0.56
1:J:745:LEU:CD1	2:J:1999:APJ:H18A	2.36	0.56
1:E:709:CYS:O	1:E:713:LEU:HD13	2.06	0.56
1:I:672:ASN:HD22	1:I:672:ASN:N	2.04	0.56
1:N:861:LEU:O	1:N:862:GLU:HB3	2.06	0.56
1:E:897:LEU:HD12	1:E:897:LEU:N	2.21	0.56
1:C:1055:LEU:C	1:C:1055:LEU:HD23	2.26	0.56
1:A:861:LEU:O	1:A:862:GLU:HB3	2.06	0.55
1:C:824:ILE:O	1:C:825:LEU:HD23	2.05	0.55
1:E:672:ASN:HD22	1:E:672:ASN:N	2.03	0.55
1:B:745:LEU:HD12	2:B:1999:APJ:H18A	1.87	0.55
1:K:781:ILE:HG12	1:K:824:ILE:HG21	1.87	0.55
1:F:781:ILE:HG12	1:F:824:ILE:HG21	1.88	0.55
1:C:772:TYR:O	1:C:772:TYR:CG	2.58	0.55
2:D:1999:APJ:H17	2:D:1999:APJ:N8	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:745:LEU:HD12	2:L:1999:APJ:H18A	1.88	0.55
1:D:781:ILE:HG12	1:D:824:ILE:HG21	1.87	0.55
1:B:749:ASN:OD1	1:B:749:ASN:N	2.39	0.55
1:G:771:GLU:HB2	1:G:821:ASN:HD21	1.70	0.55
1:A:781:ILE:HG12	1:A:824:ILE:HG21	1.88	0.55
1:D:709:CYS:O	1:D:713:LEU:HD13	2.05	0.55
1:D:668:GLN:NE2	1:D:739:ARG:NH2	2.52	0.55
1:F:861:LEU:O	1:F:862:GLU:HB3	2.06	0.55
1:G:861:LEU:O	1:G:862:GLU:HB3	2.06	0.55
1:M:861:LEU:O	1:M:862:GLU:HB3	2.06	0.55
1:K:970:THR:CB	1:M:762:SER:HB2	2.36	0.55
1:M:1034:MET:HE2	1:M:1037:LEU:HD23	1.89	0.55
1:K:843:ARG:NH2	1:M:678:LYS:HD3	2.17	0.55
1:K:861:LEU:O	1:K:862:GLU:HB3	2.06	0.55
1:D:752:LEU:HD21	1:D:913:ILE:HD11	1.87	0.55
1:N:709:CYS:O	1:N:713:LEU:HD13	2.06	0.55
1:E:861:LEU:O	1:E:862:GLU:HB3	2.07	0.55
1:D:729:ILE:CD1	1:D:745:LEU:HB3	2.37	0.55
1:D:731:TYR:HA	1:D:745:LEU:HD23	1.89	0.55
1:N:745:LEU:CD1	2:N:1999:APJ:H18A	2.36	0.55
1:A:795:HIS:HA	1:A:832:CYS:CB	2.36	0.55
1:A:897:LEU:N	1:A:897:LEU:HD12	2.21	0.55
1:G:897:LEU:HD12	1:G:897:LEU:N	2.22	0.55
1:A:781:ILE:HG22	1:A:906:MET:HE2	1.89	0.55
1:I:861:LEU:O	1:I:862:GLU:HB3	2.06	0.55
1:F:723:ASP:HB2	1:F:730:ARG:HA	1.89	0.55
1:I:970:THR:HG23	1:I:973:LYS:HB2	1.88	0.55
1:G:752:LEU:HD21	1:G:913:ILE:HD11	1.88	0.55
1:H:861:LEU:O	1:H:862:GLU:HB3	2.06	0.55
1:D:745:LEU:HD12	2:D:1999:APJ:H18A	1.88	0.55
1:A:729:ILE:CD1	1:A:745:LEU:HB3	2.37	0.55
1:A:731:TYR:HA	1:A:745:LEU:HD23	1.89	0.55
1:G:1034:MET:HA	1:G:1034:MET:HE3	1.89	0.55
1:B:709:CYS:O	1:B:713:LEU:HD13	2.06	0.55
1:J:861:LEU:O	1:J:862:GLU:HB3	2.06	0.55
1:K:745:LEU:HD12	2:K:1999:APJ:H18A	1.88	0.55
1:N:897:LEU:HD12	1:N:897:LEU:N	2.22	0.55
1:H:745:LEU:HD12	2:H:1999:APJ:H18A	1.88	0.55
1:H:731:TYR:HA	1:H:745:LEU:HD23	1.88	0.55
1:F:781:ILE:HG22	1:F:906:MET:HE2	1.88	0.55
1:K:673:LEU:C	1:K:673:LEU:HD23	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:752:LEU:HD21	1:I:913:ILE:HD11	1.88	0.55
1:C:723:ASP:HB2	1:C:730:ARG:HA	1.90	0.54
1:K:709:CYS:O	1:K:713:LEU:HD13	2.07	0.54
1:D:1055:LEU:C	1:D:1055:LEU:HD23	2.27	0.54
1:C:897:LEU:HD12	1:C:897:LEU:N	2.21	0.54
1:G:729:ILE:CD1	1:G:745:LEU:HB3	2.37	0.54
1:F:757:GLU:O	1:F:759:LYS:HE3	2.08	0.54
1:C:749:ASN:N	1:C:749:ASN:OD1	2.40	0.54
1:J:672:ASN:HD22	1:J:672:ASN:N	2.05	0.54
1:I:745:LEU:CD1	2:I:1999:APJ:H18A	2.38	0.54
1:G:1002:ARG:HH12	1:G:1041:ARG:CZ	2.21	0.54
1:E:1034:MET:HE2	1:E:1037:LEU:HD23	1.90	0.54
1:E:749:ASN:OD1	1:E:749:ASN:N	2.38	0.54
1:M:749:ASN:OD1	1:M:749:ASN:N	2.41	0.54
1:L:745:LEU:CD1	2:L:1999:APJ:H18A	2.38	0.54
1:E:745:LEU:HD12	2:E:1999:APJ:H18A	1.87	0.54
1:G:737:THR:HG23	1:G:740:PHE:H	1.72	0.54
1:E:729:ILE:CD1	1:E:745:LEU:HB3	2.37	0.54
1:E:757:GLU:O	1:E:759:LYS:HE3	2.08	0.54
1:D:749:ASN:OD1	1:D:749:ASN:N	2.40	0.54
1:B:745:LEU:CD1	2:B:1999:APJ:H18A	2.38	0.54
1:E:745:LEU:CD1	2:E:1999:APJ:H18A	2.38	0.54
1:D:1111:GLU:O	1:D:1115:SER:HB3	2.08	0.54
1:E:970:THR:OG1	1:G:762:SER:CB	2.56	0.54
1:G:745:LEU:CD1	2:G:1999:APJ:H18A	2.38	0.54
1:J:1037:LEU:HB2	1:J:1058:LYS:HZ3	1.72	0.54
1:I:1111:GLU:O	1:I:1115:SER:HB3	2.08	0.54
1:M:709:CYS:O	1:M:713:LEU:HD13	2.07	0.54
1:B:737:THR:HG23	1:B:740:PHE:H	1.73	0.54
1:K:672:ASN:ND2	1:K:672:ASN:H	2.06	0.54
2:K:1999:APJ:H17	2:K:1999:APJ:N8	2.23	0.54
1:K:729:ILE:CD1	1:K:745:LEU:HB3	2.38	0.54
1:D:757:GLU:O	1:D:759:LYS:HE3	2.08	0.54
1:G:1111:GLU:O	1:G:1115:SER:HB3	2.08	0.54
1:I:737:THR:HG23	1:I:740:PHE:H	1.73	0.54
1:L:749:ASN:OD1	1:L:749:ASN:N	2.41	0.54
1:K:737:THR:HG23	1:K:740:PHE:H	1.73	0.54
1:I:1034:MET:HA	1:I:1034:MET:HE3	1.89	0.54
1:J:897:LEU:N	1:J:897:LEU:HD12	2.23	0.54
1:J:737:THR:HG23	1:J:740:PHE:H	1.73	0.54
1:M:757:GLU:O	1:M:759:LYS:HE3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:ASN:OD1	1:A:749:ASN:N	2.40	0.54
1:K:745:LEU:CD1	2:K:1999:APJ:H18A	2.38	0.53
1:K:897:LEU:N	1:K:897:LEU:HD12	2.23	0.53
1:J:729:ILE:CD1	1:J:745:LEU:HB3	2.38	0.53
1:I:897:LEU:HD12	1:I:897:LEU:N	2.23	0.53
2:B:1999:APJ:H17	2:B:1999:APJ:N8	2.22	0.53
1:C:1037:LEU:HD21	1:C:1054:ALA:HB1	1.89	0.53
1:B:671:LYS:O	1:B:671:LYS:HD2	2.08	0.53
1:B:1055:LEU:C	1:B:1055:LEU:HD23	2.29	0.53
1:H:757:GLU:O	1:H:759:LYS:HE3	2.08	0.53
1:D:667:GLU:C	1:D:668:GLN:NE2	2.62	0.53
1:J:723:ASP:HB2	1:J:730:ARG:HA	1.89	0.53
1:M:745:LEU:CD1	2:M:1999:APJ:H18A	2.38	0.53
1:H:897:LEU:N	1:H:897:LEU:HD12	2.23	0.53
1:G:731:TYR:HA	1:G:745:LEU:HD23	1.91	0.53
1:E:1093:ILE:O	1:E:1097:MET:HG3	2.08	0.53
1:I:757:GLU:O	1:I:759:LYS:HE3	2.08	0.53
1:F:752:LEU:HD21	1:F:913:ILE:HD11	1.90	0.53
1:K:1111:GLU:O	1:K:1115:SER:HB3	2.08	0.53
1:D:1093:ILE:O	1:D:1097:MET:HG3	2.08	0.53
1:I:787:HIS:CD2	1:J:814:ASP:CG	2.77	0.53
1:M:723:ASP:HB2	1:M:730:ARG:HA	1.90	0.53
1:E:672:ASN:ND2	1:E:672:ASN:N	2.56	0.53
1:M:672:ASN:HD22	1:M:672:ASN:H	1.55	0.53
1:E:1111:GLU:O	1:E:1115:SER:HB3	2.09	0.53
1:B:909:VAL:O	1:B:913:ILE:HG12	2.08	0.53
1:I:1093:ILE:O	1:I:1097:MET:HG3	2.08	0.53
1:N:671:LYS:O	1:N:671:LYS:HD2	2.09	0.53
1:B:1111:GLU:O	1:B:1115:SER:HB3	2.09	0.53
1:N:729:ILE:CD1	1:N:745:LEU:HB3	2.39	0.53
1:D:824:ILE:O	1:D:825:LEU:HD23	2.08	0.53
1:H:729:ILE:CD1	1:H:745:LEU:HB3	2.38	0.53
1:L:824:ILE:O	1:L:825:LEU:HD23	2.09	0.53
1:B:752:LEU:HD21	1:B:913:ILE:HD11	1.90	0.53
1:B:757:GLU:O	1:B:759:LYS:HE3	2.07	0.53
1:L:757:GLU:O	1:L:759:LYS:HE3	2.08	0.53
1:H:737:THR:HG23	1:H:740:PHE:H	1.72	0.53
1:M:729:ILE:CD1	1:M:745:LEU:HB3	2.38	0.53
1:B:824:ILE:O	1:B:825:LEU:HD23	2.08	0.53
1:J:1111:GLU:O	1:J:1115:SER:HB3	2.09	0.53
1:L:737:THR:HG23	1:L:740:PHE:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1025:TRP:CD1	1:J:1045:SER:O	2.61	0.53
1:N:731:TYR:HA	1:N:745:LEU:HD23	1.91	0.53
1:C:1041:ARG:HH22	1:C:1053:ARG:HG2	1.74	0.53
1:G:672:ASN:H	1:G:672:ASN:HD22	1.57	0.53
1:N:811:PHE:HB3	1:N:823:ARG:NH1	2.24	0.53
1:C:781:ILE:HG22	1:C:906:MET:CE	2.39	0.53
1:J:757:GLU:O	1:J:759:LYS:HE3	2.08	0.53
1:G:1093:ILE:O	1:G:1097:MET:HG3	2.09	0.53
1:N:1111:GLU:O	1:N:1115:SER:HB3	2.08	0.53
1:K:757:GLU:O	1:K:759:LYS:HE3	2.09	0.53
1:C:737:THR:HG23	1:C:740:PHE:H	1.74	0.53
1:D:665:ASN:O	1:D:666:PHE:CB	2.57	0.53
2:L:1999:APJ:N8	2:L:1999:APJ:H17	2.24	0.53
1:H:745:LEU:CD1	2:H:1999:APJ:H18A	2.38	0.53
1:H:1034:MET:HE2	1:H:1037:LEU:HD23	1.90	0.53
1:H:671:LYS:O	1:H:671:LYS:HD2	2.09	0.53
1:D:668:GLN:O	1:D:669:SER:C	2.47	0.53
1:M:1055:LEU:C	1:M:1055:LEU:HD23	2.30	0.53
1:M:737:THR:HG23	1:M:740:PHE:H	1.73	0.53
1:G:757:GLU:O	1:G:759:LYS:HE3	2.08	0.53
1:A:1016:SER:C	1:A:1018:PHE:H	2.12	0.53
1:J:1055:LEU:C	1:J:1055:LEU:HD23	2.30	0.53
1:E:723:ASP:HB2	1:E:730:ARG:HA	1.90	0.52
1:L:729:ILE:CD1	1:L:745:LEU:HB3	2.38	0.52
1:N:1034:MET:HA	1:N:1034:MET:HE2	1.91	0.52
1:E:909:VAL:O	1:E:913:ILE:HG12	2.09	0.52
1:A:757:GLU:O	1:A:759:LYS:HE3	2.08	0.52
1:M:824:ILE:O	1:M:825:LEU:HD23	2.09	0.52
1:I:1034:MET:CE	1:I:1037:LEU:HD23	2.38	0.52
1:I:729:ILE:CD1	1:I:745:LEU:HB3	2.39	0.52
1:C:731:TYR:HA	1:C:745:LEU:HD23	1.91	0.52
1:G:1002:ARG:HH12	1:G:1041:ARG:NH2	2.07	0.52
1:B:1093:ILE:O	1:B:1097:MET:HG3	2.09	0.52
1:F:680:LEU:HB2	1:F:689:VAL:HG12	1.91	0.52
1:G:723:ASP:HB2	1:G:730:ARG:HA	1.91	0.52
1:C:729:ILE:CD1	1:C:745:LEU:HB3	2.39	0.52
1:D:897:LEU:N	1:D:897:LEU:HD12	2.24	0.52
1:F:824:ILE:O	1:F:825:LEU:HD23	2.10	0.52
1:E:737:THR:HG23	1:E:740:PHE:H	1.75	0.52
1:I:749:ASN:N	1:I:749:ASN:OD1	2.41	0.52
1:E:673:LEU:HD23	1:E:673:LEU:C	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:723:ASP:HB2	1:L:730:ARG:HA	1.91	0.52
1:A:811:PHE:HB3	1:A:823:ARG:NH1	2.25	0.52
1:E:731:TYR:HA	1:E:745:LEU:HD23	1.92	0.52
1:G:1059:TYR:OH	1:H:992:LYS:HE3	2.09	0.52
1:K:1093:ILE:O	1:K:1097:MET:HG3	2.09	0.52
1:L:1111:GLU:O	1:L:1115:SER:HB3	2.09	0.52
1:F:749:ASN:OD1	1:F:749:ASN:N	2.43	0.52
1:N:723:ASP:HB2	1:N:730:ARG:HA	1.90	0.52
1:L:897:LEU:HD12	1:L:897:LEU:N	2.24	0.52
1:K:909:VAL:O	1:K:913:ILE:HG12	2.10	0.52
1:E:914:LEU:O	1:E:943:CYS:HB2	2.10	0.52
1:M:811:PHE:HB3	1:M:823:ARG:NH1	2.25	0.52
1:H:1111:GLU:O	1:H:1115:SER:HB3	2.10	0.52
1:A:1020:ILE:HG22	1:A:1021:PRO:C	2.30	0.52
1:F:682:TYR:O	2:F:1999:APJ:H23	2.10	0.52
1:C:1111:GLU:O	1:C:1115:SER:HB3	2.09	0.52
1:F:737:THR:HG23	1:F:740:PHE:H	1.74	0.52
1:I:1055:LEU:HD23	1:I:1055:LEU:C	2.30	0.52
1:H:749:ASN:OD1	1:H:749:ASN:N	2.41	0.52
1:E:970:THR:OG1	1:G:762:SER:HB2	2.10	0.52
1:K:731:TYR:HA	1:K:745:LEU:HD23	1.90	0.52
1:M:1034:MET:HA	1:M:1034:MET:CE	2.40	0.52
1:E:853:SER:HA	1:E:856:ARG:HG3	1.92	0.52
1:A:737:THR:HG23	1:A:740:PHE:H	1.74	0.52
1:N:757:GLU:O	1:N:759:LYS:HE3	2.10	0.52
1:H:673:LEU:C	1:H:673:LEU:HD23	2.30	0.52
1:D:723:ASP:HB2	1:D:730:ARG:HA	1.90	0.52
1:F:897:LEU:HD12	1:F:897:LEU:N	2.24	0.52
1:M:1034:MET:HA	1:M:1034:MET:HE3	1.91	0.52
1:A:853:SER:HA	1:A:856:ARG:HG3	1.92	0.52
1:N:749:ASN:OD1	1:N:749:ASN:N	2.40	0.52
1:N:794:ILE:HG22	1:N:795:HIS:O	2.10	0.52
1:N:682:TYR:O	2:N:1999:APJ:H23	2.10	0.52
1:B:729:ILE:CD1	1:B:745:LEU:HB3	2.40	0.52
1:L:1034:MET:CE	1:L:1037:LEU:HD23	2.38	0.52
1:C:928:GLU:O	1:C:932:ILE:HG13	2.10	0.52
1:D:928:GLU:O	1:D:932:ILE:HG13	2.10	0.52
1:H:811:PHE:HB3	1:H:823:ARG:NH1	2.25	0.52
1:I:811:PHE:HB3	1:I:823:ARG:NH1	2.25	0.52
1:A:928:GLU:O	1:A:932:ILE:HG13	2.09	0.52
1:B:928:GLU:O	1:B:932:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:752:LEU:HD21	1:N:913:ILE:HD11	1.92	0.52
1:G:749:ASN:OD1	1:G:749:ASN:N	2.41	0.52
1:I:787:HIS:CD2	1:J:814:ASP:OD2	2.57	0.52
1:I:723:ASP:HB2	1:I:730:ARG:HA	1.91	0.52
1:J:824:ILE:O	1:J:825:LEU:HD23	2.10	0.52
1:B:731:TYR:HA	1:B:745:LEU:HD23	1.92	0.52
1:L:1034:MET:HE3	1:L:1034:MET:HA	1.92	0.52
1:I:909:VAL:O	1:I:913:ILE:HG12	2.10	0.52
1:I:928:GLU:O	1:I:932:ILE:HG13	2.10	0.52
1:J:928:GLU:O	1:J:932:ILE:HG13	2.10	0.52
1:F:811:PHE:HB3	1:F:823:ARG:NH1	2.25	0.52
1:N:924:LYS:HG3	1:N:925:TYR:CD2	2.45	0.52
1:M:671:LYS:HD2	1:M:671:LYS:O	2.09	0.52
1:L:671:LYS:O	1:L:671:LYS:HD2	2.09	0.52
1:G:673:LEU:C	1:G:673:LEU:HD23	2.30	0.52
1:H:723:ASP:HB2	1:H:730:ARG:HA	1.91	0.51
1:I:731:TYR:HA	1:I:745:LEU:HD23	1.91	0.51
2:F:1999:APJ:N8	2:F:1999:APJ:H17	2.25	0.51
1:M:731:TYR:HA	1:M:745:LEU:HD23	1.92	0.51
1:C:1034:MET:HA	1:C:1034:MET:CE	2.40	0.51
1:D:671:LYS:HD2	1:D:671:LYS:O	2.10	0.51
1:F:1055:LEU:HD23	1:F:1055:LEU:C	2.30	0.51
1:K:749:ASN:OD1	1:K:749:ASN:N	2.41	0.51
1:G:824:ILE:O	1:G:825:LEU:HD23	2.10	0.51
2:H:1999:APJ:N8	2:H:1999:APJ:H17	2.25	0.51
1:K:1034:MET:CE	1:K:1037:LEU:HD23	2.39	0.51
1:A:824:ILE:O	1:A:825:LEU:HD23	2.10	0.51
1:L:928:GLU:O	1:L:932:ILE:HG13	2.10	0.51
1:C:848:ASN:CB	1:C:849:PRO:HA	2.29	0.51
1:F:794:ILE:HG22	1:F:795:HIS:O	2.10	0.51
1:C:794:ILE:N	1:C:794:ILE:HD12	2.25	0.51
1:H:824:ILE:O	1:H:825:LEU:HD23	2.10	0.51
1:D:970:THR:HG23	1:D:973:LYS:CB	2.41	0.51
1:H:928:GLU:O	1:H:932:ILE:HG13	2.09	0.51
1:F:1093:ILE:O	1:F:1097:MET:HG3	2.11	0.51
1:N:1093:ILE:O	1:N:1097:MET:HG3	2.10	0.51
1:N:914:LEU:O	1:N:943:CYS:HB2	2.10	0.51
1:C:924:LYS:HG3	1:C:925:TYR:CD2	2.45	0.51
1:D:668:GLN:N	1:D:668:GLN:NE2	2.59	0.51
1:A:723:ASP:HB2	1:A:730:ARG:HA	1.92	0.51
1:J:909:VAL:O	1:J:913:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:758:SER:HB3	1:B:768:LEU:HD21	1.93	0.51
1:M:1111:GLU:O	1:M:1115:SER:HB3	2.10	0.51
1:B:861:LEU:O	1:B:862:GLU:CB	2.59	0.51
1:A:1034:MET:CE	1:A:1034:MET:HA	2.41	0.51
1:M:928:GLU:O	1:M:932:ILE:HG13	2.09	0.51
1:G:928:GLU:O	1:G:932:ILE:HG13	2.09	0.51
1:L:1055:LEU:C	1:L:1055:LEU:HD23	2.31	0.51
1:B:762:SER:HB2	1:M:970:THR:HB	1.93	0.51
1:J:731:TYR:HA	1:J:745:LEU:HD23	1.92	0.51
2:G:1999:APJ:H17	2:G:1999:APJ:N8	2.26	0.51
1:F:1034:MET:HA	1:F:1034:MET:CE	2.41	0.51
1:L:909:VAL:O	1:L:913:ILE:HG12	2.10	0.51
1:N:853:SER:HA	1:N:856:ARG:HG3	1.93	0.51
1:B:723:ASP:HB2	1:B:730:ARG:HA	1.91	0.51
1:D:745:LEU:CD1	2:D:1999:APJ:H18A	2.40	0.51
1:F:745:LEU:HD12	2:F:1999:APJ:H18A	1.91	0.51
2:E:1999:APJ:H17	2:E:1999:APJ:N8	2.25	0.51
1:F:853:SER:HA	1:F:856:ARG:HG3	1.92	0.51
1:K:811:PHE:HB3	1:K:823:ARG:NH1	2.25	0.51
1:J:811:PHE:HB3	1:J:823:ARG:NH1	2.26	0.51
1:D:1034:MET:HA	1:D:1034:MET:CE	2.40	0.51
1:E:682:TYR:O	2:E:1999:APJ:H23	2.11	0.51
1:M:1059:TYR:OH	1:N:992:LYS:HE3	2.11	0.51
1:K:1055:LEU:C	1:K:1055:LEU:HD23	2.31	0.51
1:A:725:HIS:CG	1:A:726:PRO:HD2	2.46	0.51
1:A:745:LEU:HD12	2:A:1999:APJ:H18A	1.93	0.51
1:L:1034:MET:HA	1:L:1034:MET:CE	2.41	0.51
1:M:1037:LEU:C	1:M:1039:ARG:H	2.14	0.51
1:C:757:GLU:O	1:C:759:LYS:HE3	2.10	0.51
1:C:811:PHE:HB3	1:C:823:ARG:NH1	2.26	0.51
1:J:1093:ILE:O	1:J:1097:MET:HG3	2.10	0.51
1:H:1055:LEU:C	1:H:1055:LEU:HD23	2.31	0.51
1:K:671:LYS:O	1:K:671:LYS:HD2	2.11	0.51
1:E:1034:MET:HE3	1:E:1034:MET:HA	1.91	0.51
1:L:811:PHE:HB3	1:L:823:ARG:NH1	2.26	0.51
1:K:924:LYS:HG3	1:K:925:TYR:CD2	2.46	0.51
1:K:837:SER:HB3	1:K:838:GLY:HA2	1.93	0.51
1:F:928:GLU:O	1:F:932:ILE:HG13	2.11	0.51
1:G:853:SER:HA	1:G:856:ARG:HG3	1.93	0.51
1:L:731:TYR:HA	1:L:745:LEU:HD23	1.91	0.50
2:C:1999:APJ:H17	2:C:1999:APJ:N8	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:673:LEU:HD23	1:D:673:LEU:C	2.32	0.50
1:H:845:ASN:N	1:H:845:ASN:HD22	2.09	0.50
1:E:928:GLU:O	1:E:932:ILE:HG13	2.10	0.50
1:I:685:SER:HB3	1:I:708:PHE:CZ	2.46	0.50
1:L:853:SER:HA	1:L:856:ARG:HG3	1.92	0.50
1:C:845:ASN:HD22	1:C:845:ASN:N	2.09	0.50
1:H:977:HIS:CG	1:H:978:PRO:HD2	2.46	0.50
1:J:749:ASN:N	1:J:749:ASN:OD1	2.41	0.50
1:E:1055:LEU:C	1:E:1055:LEU:HD23	2.31	0.50
1:D:737:THR:HG23	1:D:740:PHE:H	1.75	0.50
2:I:1999:APJ:N8	2:I:1999:APJ:H17	2.26	0.50
1:E:824:ILE:O	1:E:825:LEU:HD23	2.10	0.50
1:B:853:SER:HA	1:B:856:ARG:HG3	1.93	0.50
1:M:845:ASN:N	1:M:845:ASN:HD22	2.09	0.50
1:B:1000:GLU:HB2	1:B:1009:LEU:HD21	1.93	0.50
1:G:1055:LEU:C	1:G:1055:LEU:HD23	2.32	0.50
1:E:811:PHE:HB3	1:E:823:ARG:NH1	2.26	0.50
1:F:977:HIS:CG	1:F:978:PRO:HD2	2.47	0.50
1:C:1000:GLU:HB2	1:C:1009:LEU:HD21	1.93	0.50
1:M:970:THR:HG23	1:M:973:LYS:CB	2.41	0.50
1:B:794:ILE:HG22	1:B:795:HIS:O	2.12	0.50
1:C:794:ILE:HG22	1:C:795:HIS:O	2.12	0.50
1:M:909:VAL:O	1:M:913:ILE:HG12	2.11	0.50
1:D:909:VAL:O	1:D:913:ILE:HG12	2.12	0.50
1:E:1095:VAL:O	1:E:1099:VAL:HG23	2.12	0.50
1:K:928:GLU:O	1:K:932:ILE:HG13	2.11	0.50
1:B:845:ASN:N	1:B:845:ASN:HD22	2.08	0.50
1:M:781:ILE:HG22	1:M:906:MET:CE	2.41	0.50
1:B:864:SER:O	1:B:893:THR:OG1	2.29	0.50
1:F:745:LEU:CD1	2:F:1999:APJ:H18A	2.41	0.50
1:F:758:SER:HB3	1:F:768:LEU:HD21	1.93	0.50
1:N:758:SER:HB3	1:N:768:LEU:HD21	1.94	0.50
1:E:1000:GLU:HB2	1:E:1009:LEU:HD21	1.94	0.50
1:L:1000:GLU:HB2	1:L:1009:LEU:HD21	1.93	0.50
1:F:924:LYS:HG3	1:F:925:TYR:CD2	2.46	0.50
1:D:682:TYR:O	2:D:1999:APJ:H23	2.12	0.50
1:J:794:ILE:N	1:J:794:ILE:HD12	2.26	0.50
1:L:682:TYR:O	2:L:1999:APJ:H23	2.11	0.50
1:D:1034:MET:HE3	1:D:1034:MET:HA	1.92	0.50
1:J:864:SER:O	1:J:893:THR:OG1	2.29	0.50
2:M:1999:APJ:N8	2:M:1999:APJ:H17	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:845:ASN:N	1:N:845:ASN:HD22	2.10	0.50
1:G:1034:MET:CE	1:G:1034:MET:HA	2.41	0.50
1:D:758:SER:HB3	1:D:768:LEU:HD21	1.94	0.50
1:N:909:VAL:O	1:N:913:ILE:HG12	2.11	0.50
1:C:1016:SER:C	1:C:1018:PHE:H	2.14	0.50
1:A:1059:TYR:OH	1:B:1108:ILE:HD12	2.12	0.50
1:L:1093:ILE:O	1:L:1097:MET:HG3	2.11	0.50
1:L:924:LYS:HG3	1:L:925:TYR:CD2	2.47	0.50
1:H:1093:ILE:O	1:H:1097:MET:HG3	2.12	0.50
1:B:811:PHE:HB3	1:B:823:ARG:NH1	2.26	0.50
1:G:845:ASN:HD22	1:G:845:ASN:N	2.09	0.50
1:D:781:ILE:HG22	1:D:906:MET:CE	2.42	0.50
1:C:673:LEU:O	1:C:673:LEU:HD23	2.11	0.50
1:K:758:SER:HB3	1:K:768:LEU:HD21	1.94	0.50
1:M:671:LYS:HA	1:M:673:LEU:H	1.76	0.50
1:L:1016:SER:C	1:L:1018:PHE:H	2.16	0.50
1:F:1111:GLU:O	1:F:1115:SER:HB3	2.11	0.50
1:M:1016:SER:C	1:M:1018:PHE:H	2.15	0.50
1:A:1111:GLU:O	1:A:1115:SER:HB3	2.10	0.50
1:D:861:LEU:O	1:D:862:GLU:CB	2.60	0.49
1:K:841:SEP:P	1:M:678:LYS:HZ1	2.35	0.49
1:D:794:ILE:N	1:D:794:ILE:HD12	2.27	0.49
1:L:794:ILE:N	1:L:794:ILE:HD12	2.27	0.49
1:G:781:ILE:HG22	1:G:906:MET:CE	2.41	0.49
1:F:909:VAL:O	1:F:913:ILE:HG12	2.12	0.49
1:A:924:LYS:HG3	1:A:925:TYR:CD2	2.47	0.49
1:K:977:HIS:CG	1:K:978:PRO:HD2	2.47	0.49
1:N:928:GLU:O	1:N:932:ILE:HG13	2.12	0.49
1:A:1034:MET:HA	1:A:1034:MET:HE2	1.94	0.49
1:F:729:ILE:CD1	1:F:745:LEU:HB3	2.42	0.49
1:H:909:VAL:O	1:H:913:ILE:HG12	2.12	0.49
1:B:678:LYS:HE3	1:M:896:ARG:HE	1.77	0.49
1:D:1000:GLU:HB2	1:D:1009:LEU:HD21	1.94	0.49
1:N:977:HIS:CG	1:N:978:PRO:HD2	2.47	0.49
1:B:673:LEU:HD23	1:B:673:LEU:C	2.33	0.49
1:N:861:LEU:O	1:N:862:GLU:CB	2.60	0.49
1:L:794:ILE:HG22	1:L:795:HIS:O	2.11	0.49
1:C:970:THR:HG23	1:C:973:LYS:CB	2.41	0.49
1:F:1000:GLU:HB2	1:F:1009:LEU:HD21	1.94	0.49
1:J:1041:ARG:NH2	1:J:1053:ARG:HG2	2.27	0.49
1:G:1000:GLU:HB2	1:G:1009:LEU:HD21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:924:LYS:HG3	1:H:925:TYR:CD2	2.47	0.49
1:F:673:LEU:C	1:F:673:LEU:CD2	2.81	0.49
1:D:672:ASN:HD22	1:D:672:ASN:H	1.59	0.49
1:H:1034:MET:CE	1:H:1034:MET:HA	2.42	0.49
1:J:1000:GLU:HB2	1:J:1009:LEU:HD21	1.94	0.49
1:D:924:LYS:HG3	1:D:925:TYR:CD2	2.48	0.49
1:E:845:ASN:HD22	1:E:845:ASN:N	2.09	0.49
1:L:837:SER:HB3	1:L:838:GLY:HA2	1.94	0.49
1:K:685:SER:HB3	1:K:708:PHE:CZ	2.47	0.49
1:I:924:LYS:HG3	1:I:925:TYR:CD2	2.47	0.49
1:L:685:SER:HB3	1:L:708:PHE:CZ	2.47	0.49
1:M:853:SER:HA	1:M:856:ARG:HG3	1.94	0.49
1:K:723:ASP:HB2	1:K:730:ARG:HA	1.92	0.49
2:J:1999:APJ:H17	2:J:1999:APJ:N8	2.28	0.49
1:G:682:TYR:O	2:G:1999:APJ:H23	2.12	0.49
1:M:758:SER:HB3	1:M:768:LEU:HD21	1.94	0.49
1:G:758:SER:HB3	1:G:768:LEU:HD21	1.94	0.49
1:M:685:SER:HB3	1:M:708:PHE:CZ	2.48	0.49
1:F:1016:SER:C	1:F:1018:PHE:H	2.16	0.49
1:A:1000:GLU:HB2	1:A:1009:LEU:HD21	1.94	0.49
1:H:837:SER:HB3	1:H:838:GLY:HA2	1.95	0.49
1:B:924:LYS:HG3	1:B:925:TYR:CD2	2.47	0.49
1:B:837:SER:HB3	1:B:838:GLY:HA2	1.93	0.49
1:A:1037:LEU:O	1:A:1037:LEU:HD12	2.12	0.49
1:I:824:ILE:O	1:I:825:LEU:HD23	2.13	0.49
1:A:909:VAL:O	1:A:913:ILE:HG12	2.12	0.49
1:E:758:SER:HB3	1:E:768:LEU:HD21	1.95	0.49
1:I:758:SER:HB3	1:I:768:LEU:HD21	1.95	0.49
1:J:685:SER:HB3	1:J:708:PHE:CZ	2.47	0.49
1:I:992:LYS:HE3	1:J:1059:TYR:OH	2.13	0.49
1:M:861:LEU:O	1:M:862:GLU:CB	2.61	0.49
1:I:794:ILE:HG22	1:I:795:HIS:O	2.13	0.49
1:I:682:TYR:O	2:I:1999:APJ:H23	2.13	0.49
1:E:864:SER:O	1:E:893:THR:OG1	2.29	0.49
1:A:745:LEU:CD1	2:A:1999:APJ:H18A	2.42	0.49
1:B:781:ILE:HG22	1:B:906:MET:CE	2.42	0.49
1:G:672:ASN:N	1:G:672:ASN:ND2	2.59	0.49
1:G:909:VAL:O	1:G:913:ILE:HG12	2.12	0.49
1:D:845:ASN:HD22	1:D:845:ASN:N	2.10	0.49
1:F:845:ASN:N	1:F:845:ASN:HD22	2.09	0.49
1:A:845:ASN:HD22	1:A:845:ASN:N	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:837:SER:HB3	1:I:838:GLY:HA2	1.94	0.49
1:B:1034:MET:HA	1:B:1034:MET:CE	2.42	0.49
1:K:794:ILE:N	1:K:794:ILE:HD12	2.28	0.49
1:G:794:ILE:HD12	1:G:794:ILE:N	2.28	0.49
1:I:781:ILE:HG22	1:I:906:MET:CE	2.43	0.49
1:E:1034:MET:HA	1:E:1034:MET:CE	2.42	0.49
1:J:758:SER:HB3	1:J:768:LEU:HD21	1.94	0.49
1:I:845:ASN:HD22	1:I:845:ASN:N	2.09	0.49
1:J:924:LYS:HG3	1:J:925:TYR:CD2	2.48	0.49
1:G:861:LEU:O	1:G:862:GLU:CB	2.61	0.49
1:J:794:ILE:HG22	1:J:795:HIS:O	2.12	0.49
1:J:770:LYS:HG2	1:J:771:GLU:N	2.28	0.49
1:D:671:LYS:HA	1:D:673:LEU:H	1.78	0.49
1:I:853:SER:HA	1:I:856:ARG:HG3	1.94	0.49
1:C:1076:VAL:HG11	1:D:1108:ILE:HD11	1.94	0.49
1:B:1016:SER:C	1:B:1018:PHE:H	2.15	0.49
1:G:924:LYS:HG3	1:G:925:TYR:CD2	2.48	0.49
1:E:794:ILE:HG22	1:E:795:HIS:O	2.12	0.49
1:C:745:LEU:HD12	2:C:1999:APJ:H18A	1.94	0.49
1:N:824:ILE:O	1:N:825:LEU:HD23	2.12	0.49
1:A:785:VAL:HG21	1:A:906:MET:HE1	1.94	0.49
1:C:758:SER:HB3	1:C:768:LEU:HD21	1.94	0.49
1:K:914:LEU:O	1:K:943:CYS:HB2	2.13	0.49
1:L:914:LEU:O	1:L:943:CYS:HB2	2.13	0.49
1:A:837:SER:HB3	1:A:838:GLY:HA2	1.94	0.49
1:H:853:SER:HA	1:H:856:ARG:HG3	1.94	0.49
1:L:861:LEU:O	1:L:862:GLU:CB	2.61	0.48
1:F:861:LEU:O	1:F:862:GLU:CB	2.60	0.48
1:M:682:TYR:O	2:M:1999:APJ:H23	2.13	0.48
1:J:682:TYR:O	2:J:1999:APJ:H23	2.13	0.48
1:I:695:GLN:HG2	1:J:731:TYR:OH	2.13	0.48
1:D:770:LYS:HG2	1:D:771:GLU:N	2.28	0.48
1:J:914:LEU:O	1:J:943:CYS:HB2	2.13	0.48
1:C:914:LEU:O	1:C:943:CYS:HB2	2.12	0.48
1:D:685:SER:HB3	1:D:708:PHE:CZ	2.48	0.48
1:F:794:ILE:N	1:F:794:ILE:HD12	2.29	0.48
1:C:794:ILE:O	1:C:832:CYS:HB2	2.13	0.48
1:N:1034:MET:HA	1:N:1034:MET:CE	2.43	0.48
1:J:853:SER:HA	1:J:856:ARG:HG3	1.94	0.48
1:E:837:SER:HB3	1:E:838:GLY:HA2	1.94	0.48
1:G:837:SER:HB3	1:G:838:GLY:HA2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:685:SER:HB3	1:F:708:PHE:CZ	2.48	0.48
1:A:674:VAL:CG1	1:A:675:VAL:N	2.76	0.48
1:K:861:LEU:O	1:K:862:GLU:CB	2.61	0.48
1:C:804:LEU:HB2	1:C:825:LEU:HB2	1.96	0.48
1:G:977:HIS:CG	1:G:978:PRO:HD2	2.48	0.48
1:G:823:ARG:NH2	1:H:724:ASP:OD2	2.46	0.48
1:G:794:ILE:HG22	1:G:795:HIS:O	2.13	0.48
1:N:781:ILE:HG22	1:N:906:MET:CE	2.43	0.48
1:G:970:THR:HG23	1:G:973:LYS:CB	2.43	0.48
1:I:914:LEU:O	1:I:943:CYS:HB2	2.14	0.48
1:N:1055:LEU:C	1:N:1055:LEU:HD23	2.33	0.48
1:E:924:LYS:HG3	1:E:925:TYR:CD2	2.48	0.48
1:K:845:ASN:HD22	1:K:845:ASN:N	2.10	0.48
1:I:861:LEU:O	1:I:862:GLU:CB	2.61	0.48
1:M:804:LEU:HB2	1:M:825:LEU:HB2	1.96	0.48
1:I:864:SER:O	1:I:893:THR:OG1	2.30	0.48
1:C:745:LEU:CD1	2:C:1999:APJ:H18A	2.43	0.48
1:K:824:ILE:O	1:K:825:LEU:HD23	2.13	0.48
1:A:682:TYR:O	2:A:1999:APJ:H23	2.13	0.48
1:J:837:SER:HB3	1:J:838:GLY:HA2	1.95	0.48
1:D:1016:SER:C	1:D:1018:PHE:H	2.15	0.48
1:K:1016:SER:C	1:K:1018:PHE:H	2.17	0.48
1:D:977:HIS:CG	1:D:978:PRO:HD2	2.48	0.48
1:N:837:SER:HB3	1:N:838:GLY:HA2	1.95	0.48
1:N:1016:SER:C	1:N:1018:PHE:H	2.17	0.48
1:D:667:GLU:C	1:D:668:GLN:HE21	2.17	0.48
1:E:970:THR:HG23	1:E:973:LYS:CB	2.43	0.48
1:J:861:LEU:O	1:J:862:GLU:CB	2.61	0.48
1:A:794:ILE:HG22	1:A:795:HIS:O	2.13	0.48
1:J:1034:MET:CE	1:J:1034:MET:HA	2.42	0.48
1:B:770:LYS:HG2	1:B:771:GLU:N	2.28	0.48
1:B:970:THR:HG23	1:B:973:LYS:CB	2.44	0.48
1:H:685:SER:HB3	1:H:708:PHE:CZ	2.49	0.48
1:A:685:SER:HB3	1:A:708:PHE:CZ	2.49	0.48
1:L:845:ASN:N	1:L:845:ASN:HD22	2.10	0.48
1:A:914:LEU:O	1:A:943:CYS:HB2	2.14	0.48
1:A:1055:LEU:C	1:A:1055:LEU:HD23	2.33	0.48
1:F:848:ASN:CB	1:F:849:PRO:HA	2.30	0.48
1:B:828:ASP:HB2	2:B:1999:APJ:H25	1.95	0.48
1:G:673:LEU:HD23	1:G:673:LEU:O	2.13	0.48
1:D:837:SER:HB3	1:D:838:GLY:HA2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:685:SER:HB3	1:G:708:PHE:CZ	2.48	0.48
1:H:670:LEU:O	1:H:735:GLU:OE2	2.32	0.48
1:G:1016:SER:C	1:G:1018:PHE:H	2.17	0.48
1:C:1093:ILE:O	1:C:1097:MET:HG3	2.12	0.48
1:H:861:LEU:O	1:H:862:GLU:CB	2.61	0.48
1:H:794:ILE:HG22	1:H:795:HIS:O	2.14	0.48
1:I:1034:MET:HA	1:I:1034:MET:CE	2.43	0.48
1:C:682:TYR:O	2:C:1999:APJ:H23	2.14	0.48
1:E:804:LEU:HB2	1:E:825:LEU:HB2	1.95	0.48
1:K:663:ILE:O	1:K:664:PRO:C	2.52	0.48
1:C:1037:LEU:C	1:C:1039:ARG:H	2.17	0.48
1:L:758:SER:HB3	1:L:768:LEU:HD21	1.94	0.48
1:D:914:LEU:O	1:D:943:CYS:HB2	2.13	0.48
1:K:853:SER:HA	1:K:856:ARG:HG3	1.94	0.48
1:H:1025:TRP:HB2	1:H:1088:PHE:CZ	2.48	0.48
1:J:977:HIS:CG	1:J:978:PRO:HD2	2.49	0.48
1:M:1000:GLU:HB2	1:M:1009:LEU:HD21	1.95	0.48
1:H:914:LEU:O	1:H:943:CYS:HB2	2.13	0.48
1:H:1000:GLU:HB2	1:H:1009:LEU:HD21	1.94	0.48
1:M:794:ILE:O	1:M:832:CYS:HB2	2.13	0.48
1:E:794:ILE:O	1:E:832:CYS:HB2	2.14	0.48
1:H:864:SER:O	1:H:893:THR:OG1	2.30	0.48
1:J:1036:ASN:O	1:J:1039:ARG:HB3	2.14	0.48
1:A:946:ASP:HB3	1:A:949:LEU:HD12	1.94	0.48
1:D:668:GLN:CD	1:D:739:ARG:NH2	2.58	0.48
1:D:794:ILE:HG22	1:D:795:HIS:O	2.13	0.48
1:F:725:HIS:CG	1:F:726:PRO:HD2	2.49	0.48
1:I:794:ILE:N	1:I:794:ILE:HD12	2.29	0.48
1:K:781:ILE:HG22	1:K:906:MET:CE	2.44	0.48
1:G:1037:LEU:C	1:G:1039:ARG:H	2.15	0.48
1:G:811:PHE:HB3	1:G:823:ARG:NH1	2.29	0.48
1:E:1016:SER:C	1:E:1018:PHE:H	2.16	0.48
1:M:837:SER:HB3	1:M:838:GLY:HA2	1.95	0.48
1:A:671:LYS:HD2	1:A:671:LYS:O	2.14	0.48
1:C:861:LEU:O	1:C:862:GLU:CB	2.60	0.47
1:F:794:ILE:O	1:F:832:CYS:HB2	2.14	0.47
1:M:673:LEU:C	1:M:673:LEU:HD23	2.34	0.47
1:C:946:ASP:HB3	1:C:949:LEU:HD12	1.95	0.47
1:J:845:ASN:N	1:J:845:ASN:HD22	2.10	0.47
1:M:1093:ILE:O	1:M:1097:MET:HG3	2.14	0.47
1:A:794:ILE:N	1:A:794:ILE:HD12	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1037:LEU:C	1:I:1039:ARG:H	2.18	0.47
1:H:781:ILE:HG22	1:H:906:MET:CE	2.43	0.47
1:L:893:THR:O	1:L:895:ARG:HG3	2.14	0.47
1:I:893:THR:O	1:I:895:ARG:HG3	2.14	0.47
1:C:864:SER:O	1:C:893:THR:OG1	2.29	0.47
1:A:828:ASP:HB2	2:A:1999:APJ:H25	1.96	0.47
1:I:804:LEU:HB2	1:I:825:LEU:HB2	1.96	0.47
1:E:906:MET:HB2	1:E:906:MET:HE3	1.78	0.47
1:C:770:LYS:HG2	1:C:771:GLU:N	2.29	0.47
1:B:674:VAL:CG1	1:B:675:VAL:N	2.76	0.47
1:L:977:HIS:CG	1:L:978:PRO:HD2	2.50	0.47
1:G:687:THR:HG23	1:G:704:MET:HG2	1.96	0.47
1:B:1025:TRP:HB2	1:B:1088:PHE:CZ	2.49	0.47
1:N:1000:GLU:HB2	1:N:1009:LEU:HD21	1.95	0.47
1:H:893:THR:O	1:H:895:ARG:HG3	2.14	0.47
1:G:770:LYS:HG2	1:G:771:GLU:N	2.29	0.47
1:L:970:THR:HG23	1:L:973:LYS:CB	2.43	0.47
1:K:970:THR:HG23	1:K:973:LYS:CB	2.44	0.47
1:A:1059:TYR:OH	1:B:1108:ILE:CD1	2.63	0.47
1:M:1095:VAL:O	1:M:1099:VAL:HG23	2.14	0.47
1:I:1000:GLU:HB2	1:I:1009:LEU:HD21	1.95	0.47
1:I:787:HIS:CD2	1:J:814:ASP:HB2	2.50	0.47
1:G:864:SER:O	1:G:893:THR:OG1	2.30	0.47
1:L:864:SER:O	1:L:893:THR:OG1	2.30	0.47
1:K:804:LEU:HB2	1:K:825:LEU:HB2	1.97	0.47
1:J:1037:LEU:C	1:J:1039:ARG:H	2.16	0.47
1:C:670:LEU:HD23	1:C:735:GLU:OE2	2.14	0.47
1:K:1025:TRP:HB2	1:K:1088:PHE:CZ	2.49	0.47
1:J:1016:SER:C	1:J:1018:PHE:H	2.17	0.47
1:B:977:HIS:CG	1:B:978:PRO:HD2	2.49	0.47
1:A:861:LEU:O	1:A:862:GLU:CB	2.61	0.47
1:I:725:HIS:HE1	1:J:816:GLN:NE2	2.12	0.47
1:K:682:TYR:O	2:K:1999:APJ:H23	2.15	0.47
1:E:828:ASP:HB2	2:E:1999:APJ:H25	1.96	0.47
1:A:758:SER:HB3	1:A:768:LEU:HD21	1.96	0.47
1:D:853:SER:HA	1:D:856:ARG:HG3	1.96	0.47
1:F:837:SER:HB3	1:F:838:GLY:HA2	1.96	0.47
1:M:924:LYS:HG3	1:M:925:TYR:CD2	2.49	0.47
1:F:671:LYS:O	1:F:671:LYS:HD2	2.15	0.47
1:L:1032:THR:CG2	1:M:1027:VAL:HB	2.44	0.47
2:N:1999:APJ:N8	2:N:1999:APJ:H17	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:906:MET:HE3	1:G:906:MET:HB2	1.76	0.47
1:N:673:LEU:O	1:N:673:LEU:HD23	2.14	0.47
1:F:1034:MET:CE	1:F:1037:LEU:HD23	2.44	0.47
1:K:1034:MET:CE	1:K:1034:MET:HA	2.44	0.47
1:N:685:SER:HB3	1:N:708:PHE:CZ	2.48	0.47
1:H:1095:VAL:O	1:H:1099:VAL:HG23	2.14	0.47
1:M:794:ILE:HG22	1:M:795:HIS:O	2.14	0.47
1:J:804:LEU:HB2	1:J:825:LEU:HB2	1.96	0.47
1:K:794:ILE:HG22	1:K:795:HIS:O	2.14	0.47
1:N:893:THR:O	1:N:895:ARG:HG3	2.15	0.47
1:B:893:THR:O	1:B:895:ARG:HG3	2.14	0.47
1:M:893:THR:O	1:M:895:ARG:HG3	2.15	0.47
1:B:682:TYR:O	2:B:1999:APJ:H23	2.15	0.47
1:H:682:TYR:O	2:H:1999:APJ:H23	2.13	0.47
1:L:781:ILE:HG22	1:L:906:MET:CE	2.43	0.47
1:H:970:THR:HG23	1:H:973:LYS:CB	2.45	0.47
1:F:804:LEU:HB2	1:F:825:LEU:HB2	1.97	0.47
1:H:758:SER:HB3	1:H:768:LEU:HD21	1.95	0.47
1:A:814:ASP:OD2	1:B:787:HIS:HD2	1.98	0.47
1:A:1025:TRP:HB2	1:A:1088:PHE:CZ	2.50	0.47
1:N:946:ASP:HB3	1:N:949:LEU:HD12	1.96	0.47
1:G:1025:TRP:HB2	1:G:1088:PHE:CZ	2.50	0.47
1:K:737:THR:C	1:K:739:ARG:H	2.19	0.47
1:J:970:THR:HG23	1:J:973:LYS:CB	2.45	0.47
1:K:906:MET:HE3	1:K:906:MET:HB2	1.75	0.47
1:F:1034:MET:HE3	1:F:1034:MET:HA	1.96	0.47
1:J:1025:TRP:HB2	1:J:1088:PHE:CZ	2.50	0.47
1:C:737:THR:C	1:C:739:ARG:H	2.17	0.47
1:L:1095:VAL:O	1:L:1099:VAL:HG23	2.15	0.47
1:E:946:ASP:HB3	1:E:949:LEU:HD12	1.97	0.47
1:B:725:HIS:CG	1:B:726:PRO:HD2	2.50	0.47
1:M:864:SER:O	1:M:893:THR:OG1	2.28	0.47
1:E:770:LYS:HG2	1:E:771:GLU:N	2.30	0.47
1:G:737:THR:C	1:G:739:ARG:H	2.18	0.47
1:L:737:THR:C	1:L:739:ARG:H	2.19	0.47
1:A:814:ASP:HB2	1:B:787:HIS:CD2	2.50	0.47
1:I:1016:SER:C	1:I:1018:PHE:H	2.17	0.47
1:G:914:LEU:O	1:G:943:CYS:HB2	2.15	0.47
1:N:1008:LEU:HA	1:N:1008:LEU:HD23	1.78	0.47
1:D:725:HIS:CG	1:D:726:PRO:HD2	2.49	0.47
1:M:906:MET:HG3	1:M:910:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:893:THR:O	1:K:895:ARG:HG3	2.15	0.47
1:E:781:ILE:HG22	1:E:906:MET:CE	2.44	0.47
1:K:970:THR:HB	1:M:762:SER:HB2	1.96	0.47
1:N:770:LYS:HG2	1:N:771:GLU:N	2.30	0.47
1:C:1055:LEU:HD23	1:C:1055:LEU:O	2.15	0.47
1:C:685:SER:HB3	1:C:708:PHE:CZ	2.50	0.47
1:A:687:THR:HG23	1:A:704:MET:HG2	1.97	0.47
1:D:665:ASN:ND2	1:D:665:ASN:N	2.59	0.46
1:F:893:THR:O	1:F:895:ARG:HG3	2.15	0.46
1:E:893:THR:O	1:E:895:ARG:HG3	2.15	0.46
1:A:864:SER:O	1:A:893:THR:OG1	2.28	0.46
1:H:770:LYS:HG2	1:H:771:GLU:N	2.30	0.46
1:D:837:SER:CB	1:D:838:GLY:HA2	2.46	0.46
1:E:687:THR:HG23	1:E:704:MET:HG2	1.98	0.46
1:H:804:LEU:HB2	1:H:825:LEU:HB2	1.98	0.46
1:A:729:ILE:HD12	1:A:745:LEU:HB3	1.98	0.46
1:M:770:LYS:HG2	1:M:771:GLU:N	2.31	0.46
1:J:737:THR:C	1:J:739:ARG:H	2.18	0.46
1:C:853:SER:HA	1:C:856:ARG:HG3	1.96	0.46
1:E:685:SER:HB3	1:E:708:PHE:CZ	2.51	0.46
1:J:1044:HIS:ND1	1:J:1050:ASP:OD2	2.47	0.46
1:I:1095:VAL:O	1:I:1099:VAL:HG23	2.15	0.46
1:L:842:PHE:O	1:L:842:PHE:CG	2.69	0.46
1:A:725:HIS:HD2	1:A:727:ASN:H	1.61	0.46
1:N:794:ILE:O	1:N:832:CYS:HB2	2.15	0.46
1:M:794:ILE:N	1:M:794:ILE:HD12	2.29	0.46
1:K:748:CYS:N	2:K:1999:APJ:HN4	2.12	0.46
1:K:770:LYS:HG2	1:K:771:GLU:N	2.30	0.46
1:L:770:LYS:HG2	1:L:771:GLU:N	2.29	0.46
1:F:1037:LEU:C	1:F:1039:ARG:H	2.17	0.46
1:A:804:LEU:HB2	1:A:825:LEU:HB2	1.97	0.46
1:A:737:THR:C	1:A:739:ARG:H	2.18	0.46
1:B:837:SER:CB	1:B:838:GLY:HA2	2.45	0.46
1:K:1000:GLU:HB2	1:K:1009:LEU:HD21	1.96	0.46
1:C:687:THR:HG23	1:C:704:MET:HG2	1.98	0.46
1:B:842:PHE:CG	1:B:842:PHE:O	2.68	0.46
1:C:842:PHE:CG	1:C:842:PHE:O	2.68	0.46
1:D:748:CYS:N	2:D:1999:APJ:HN4	2.11	0.46
1:J:893:THR:O	1:J:895:ARG:HG3	2.16	0.46
1:K:864:SER:O	1:K:893:THR:OG1	2.29	0.46
1:E:1037:LEU:C	1:E:1039:ARG:H	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:837:SER:CB	1:I:838:GLY:HA2	2.46	0.46
1:C:1076:VAL:CG1	1:D:1108:ILE:HD11	2.45	0.46
1:A:837:SER:CB	1:A:838:GLY:HA2	2.45	0.46
1:I:1025:TRP:HB2	1:I:1088:PHE:CZ	2.50	0.46
1:B:687:THR:HG23	1:B:704:MET:HG2	1.98	0.46
1:K:842:PHE:O	1:K:842:PHE:CG	2.69	0.46
1:E:861:LEU:O	1:E:862:GLU:CB	2.61	0.46
1:C:729:ILE:HD12	1:C:745:LEU:HB3	1.98	0.46
1:E:964:ASP:HA	1:E:965:PRO:HD2	1.84	0.46
1:K:1095:VAL:O	1:K:1099:VAL:HG23	2.16	0.46
1:C:1108:ILE:HD11	1:D:1076:VAL:HG11	1.96	0.46
1:E:977:HIS:CG	1:E:978:PRO:HD2	2.49	0.46
1:C:761:VAL:CG1	1:F:840:SEP:O2P	2.55	0.46
1:B:1037:LEU:C	1:B:1039:ARG:H	2.18	0.46
1:M:906:MET:HB2	1:M:906:MET:HE3	1.78	0.46
1:D:804:LEU:HB2	1:D:825:LEU:HB2	1.97	0.46
1:F:864:SER:O	1:F:893:THR:OG1	2.29	0.46
1:J:748:CYS:N	2:J:1999:APJ:HN4	2.13	0.46
1:A:893:THR:O	1:A:895:ARG:HG3	2.16	0.46
1:L:804:LEU:HB2	1:L:825:LEU:HB2	1.98	0.46
1:K:837:SER:CB	1:K:838:GLY:HA2	2.45	0.46
1:J:837:SER:CB	1:J:838:GLY:HA2	2.46	0.46
1:B:947:ARG:HB2	1:N:1071:GLU:OE1	2.15	0.46
1:J:687:THR:HG23	1:J:704:MET:HG2	1.97	0.46
1:C:837:SER:HB3	1:C:838:GLY:HA2	1.96	0.46
1:E:671:LYS:O	1:E:671:LYS:HD2	2.16	0.46
1:A:842:PHE:O	1:A:842:PHE:CG	2.68	0.46
1:B:794:ILE:O	1:B:832:CYS:HB2	2.16	0.46
1:D:906:MET:HE3	1:D:906:MET:HB2	1.80	0.46
1:F:970:THR:HG23	1:F:973:LYS:CB	2.45	0.46
1:B:737:THR:C	1:B:739:ARG:H	2.19	0.46
1:E:823:ARG:NH2	1:F:724:ASP:OD2	2.49	0.46
1:F:1025:TRP:HB2	1:F:1088:PHE:CZ	2.50	0.46
1:N:1095:VAL:O	1:N:1099:VAL:HG23	2.16	0.46
1:M:1103:LEU:C	1:M:1105:ASP:H	2.19	0.46
1:D:737:THR:C	1:D:739:ARG:H	2.18	0.46
1:L:725:HIS:CG	1:L:726:PRO:HD2	2.51	0.46
1:C:893:THR:O	1:C:895:ARG:HG3	2.15	0.46
1:A:781:ILE:HG22	1:A:906:MET:CE	2.45	0.46
1:M:737:THR:C	1:M:739:ARG:H	2.19	0.46
1:E:737:THR:C	1:E:739:ARG:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:671:LYS:CA	1:M:673:LEU:H	2.28	0.46
1:M:977:HIS:CG	1:M:978:PRO:HD2	2.51	0.46
1:D:1025:TRP:HB2	1:D:1088:PHE:CZ	2.51	0.46
1:M:914:LEU:O	1:M:943:CYS:HB2	2.16	0.46
1:C:1063:MET:HE3	1:D:999:ILE:HD11	1.98	0.46
1:G:946:ASP:HB3	1:G:949:LEU:HD12	1.98	0.46
1:I:673:LEU:HD23	1:I:673:LEU:C	2.36	0.46
1:H:725:HIS:CG	1:H:726:PRO:HD2	2.51	0.46
1:K:1037:LEU:C	1:K:1039:ARG:H	2.19	0.46
1:L:837:SER:CB	1:L:838:GLY:HA2	2.45	0.46
1:L:687:THR:HG23	1:L:704:MET:HG2	1.98	0.46
1:B:672:ASN:ND2	1:B:672:ASN:H	2.13	0.46
1:G:842:PHE:O	1:G:842:PHE:CG	2.69	0.46
1:B:914:LEU:O	1:B:943:CYS:HB2	2.16	0.46
1:G:893:THR:O	1:G:895:ARG:HG3	2.16	0.46
1:I:737:THR:C	1:I:739:ARG:H	2.19	0.46
1:H:687:THR:HG23	1:H:704:MET:HG2	1.98	0.46
1:G:1095:VAL:O	1:G:1099:VAL:HG23	2.16	0.46
1:N:929:SER:O	1:N:933:ARG:HG3	2.17	0.46
1:C:725:HIS:CG	1:C:726:PRO:HD2	2.51	0.45
1:H:794:ILE:N	1:H:794:ILE:HD12	2.31	0.45
1:H:794:ILE:O	1:H:832:CYS:HB2	2.15	0.45
1:N:804:LEU:HB2	1:N:825:LEU:HB2	1.98	0.45
1:F:770:LYS:HG2	1:F:771:GLU:N	2.31	0.45
1:H:837:SER:CB	1:H:838:GLY:HA2	2.46	0.45
1:A:1095:VAL:O	1:A:1099:VAL:HG23	2.16	0.45
1:D:799:LYS:NZ	1:D:852:THR:HG23	2.31	0.45
1:D:898:THR:HG23	1:D:900:SER:OG	2.16	0.45
1:D:794:ILE:O	1:D:832:CYS:HB2	2.15	0.45
1:L:794:ILE:O	1:L:832:CYS:HB2	2.17	0.45
1:K:794:ILE:O	1:K:832:CYS:HB2	2.16	0.45
1:L:729:ILE:HD12	1:L:745:LEU:HB3	1.98	0.45
1:A:770:LYS:HG2	1:A:771:GLU:N	2.31	0.45
1:B:804:LEU:HB2	1:B:825:LEU:HB2	1.97	0.45
1:E:729:ILE:HD12	1:E:745:LEU:HB3	1.97	0.45
1:I:770:LYS:HG2	1:I:771:GLU:N	2.30	0.45
1:A:970:THR:HG23	1:A:973:LYS:CB	2.46	0.45
1:F:761:VAL:HG11	1:H:840:SEP:P	2.57	0.45
1:E:1025:TRP:HB2	1:E:1088:PHE:CZ	2.51	0.45
1:F:946:ASP:HB3	1:F:949:LEU:HD12	1.97	0.45
1:N:794:ILE:N	1:N:794:ILE:HD12	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:748:CYS:N	2:N:1999:APJ:HN4	2.11	0.45
1:I:725:HIS:CG	1:I:726:PRO:HD2	2.51	0.45
1:B:748:CYS:N	2:B:1999:APJ:HN4	2.12	0.45
1:H:737:THR:C	1:H:739:ARG:H	2.19	0.45
1:E:837:SER:CB	1:E:838:GLY:HA2	2.46	0.45
1:B:1082:ASP:HA	1:B:1085:THR:HB	1.98	0.45
1:M:719:LEU:HA	1:M:719:LEU:HD23	1.72	0.45
1:E:842:PHE:O	1:E:842:PHE:CG	2.69	0.45
1:M:1008:LEU:HA	1:M:1008:LEU:HD23	1.80	0.45
1:D:666:PHE:HD1	1:D:742:TYR:HH	1.60	0.45
1:M:729:ILE:HD12	1:M:745:LEU:HB3	1.98	0.45
1:I:906:MET:HB2	1:I:906:MET:HE3	1.75	0.45
1:F:1033:PHE:CE1	1:F:1058:LYS:HE2	2.52	0.45
1:D:1093:ILE:HG23	1:D:1094:GLY:N	2.31	0.45
1:H:1016:SER:C	1:H:1018:PHE:H	2.17	0.45
1:I:687:THR:HG23	1:I:704:MET:HG2	1.98	0.45
1:C:1043:TYR:OH	1:C:1057:ASN:ND2	2.45	0.45
1:I:828:ASP:HB2	2:I:1999:APJ:H25	1.98	0.45
1:F:748:CYS:N	2:F:1999:APJ:HN4	2.12	0.45
1:C:828:ASP:HB2	2:C:1999:APJ:H25	1.99	0.45
1:N:837:SER:CB	1:N:838:GLY:HA2	2.46	0.45
1:N:828:ASP:HB2	2:N:1999:APJ:H25	1.99	0.45
1:L:1037:LEU:C	1:L:1039:ARG:H	2.19	0.45
1:G:1034:MET:CE	1:G:1037:LEU:HD23	2.46	0.45
1:M:823:ARG:NH2	1:N:724:ASP:OD2	2.50	0.45
1:K:946:ASP:HB3	1:K:949:LEU:HD12	1.98	0.45
1:D:694:PHE:CG	1:D:695:GLN:N	2.84	0.45
1:F:1032:THR:HG23	1:G:1027:VAL:O	2.16	0.45
1:M:946:ASP:HB3	1:M:949:LEU:HD12	1.98	0.45
1:H:842:PHE:CG	1:H:842:PHE:O	2.69	0.45
1:F:842:PHE:O	1:F:842:PHE:CG	2.69	0.45
1:D:666:PHE:HZ	1:D:690:PHE:CZ	2.33	0.45
1:J:781:ILE:HG22	1:J:906:MET:CE	2.44	0.45
1:J:782:ALA:HA	1:J:906:MET:HE1	1.97	0.45
1:D:1037:LEU:C	1:D:1039:ARG:H	2.19	0.45
1:I:729:ILE:HD12	1:I:745:LEU:HB3	1.99	0.45
1:M:748:CYS:N	2:M:1999:APJ:HN4	2.13	0.45
1:N:970:THR:HG23	1:N:973:LYS:CB	2.44	0.45
1:K:1034:MET:HE3	1:K:1034:MET:HA	1.98	0.45
1:H:1037:LEU:C	1:H:1039:ARG:H	2.20	0.45
1:A:785:VAL:CG2	1:A:906:MET:HE1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:805:VAL:HA	1:B:823:ARG:O	2.17	0.45
1:G:837:SER:CB	1:G:838:GLY:HA2	2.46	0.45
1:F:837:SER:CB	1:F:838:GLY:HA2	2.47	0.45
1:C:837:SER:CB	1:C:838:GLY:HA2	2.47	0.45
1:B:857:ALA:O	1:B:860:LEU:HB2	2.16	0.45
1:B:1095:VAL:O	1:B:1099:VAL:HG23	2.17	0.45
1:M:842:PHE:CG	1:M:842:PHE:O	2.69	0.45
1:N:842:PHE:CG	1:N:842:PHE:O	2.70	0.45
1:K:848:ASN:CB	1:K:849:PRO:HA	2.30	0.45
1:B:794:ILE:N	1:B:794:ILE:HD12	2.32	0.45
1:J:729:ILE:HD12	1:J:745:LEU:HB3	1.98	0.45
1:D:1055:LEU:HD23	1:D:1055:LEU:O	2.15	0.45
1:M:992:LYS:HE3	1:N:1059:TYR:OH	2.17	0.45
1:C:1095:VAL:O	1:C:1099:VAL:HG23	2.17	0.45
1:E:794:ILE:N	1:E:794:ILE:HD12	2.31	0.45
1:I:794:ILE:O	1:I:832:CYS:HB2	2.17	0.45
1:F:673:LEU:HD23	1:F:674:VAL:N	2.31	0.45
1:J:725:HIS:CG	1:J:726:PRO:HD2	2.52	0.45
1:G:804:LEU:HB2	1:G:825:LEU:HB2	1.97	0.45
1:D:893:THR:O	1:D:895:ARG:HG3	2.17	0.45
1:B:946:ASP:HB3	1:B:949:LEU:HD12	1.99	0.45
1:K:666:PHE:HE1	1:K:703:ARG:HD3	1.82	0.45
1:I:799:LYS:NZ	1:I:852:THR:HG23	2.32	0.45
1:G:798:LEU:HA	1:G:798:LEU:HD23	1.83	0.45
1:J:842:PHE:CG	1:J:842:PHE:O	2.69	0.45
1:B:798:LEU:HA	1:B:798:LEU:HD23	1.80	0.45
1:M:725:HIS:CG	1:M:726:PRO:HD2	2.52	0.45
1:D:729:ILE:HD12	1:D:745:LEU:HB3	1.98	0.45
1:G:729:ILE:HD12	1:G:745:LEU:HB3	1.99	0.45
1:M:1025:TRP:HB2	1:M:1088:PHE:CZ	2.51	0.45
1:J:1095:VAL:O	1:J:1099:VAL:HG23	2.17	0.45
1:G:748:CYS:N	2:G:1999:APJ:HN4	2.14	0.44
1:B:785:VAL:HG21	1:B:906:MET:HE1	1.99	0.44
1:G:758:SER:O	1:G:759:LYS:HB3	2.17	0.44
1:N:925:TYR:N	1:N:925:TYR:CD2	2.85	0.44
1:G:992:LYS:HE3	1:H:1059:TYR:OH	2.17	0.44
1:A:797:ASP:O	1:A:802:ASN:ND2	2.49	0.44
1:H:1082:ASP:HA	1:H:1085:THR:HB	2.00	0.44
1:C:1030:ASP:N	1:C:1030:ASP:OD1	2.50	0.44
1:D:864:SER:O	1:D:893:THR:OG1	2.28	0.44
1:F:906:MET:HB2	1:F:906:MET:HE3	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:906:MET:HG3	1:F:910:PHE:CE1	2.53	0.44
1:I:970:THR:HG23	1:I:973:LYS:CB	2.48	0.44
1:L:758:SER:O	1:L:759:LYS:HB3	2.18	0.44
1:H:740:PHE:HB3	1:H:741:LEU:H	1.63	0.44
1:F:925:TYR:CD2	1:F:925:TYR:N	2.84	0.44
1:J:978:PRO:HA	1:J:981:TRP:CD1	2.53	0.44
1:B:685:SER:HB3	1:B:708:PHE:CZ	2.51	0.44
1:K:687:THR:HG23	1:K:704:MET:HG2	1.99	0.44
1:D:1095:VAL:O	1:D:1099:VAL:HG23	2.17	0.44
1:K:841:SEP:P	1:M:678:LYS:NZ	2.91	0.44
1:G:725:HIS:CG	1:G:726:PRO:HD2	2.53	0.44
1:H:729:ILE:HD12	1:H:745:LEU:HB3	1.99	0.44
1:L:906:MET:HE3	1:L:906:MET:HB2	1.78	0.44
1:N:906:MET:HG3	1:N:910:PHE:CE1	2.52	0.44
1:B:670:LEU:O	1:B:735:GLU:OE2	2.35	0.44
1:L:1025:TRP:HB2	1:L:1088:PHE:CZ	2.52	0.44
1:E:1103:LEU:C	1:E:1105:ASP:H	2.21	0.44
1:D:828:ASP:HB2	2:D:1999:APJ:H25	1.99	0.44
1:F:781:ILE:HG22	1:F:906:MET:CE	2.47	0.44
1:B:1093:ILE:HG23	1:B:1094:GLY:N	2.33	0.44
1:A:925:TYR:CD2	1:A:925:TYR:N	2.85	0.44
1:M:837:SER:CB	1:M:838:GLY:HA2	2.47	0.44
1:M:1048:LEU:HD23	1:M:1048:LEU:O	2.18	0.44
1:M:964:ASP:HA	1:M:965:PRO:HD2	1.85	0.44
1:H:946:ASP:HB3	1:H:949:LEU:HD12	1.99	0.44
1:F:758:SER:O	1:F:759:LYS:HB3	2.17	0.44
1:M:978:PRO:HA	1:M:981:TRP:CD1	2.53	0.44
1:B:1033:PHE:CE1	1:B:1058:LYS:HE2	2.53	0.44
1:F:670:LEU:HD23	1:F:735:GLU:OE2	2.18	0.44
1:D:687:THR:HG23	1:D:704:MET:HG2	2.00	0.44
1:E:799:LYS:NZ	1:E:852:THR:HG23	2.33	0.44
1:C:909:VAL:O	1:C:913:ILE:HG12	2.18	0.44
1:H:1034:MET:CE	1:H:1037:LEU:HD23	2.48	0.44
1:K:672:ASN:ND2	1:K:672:ASN:N	2.65	0.44
1:A:758:SER:O	1:A:759:LYS:HB3	2.17	0.44
1:C:758:SER:O	1:C:759:LYS:HB3	2.18	0.44
1:K:1106:ASP:O	1:K:1110:ARG:HG3	2.18	0.44
1:A:1103:LEU:C	1:A:1105:ASP:H	2.20	0.44
1:M:857:ALA:O	1:M:860:LEU:HB2	2.17	0.44
1:G:906:MET:HG3	1:G:910:PHE:CE1	2.53	0.44
1:M:828:ASP:HB2	2:M:1999:APJ:H25	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:906:MET:HG3	1:E:910:PHE:CE1	2.53	0.44
1:I:672:ASN:ND2	1:I:672:ASN:N	2.64	0.44
1:C:925:TYR:CD2	1:C:925:TYR:N	2.83	0.44
1:K:978:PRO:HA	1:K:981:TRP:CD1	2.53	0.44
1:F:898:THR:OG1	1:F:899:ARG:N	2.51	0.44
1:N:687:THR:HG23	1:N:704:MET:HG2	2.00	0.44
1:K:1103:LEU:C	1:K:1105:ASP:H	2.21	0.44
1:F:914:LEU:O	1:F:943:CYS:HB2	2.18	0.44
1:A:1106:ASP:O	1:A:1110:ARG:HG3	2.18	0.44
1:N:1103:LEU:C	1:N:1105:ASP:H	2.21	0.44
1:N:1030:ASP:OD1	1:N:1030:ASP:N	2.51	0.44
1:I:1030:ASP:N	1:I:1030:ASP:OD1	2.51	0.44
1:H:1020:ILE:HG22	1:H:1021:PRO:C	2.37	0.44
1:A:805:VAL:HA	1:A:823:ARG:O	2.18	0.44
1:N:737:THR:C	1:N:739:ARG:H	2.21	0.44
1:K:672:ASN:HD22	1:K:672:ASN:N	2.16	0.44
1:A:1082:ASP:HA	1:A:1085:THR:HB	2.00	0.44
1:I:1033:PHE:CE1	1:I:1058:LYS:HE2	2.53	0.44
1:L:799:LYS:NZ	1:L:852:THR:HG23	2.33	0.44
1:C:898:THR:OG1	1:C:899:ARG:N	2.51	0.44
1:L:946:ASP:HB3	1:L:949:LEU:HD12	1.99	0.44
1:A:999:ILE:N	1:A:999:ILE:HD12	2.33	0.44
1:D:767:LYS:HE2	1:D:767:LYS:HB2	1.82	0.44
1:L:1008:LEU:HA	1:L:1008:LEU:HD23	1.79	0.44
1:K:1030:ASP:OD1	1:K:1030:ASP:N	2.51	0.44
1:K:788:LEU:HA	1:K:788:LEU:HD13	1.87	0.44
1:L:828:ASP:HB2	2:L:1999:APJ:H25	2.00	0.44
1:E:1020:ILE:HG22	1:E:1021:PRO:C	2.39	0.44
1:E:748:CYS:N	2:E:1999:APJ:HN4	2.14	0.44
1:D:758:SER:O	1:D:759:LYS:HB3	2.17	0.44
1:F:712:ALA:O	1:F:716:ILE:HG12	2.18	0.44
1:G:1033:PHE:CE1	1:G:1058:LYS:HE2	2.53	0.44
1:M:937:SER:O	1:M:938:LEU:HD23	2.17	0.44
1:I:842:PHE:O	1:I:842:PHE:CG	2.70	0.44
1:L:1020:ILE:HG22	1:L:1021:PRO:C	2.37	0.43
1:N:864:SER:O	1:N:893:THR:OG1	2.31	0.43
1:C:1033:PHE:CE1	1:C:1058:LYS:HE2	2.53	0.43
1:F:799:LYS:NZ	1:F:852:THR:HG23	2.33	0.43
1:E:1033:PHE:CE1	1:E:1058:LYS:HE2	2.53	0.43
1:N:672:ASN:N	1:N:672:ASN:ND2	2.66	0.43
1:C:671:LYS:HD2	1:C:671:LYS:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:842:PHE:O	1:D:842:PHE:CG	2.70	0.43
1:G:1020:ILE:HG22	1:G:1021:PRO:C	2.39	0.43
1:H:906:MET:HG3	1:H:910:PHE:CE1	2.53	0.43
1:J:828:ASP:HB2	2:J:1999:APJ:H25	2.00	0.43
1:C:821:ASN:O	1:C:822:LEU:HB3	2.18	0.43
1:G:740:PHE:HB3	1:G:741:LEU:H	1.64	0.43
1:I:758:SER:O	1:I:759:LYS:HB3	2.18	0.43
1:B:758:SER:O	1:B:759:LYS:HB3	2.17	0.43
1:K:925:TYR:N	1:K:925:TYR:CD2	2.86	0.43
1:B:1103:LEU:C	1:B:1105:ASP:H	2.22	0.43
1:C:1082:ASP:HA	1:C:1085:THR:HB	2.00	0.43
1:M:898:THR:HG23	1:M:900:SER:OG	2.18	0.43
1:N:1025:TRP:HB2	1:N:1088:PHE:CZ	2.53	0.43
1:K:1033:PHE:CE1	1:K:1058:LYS:HE2	2.54	0.43
1:J:1011:LYS:HA	1:J:1011:LYS:HE2	2.00	0.43
1:A:719:LEU:HD23	1:A:719:LEU:HA	1.72	0.43
1:A:725:HIS:CD2	1:A:727:ASN:HB2	2.53	0.43
1:C:725:HIS:CD2	1:C:727:ASN:HB2	2.54	0.43
1:K:828:ASP:HB2	2:K:1999:APJ:H25	2.00	0.43
1:L:1020:ILE:HB	1:L:1021:PRO:HA	2.00	0.43
1:K:725:HIS:CG	1:K:726:PRO:HD2	2.53	0.43
1:F:737:THR:C	1:F:739:ARG:H	2.21	0.43
1:N:1093:ILE:HG23	1:N:1094:GLY:N	2.34	0.43
1:B:845:ASN:N	1:B:845:ASN:ND2	2.66	0.43
1:N:978:PRO:HA	1:N:981:TRP:CD1	2.53	0.43
1:E:925:TYR:N	1:E:925:TYR:CD2	2.86	0.43
1:J:946:ASP:HB3	1:J:949:LEU:HD12	1.99	0.43
1:F:1095:VAL:O	1:F:1099:VAL:HG23	2.18	0.43
1:F:1106:ASP:O	1:F:1110:ARG:HG3	2.19	0.43
1:L:1030:ASP:OD1	1:L:1030:ASP:N	2.52	0.43
1:J:906:MET:HB2	1:J:906:MET:HE3	1.81	0.43
1:E:1034:MET:CE	1:E:1037:LEU:HD23	2.48	0.43
1:N:758:SER:CB	1:N:768:LEU:HD21	2.49	0.43
1:I:1082:ASP:HA	1:I:1085:THR:HB	2.00	0.43
1:D:1103:LEU:C	1:D:1105:ASP:H	2.22	0.43
1:D:946:ASP:HB3	1:D:949:LEU:HD12	2.01	0.43
1:E:857:ALA:O	1:E:860:LEU:HB2	2.19	0.43
1:C:1048:LEU:HD23	1:C:1048:LEU:O	2.19	0.43
1:J:798:LEU:HD23	1:J:798:LEU:HA	1.81	0.43
1:J:719:LEU:HD23	1:J:719:LEU:HA	1.72	0.43
1:N:729:ILE:HD12	1:N:745:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:758:SER:O	1:K:759:LYS:HB3	2.18	0.43
1:H:925:TYR:CD2	1:H:925:TYR:N	2.87	0.43
1:I:845:ASN:ND2	1:I:845:ASN:N	2.67	0.43
1:N:672:ASN:H	1:N:672:ASN:ND2	2.17	0.43
1:A:787:HIS:O	1:A:790:SER:HB2	2.19	0.43
1:C:1106:ASP:O	1:C:1110:ARG:HG3	2.18	0.43
1:N:999:ILE:N	1:N:999:ILE:HD12	2.34	0.43
1:C:1020:ILE:HG22	1:C:1021:PRO:C	2.38	0.43
1:F:964:ASP:HA	1:F:965:PRO:HD2	1.83	0.43
1:G:794:ILE:O	1:G:832:CYS:HB2	2.18	0.43
1:H:828:ASP:HB2	2:H:1999:APJ:H25	1.99	0.43
1:K:906:MET:HG3	1:K:910:PHE:CE1	2.53	0.43
1:N:906:MET:HB2	1:N:906:MET:HE3	1.78	0.43
1:C:1034:MET:CE	1:C:1037:LEU:HD23	2.48	0.43
1:K:672:ASN:H	1:K:672:ASN:HD22	1.66	0.43
1:A:845:ASN:ND2	1:A:845:ASN:N	2.66	0.43
1:M:1093:ILE:HG23	1:M:1094:GLY:N	2.34	0.43
1:E:1082:ASP:HA	1:E:1085:THR:HB	1.99	0.43
1:F:1082:ASP:HA	1:F:1085:THR:HB	2.01	0.43
1:J:1106:ASP:O	1:J:1110:ARG:HG3	2.18	0.43
1:E:937:SER:O	1:E:938:LEU:HD23	2.18	0.43
1:N:799:LYS:NZ	1:N:852:THR:HG23	2.34	0.43
1:E:843:ARG:NH2	1:G:678:LYS:HB2	2.34	0.43
1:K:719:LEU:HA	1:K:719:LEU:HD23	1.72	0.43
1:J:1020:ILE:HG22	1:J:1021:PRO:C	2.38	0.43
1:N:1020:ILE:HG22	1:N:1021:PRO:C	2.39	0.43
1:A:748:CYS:N	2:A:1999:APJ:HN4	2.13	0.43
1:L:906:MET:HG3	1:L:910:PHE:CE1	2.53	0.43
1:E:845:ASN:N	1:E:845:ASN:ND2	2.67	0.43
1:J:845:ASN:N	1:J:845:ASN:ND2	2.67	0.43
1:F:898:THR:HG23	1:F:900:SER:OG	2.18	0.43
1:G:898:THR:HG23	1:G:900:SER:OG	2.19	0.43
1:C:799:LYS:HB2	1:C:800:PRO:HD2	2.01	0.43
1:H:797:ASP:O	1:H:802:ASN:ND2	2.51	0.43
1:A:1030:ASP:N	1:A:1030:ASP:OD1	2.52	0.43
1:I:1008:LEU:HD23	1:I:1008:LEU:HA	1.81	0.43
1:J:673:LEU:HD23	1:J:673:LEU:C	2.39	0.43
1:F:1008:LEU:HD23	1:F:1008:LEU:HA	1.79	0.43
1:F:1011:LYS:HE2	1:F:1011:LYS:HA	2.01	0.43
1:N:848:ASN:CB	1:N:849:PRO:HA	2.30	0.43
1:K:729:ILE:HD12	1:K:745:LEU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:821:ASN:O	1:D:822:LEU:HB3	2.18	0.43
1:E:758:SER:O	1:E:759:LYS:HB3	2.18	0.43
1:G:1093:ILE:HG23	1:G:1094:GLY:N	2.33	0.43
1:F:680:LEU:HB2	1:F:689:VAL:CG1	2.48	0.43
1:L:805:VAL:HA	1:L:823:ARG:O	2.19	0.43
1:F:845:ASN:N	1:F:845:ASN:ND2	2.67	0.43
1:L:978:PRO:HA	1:L:981:TRP:CD1	2.54	0.43
1:M:925:TYR:CD2	1:M:925:TYR:N	2.87	0.43
1:A:799:LYS:HB2	1:A:800:PRO:HD2	2.01	0.43
1:L:1103:LEU:C	1:L:1105:ASP:H	2.22	0.43
1:D:797:ASP:O	1:D:802:ASN:ND2	2.52	0.43
1:B:767:LYS:HE2	1:B:767:LYS:HB2	1.81	0.43
1:I:1011:LYS:HE2	1:I:1011:LYS:HA	2.00	0.43
1:A:848:ASN:CB	1:A:849:PRO:HA	2.30	0.43
1:A:1033:PHE:CE1	1:A:1058:LYS:HE2	2.54	0.43
1:B:740:PHE:HB3	1:B:741:LEU:H	1.63	0.43
1:M:845:ASN:N	1:M:845:ASN:ND2	2.66	0.43
1:L:925:TYR:CD2	1:L:925:TYR:N	2.87	0.43
1:J:925:TYR:CD2	1:J:925:TYR:N	2.87	0.43
1:G:925:TYR:N	1:G:925:TYR:CD2	2.87	0.43
1:N:1055:LEU:O	1:N:1055:LEU:HD23	2.19	0.43
1:A:1048:LEU:O	1:A:1049:MET:C	2.57	0.43
1:I:1103:LEU:C	1:I:1105:ASP:H	2.22	0.43
1:N:787:HIS:O	1:N:790:SER:HB2	2.19	0.43
1:K:857:ALA:O	1:K:860:LEU:HB2	2.19	0.43
1:G:1103:LEU:C	1:G:1105:ASP:H	2.22	0.43
1:A:798:LEU:HA	1:A:798:LEU:HD23	1.79	0.43
1:G:719:LEU:HA	1:G:719:LEU:HD23	1.72	0.43
1:E:798:LEU:HD23	1:E:798:LEU:HA	1.79	0.43
1:N:725:HIS:CG	1:N:726:PRO:HD2	2.54	0.43
1:H:821:ASN:O	1:H:822:LEU:HB3	2.19	0.43
1:D:663:ILE:O	1:D:664:PRO:C	2.58	0.43
1:J:758:SER:O	1:J:759:LYS:HB3	2.18	0.43
1:G:758:SER:CB	1:G:768:LEU:HD21	2.49	0.43
1:H:845:ASN:ND2	1:H:845:ASN:N	2.67	0.43
1:D:925:TYR:CD2	1:D:925:TYR:N	2.87	0.43
1:B:925:TYR:N	1:B:925:TYR:CD2	2.87	0.43
1:K:845:ASN:ND2	1:K:845:ASN:N	2.67	0.43
1:L:845:ASN:ND2	1:L:845:ASN:N	2.67	0.43
1:M:712:ALA:O	1:M:716:ILE:HG12	2.19	0.43
1:G:1082:ASP:HA	1:G:1085:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:798:LEU:HA	1:H:798:LEU:HD23	1.80	0.43
1:D:719:LEU:HA	1:D:719:LEU:HD23	1.70	0.43
1:J:906:MET:HG3	1:J:910:PHE:CE1	2.53	0.42
1:E:725:HIS:CG	1:E:726:PRO:HD2	2.54	0.42
1:B:1020:ILE:HG22	1:B:1021:PRO:C	2.39	0.42
1:K:821:ASN:O	1:K:822:LEU:HB3	2.19	0.42
1:B:906:MET:HE3	1:B:906:MET:HB2	1.76	0.42
1:K:758:SER:CB	1:K:768:LEU:HD21	2.49	0.42
1:H:978:PRO:HA	1:H:981:TRP:CD1	2.54	0.42
1:E:978:PRO:HA	1:E:981:TRP:CD1	2.54	0.42
1:K:898:THR:HG23	1:K:900:SER:OG	2.19	0.42
1:M:687:THR:HG23	1:M:704:MET:HG2	2.01	0.42
1:H:799:LYS:NZ	1:H:852:THR:HG23	2.34	0.42
1:D:1033:PHE:CE1	1:D:1058:LYS:HE2	2.54	0.42
1:G:1030:ASP:N	1:G:1030:ASP:OD1	2.52	0.42
1:C:672:ASN:ND2	1:C:672:ASN:H	2.17	0.42
1:E:725:HIS:CD2	1:E:727:ASN:HB2	2.55	0.42
1:F:758:SER:CB	1:F:768:LEU:HD21	2.49	0.42
1:J:672:ASN:ND2	1:J:672:ASN:N	2.67	0.42
1:F:1093:ILE:HG23	1:F:1094:GLY:N	2.34	0.42
1:A:799:LYS:NZ	1:A:852:THR:HG23	2.34	0.42
1:L:898:THR:HG23	1:L:900:SER:OG	2.19	0.42
1:C:1025:TRP:HB2	1:C:1088:PHE:CZ	2.53	0.42
1:F:1103:LEU:C	1:F:1105:ASP:H	2.22	0.42
1:N:1106:ASP:O	1:N:1110:ARG:HG3	2.18	0.42
1:C:797:ASP:O	1:C:802:ASN:ND2	2.52	0.42
1:E:694:PHE:CG	1:E:695:GLN:N	2.86	0.42
1:I:798:LEU:HD23	1:I:798:LEU:HA	1.80	0.42
1:E:1030:ASP:OD1	1:E:1030:ASP:N	2.52	0.42
1:A:1020:ILE:HB	1:A:1021:PRO:HA	2.01	0.42
1:I:906:MET:HG3	1:I:910:PHE:CE1	2.53	0.42
1:G:821:ASN:O	1:G:822:LEU:HB3	2.19	0.42
1:H:758:SER:O	1:H:759:LYS:HB3	2.18	0.42
1:I:925:TYR:N	1:I:925:TYR:CD2	2.87	0.42
1:I:937:SER:O	1:I:938:LEU:HD23	2.20	0.42
1:N:1033:PHE:CE1	1:N:1058:LYS:HE2	2.54	0.42
1:L:1003:ASP:HA	1:L:1004:PRO:HA	1.91	0.42
1:J:799:LYS:NZ	1:J:852:THR:HG23	2.34	0.42
1:K:799:LYS:NZ	1:K:852:THR:HG23	2.33	0.42
1:M:1106:ASP:O	1:M:1110:ARG:HG3	2.19	0.42
1:G:1024:ASP:HA	1:G:1045:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:767:LYS:HB2	1:C:767:LYS:HE2	1.84	0.42
1:J:1030:ASP:N	1:J:1030:ASP:OD1	2.52	0.42
1:B:999:ILE:HD12	1:B:999:ILE:N	2.35	0.42
1:G:828:ASP:HB2	2:G:1999:APJ:H25	2.00	0.42
1:E:758:SER:CB	1:E:768:LEU:HD21	2.49	0.42
1:C:758:SER:CB	1:C:768:LEU:HD21	2.49	0.42
1:G:845:ASN:N	1:G:845:ASN:ND2	2.67	0.42
1:M:1103:LEU:O	1:M:1105:ASP:N	2.52	0.42
1:A:860:LEU:HA	1:A:860:LEU:HD23	1.83	0.42
1:M:1030:ASP:N	1:M:1030:ASP:OD1	2.52	0.42
1:C:798:LEU:HA	1:C:798:LEU:HD23	1.81	0.42
1:K:1020:ILE:HB	1:K:1021:PRO:HA	2.02	0.42
1:C:748:CYS:N	2:C:1999:APJ:HN4	2.12	0.42
1:D:964:ASP:HA	1:D:965:PRO:HD2	1.82	0.42
1:D:758:SER:CB	1:D:768:LEU:HD21	2.49	0.42
1:L:758:SER:CB	1:L:768:LEU:HD21	2.50	0.42
1:J:758:SER:CB	1:J:768:LEU:HD21	2.50	0.42
1:F:680:LEU:HD23	1:F:680:LEU:HA	1.87	0.42
1:N:758:SER:O	1:N:759:LYS:HB3	2.18	0.42
1:I:805:VAL:HA	1:I:823:ARG:O	2.19	0.42
1:N:845:ASN:C	1:N:846:LEU:HD22	2.40	0.42
1:J:1041:ARG:HH22	1:J:1053:ARG:HG2	1.84	0.42
1:C:898:THR:HG23	1:C:900:SER:OG	2.19	0.42
1:N:797:ASP:O	1:N:802:ASN:ND2	2.52	0.42
1:F:705:LEU:N	1:F:705:LEU:HD12	2.34	0.42
1:J:788:LEU:HA	1:J:788:LEU:HD13	1.88	0.42
1:F:1020:ILE:HG22	1:F:1021:PRO:C	2.39	0.42
1:L:821:ASN:O	1:L:822:LEU:HB3	2.19	0.42
1:M:773:ASN:O	1:M:776:SER:HB3	2.19	0.42
1:L:857:ALA:O	1:L:860:LEU:HB2	2.19	0.42
1:H:1003:ASP:HA	1:H:1004:PRO:HA	1.91	0.42
1:F:798:LEU:HA	1:F:798:LEU:HD23	1.80	0.42
1:H:857:ALA:O	1:H:860:LEU:HB2	2.19	0.42
1:E:970:THR:HG21	1:G:762:SER:CB	2.49	0.42
1:B:762:SER:O	1:B:765:ASN:HB3	2.20	0.42
1:N:725:HIS:CD2	1:N:727:ASN:HB2	2.55	0.42
1:D:1020:ILE:HB	1:D:1021:PRO:HA	2.02	0.42
1:J:740:PHE:HB3	1:J:741:LEU:H	1.64	0.42
1:G:978:PRO:HA	1:G:981:TRP:CD1	2.55	0.42
1:I:946:ASP:HB3	1:I:949:LEU:HD12	2.00	0.42
1:E:919:HIS:CE1	1:E:921:PHE:HD2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:799:LYS:NZ	1:G:852:THR:HG23	2.35	0.42
1:N:898:THR:HG23	1:N:900:SER:OG	2.20	0.42
1:H:1103:LEU:C	1:H:1105:ASP:H	2.22	0.42
1:G:1106:ASP:O	1:G:1110:ARG:HG3	2.20	0.42
1:F:687:THR:HG23	1:F:704:MET:HG2	2.01	0.42
1:L:694:PHE:CG	1:L:695:GLN:N	2.87	0.42
1:G:1076:VAL:HG11	1:H:1108:ILE:HD11	2.02	0.42
1:J:805:VAL:HA	1:J:823:ARG:O	2.19	0.42
1:H:1020:ILE:HB	1:H:1021:PRO:HA	2.02	0.42
1:E:1020:ILE:HB	1:E:1021:PRO:HA	2.01	0.42
1:F:821:ASN:O	1:F:822:LEU:HB3	2.19	0.42
1:B:758:SER:CB	1:B:768:LEU:HD21	2.49	0.42
1:M:1055:LEU:O	1:M:1055:LEU:HD23	2.20	0.42
1:C:805:VAL:HA	1:C:823:ARG:O	2.20	0.42
1:K:978:PRO:HA	1:K:981:TRP:CD2	2.55	0.42
1:D:898:THR:OG1	1:D:899:ARG:N	2.52	0.42
1:D:860:LEU:HD23	1:D:860:LEU:HA	1.84	0.42
1:H:898:THR:HG23	1:H:900:SER:OG	2.20	0.42
1:A:929:SER:O	1:A:933:ARG:HG3	2.20	0.42
1:I:898:THR:HG23	1:I:900:SER:OG	2.20	0.42
1:M:948:SER:HB3	1:M:1085:THR:HG23	2.02	0.42
1:K:1008:LEU:HA	1:K:1008:LEU:HD23	1.79	0.42
1:F:1030:ASP:OD1	1:F:1030:ASP:N	2.53	0.42
1:C:1020:ILE:HB	1:C:1021:PRO:HA	2.02	0.42
1:F:729:ILE:HD12	1:F:745:LEU:HB3	2.02	0.42
1:D:1020:ILE:HG22	1:D:1021:PRO:C	2.40	0.42
1:J:1033:PHE:CE1	1:J:1058:LYS:HE2	2.55	0.42
1:N:821:ASN:O	1:N:822:LEU:HB3	2.19	0.42
1:N:737:THR:HG23	1:N:740:PHE:N	2.35	0.42
1:M:758:SER:O	1:M:759:LYS:HB3	2.19	0.42
1:I:1093:ILE:HG23	1:I:1094:GLY:N	2.35	0.42
1:K:805:VAL:HA	1:K:823:ARG:O	2.20	0.42
1:F:845:ASN:C	1:F:846:LEU:HD22	2.41	0.42
1:K:1082:ASP:HA	1:K:1085:THR:HB	2.01	0.42
1:I:1106:ASP:O	1:I:1110:ARG:HG3	2.20	0.42
1:J:694:PHE:CG	1:J:695:GLN:N	2.87	0.42
1:J:712:ALA:O	1:J:716:ILE:HG12	2.20	0.42
1:H:1030:ASP:OD1	1:H:1030:ASP:N	2.51	0.42
1:G:792:LYS:HE2	1:G:792:LYS:HB2	1.88	0.42
1:C:999:ILE:HD12	1:C:999:ILE:N	2.35	0.42
1:G:1011:LYS:HE2	1:G:1011:LYS:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:794:ILE:O	1:J:832:CYS:HB2	2.20	0.42
1:N:1037:LEU:C	1:N:1039:ARG:H	2.24	0.42
1:A:811:PHE:HB3	1:A:823:ARG:HG3	2.01	0.42
1:E:821:ASN:O	1:E:822:LEU:HB3	2.20	0.42
1:M:811:PHE:HB3	1:M:823:ARG:HG3	2.02	0.42
1:H:811:PHE:HB3	1:H:823:ARG:HG3	2.02	0.42
1:C:845:ASN:ND2	1:C:845:ASN:N	2.67	0.42
1:D:845:ASN:N	1:D:845:ASN:ND2	2.68	0.42
1:D:857:ALA:O	1:D:860:LEU:HB2	2.20	0.42
1:E:712:ALA:O	1:E:716:ILE:HG12	2.20	0.42
1:C:929:SER:O	1:C:933:ARG:HG3	2.20	0.42
1:A:898:THR:OG1	1:A:899:ARG:N	2.53	0.42
1:L:1106:ASP:O	1:L:1110:ARG:HG3	2.20	0.42
1:E:692:GLY:O	1:E:699:VAL:HG22	2.20	0.42
1:N:860:LEU:HD23	1:N:860:LEU:HA	1.83	0.42
1:F:787:HIS:O	1:F:790:SER:HB2	2.20	0.42
1:J:1082:ASP:HA	1:J:1085:THR:HB	2.01	0.42
1:B:1030:ASP:OD1	1:B:1030:ASP:N	2.53	0.42
1:F:999:ILE:HD12	1:F:999:ILE:N	2.35	0.42
1:H:788:LEU:HD13	1:H:788:LEU:HA	1.84	0.42
1:C:761:VAL:HG12	1:F:840:SEP:P	2.59	0.41
1:K:1020:ILE:HG22	1:K:1021:PRO:C	2.39	0.41
1:C:978:PRO:HA	1:C:981:TRP:CD1	2.55	0.41
1:C:739:ARG:CG	1:C:739:ARG:HH11	2.33	0.41
1:H:805:VAL:HA	1:H:823:ARG:O	2.20	0.41
1:A:814:ASP:CG	1:B:787:HIS:HD2	2.23	0.41
1:A:799:LYS:HB2	1:A:800:PRO:CD	2.50	0.41
1:L:898:THR:OG1	1:L:899:ARG:N	2.53	0.41
1:D:929:SER:O	1:D:933:ARG:HG3	2.20	0.41
1:B:799:LYS:NZ	1:B:852:THR:HG23	2.35	0.41
1:E:1106:ASP:O	1:E:1110:ARG:HG3	2.19	0.41
1:L:929:SER:O	1:L:933:ARG:HG3	2.20	0.41
1:I:797:ASP:O	1:I:802:ASN:ND2	2.53	0.41
1:K:798:LEU:HD23	1:K:798:LEU:HA	1.82	0.41
1:B:725:HIS:CD2	1:B:727:ASN:HB2	2.56	0.41
1:I:1020:ILE:HG22	1:I:1021:PRO:C	2.40	0.41
1:M:1020:ILE:HG22	1:M:1021:PRO:C	2.39	0.41
1:J:999:ILE:N	1:J:999:ILE:HD12	2.34	0.41
1:F:761:VAL:CG1	1:H:840:SEP:O2P	2.69	0.41
1:D:823:ARG:HH11	1:D:823:ARG:CG	2.33	0.41
1:M:1052:LEU:O	1:M:1055:LEU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:805:VAL:HA	1:M:823:ARG:O	2.20	0.41
1:I:811:PHE:HB3	1:I:823:ARG:HG3	2.01	0.41
1:C:924:LYS:HG3	1:C:925:TYR:HD2	1.84	0.41
1:K:978:PRO:HA	1:K:981:TRP:CG	2.55	0.41
1:B:787:HIS:O	1:B:790:SER:HB2	2.20	0.41
1:C:1032:THR:HG23	1:E:1027:VAL:HB	2.00	0.41
1:H:1033:PHE:CE1	1:H:1058:LYS:HE2	2.55	0.41
1:M:797:ASP:O	1:M:802:ASN:ND2	2.53	0.41
1:J:857:ALA:O	1:J:860:LEU:HB2	2.20	0.41
1:C:712:ALA:O	1:C:716:ILE:HG12	2.19	0.41
1:K:792:LYS:HE2	1:K:792:LYS:HB2	1.88	0.41
1:K:712:ALA:O	1:K:716:ILE:HG12	2.20	0.41
1:J:811:PHE:HB3	1:J:823:ARG:HG3	2.01	0.41
2:K:1999:APJ:H15	2:K:1999:APJ:N1	2.36	0.41
1:F:1020:ILE:HB	1:F:1021:PRO:HA	2.02	0.41
1:H:748:CYS:N	2:H:1999:APJ:HN4	2.13	0.41
1:L:1093:ILE:HG23	1:L:1094:GLY:N	2.34	0.41
1:H:948:SER:HB3	1:H:1085:THR:HG23	2.03	0.41
1:C:799:LYS:NZ	1:C:852:THR:HG23	2.35	0.41
1:C:964:ASP:HA	1:C:965:PRO:HD2	1.84	0.41
1:N:948:SER:HB3	1:N:1085:THR:HG23	2.02	0.41
1:B:712:ALA:O	1:B:716:ILE:HG12	2.20	0.41
1:A:919:HIS:ND1	1:A:920:PRO:HD2	2.35	0.41
1:J:1008:LEU:HA	1:J:1008:LEU:HD23	1.79	0.41
1:G:767:LYS:HB2	1:G:767:LYS:HE2	1.84	0.41
1:D:666:PHE:CZ	1:D:690:PHE:CZ	3.07	0.41
1:I:694:PHE:CG	1:I:695:GLN:N	2.87	0.41
1:I:1063:MET:HB2	1:I:1063:MET:HE2	1.90	0.41
1:J:821:ASN:O	1:J:822:LEU:HB3	2.20	0.41
1:I:821:ASN:O	1:I:822:LEU:HB3	2.20	0.41
1:I:978:PRO:HA	1:I:981:TRP:CD2	2.55	0.41
1:C:978:PRO:HA	1:C:981:TRP:CE2	2.55	0.41
1:L:1055:LEU:O	1:L:1055:LEU:HD23	2.21	0.41
1:G:805:VAL:HA	1:G:823:ARG:O	2.20	0.41
1:J:978:PRO:HA	1:J:981:TRP:CE2	2.55	0.41
1:L:978:PRO:HA	1:L:981:TRP:CD2	2.55	0.41
1:L:978:PRO:HA	1:L:981:TRP:CE2	2.55	0.41
1:M:799:LYS:NZ	1:M:852:THR:HG23	2.35	0.41
1:D:680:LEU:HB2	1:D:689:VAL:HG12	2.01	0.41
1:D:968:ARG:HA	1:D:969:PRO:HD2	1.91	0.41
1:H:1011:LYS:HE2	1:H:1011:LYS:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:970:THR:CB	1:G:762:SER:CB	2.84	0.41
1:I:748:CYS:N	2:I:1999:APJ:HN4	2.13	0.41
1:H:906:MET:HE3	1:H:906:MET:HB2	1.78	0.41
1:F:1033:PHE:CD2	1:F:1034:MET:HE3	2.56	0.41
1:A:1093:ILE:HG23	1:A:1094:GLY:N	2.35	0.41
1:A:785:VAL:HG21	1:A:906:MET:CE	2.50	0.41
1:F:805:VAL:HA	1:F:823:ARG:O	2.20	0.41
1:N:845:ASN:N	1:N:845:ASN:ND2	2.67	0.41
1:E:845:ASN:C	1:E:846:LEU:HD22	2.41	0.41
1:J:978:PRO:HA	1:J:981:TRP:CD2	2.55	0.41
1:L:799:LYS:HB2	1:L:800:PRO:HD2	2.03	0.41
1:M:1082:ASP:HA	1:M:1085:THR:HB	2.03	0.41
1:A:898:THR:HG23	1:A:900:SER:OG	2.20	0.41
1:E:929:SER:O	1:E:933:ARG:HG3	2.21	0.41
1:B:898:THR:HG23	1:B:900:SER:OG	2.20	0.41
1:F:1003:ASP:HA	1:F:1004:PRO:HA	1.91	0.41
1:E:787:HIS:O	1:E:790:SER:HB2	2.20	0.41
1:N:767:LYS:HB2	1:N:767:LYS:HE2	1.83	0.41
1:M:767:LYS:HB2	1:M:767:LYS:HE2	1.83	0.41
1:K:907:GLY:HA2	1:K:960:MET:HE1	2.02	0.41
1:D:895:ARG:HH12	1:D:964:ASP:CG	2.24	0.41
1:C:1052:LEU:O	1:C:1055:LEU:HB3	2.20	0.41
1:H:758:SER:CB	1:H:768:LEU:HD21	2.51	0.41
1:D:799:LYS:HB2	1:D:800:PRO:CD	2.51	0.41
1:N:857:ALA:O	1:N:860:LEU:HB2	2.20	0.41
1:E:797:ASP:O	1:E:802:ASN:ND2	2.53	0.41
1:C:694:PHE:CG	1:C:695:GLN:N	2.88	0.41
1:H:712:ALA:O	1:H:716:ILE:HG12	2.20	0.41
1:G:857:ALA:O	1:G:860:LEU:HB2	2.19	0.41
1:N:788:LEU:HD13	1:N:788:LEU:HA	1.89	0.41
1:L:1011:LYS:HE2	1:L:1011:LYS:HA	2.01	0.41
1:I:1020:ILE:HB	1:I:1021:PRO:HA	2.03	0.41
1:I:978:PRO:HA	1:I:981:TRP:CE2	2.56	0.41
1:C:811:PHE:HB3	1:C:823:ARG:HG3	2.02	0.41
1:K:924:LYS:HG3	1:K:925:TYR:HD2	1.86	0.41
1:D:978:PRO:HA	1:D:981:TRP:CD1	2.55	0.41
1:G:799:LYS:HB2	1:G:800:PRO:HD2	2.03	0.41
1:K:948:SER:HB3	1:K:1085:THR:HG23	2.03	0.41
1:C:1103:LEU:C	1:C:1105:ASP:H	2.24	0.41
1:L:948:SER:HB3	1:L:1085:THR:HG23	2.03	0.41
1:J:1103:LEU:C	1:J:1105:ASP:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:898:THR:HG23	1:J:900:SER:OG	2.21	0.41
1:C:787:HIS:O	1:C:790:SER:HB2	2.21	0.41
1:A:915:SER:HB2	1:A:918:LYS:HB2	2.02	0.41
1:K:787:HIS:O	1:K:790:SER:HB2	2.20	0.41
1:H:672:ASN:H	1:H:672:ASN:ND2	2.18	0.41
1:E:1011:LYS:HA	1:E:1011:LYS:HE2	2.03	0.41
1:N:1011:LYS:HE2	1:N:1011:LYS:HA	2.02	0.41
1:M:1020:ILE:HB	1:M:1021:PRO:HA	2.03	0.41
1:C:1037:LEU:HB2	1:C:1058:LYS:HZ3	1.83	0.41
1:D:805:VAL:HA	1:D:823:ARG:O	2.21	0.41
1:H:737:THR:HG23	1:H:740:PHE:N	2.36	0.41
1:F:924:LYS:HG3	1:F:925:TYR:HD2	1.86	0.41
1:H:924:LYS:HG3	1:H:925:TYR:HD2	1.86	0.41
1:M:978:PRO:HA	1:M:981:TRP:CG	2.56	0.41
1:C:948:SER:HB3	1:C:1085:THR:HG23	2.03	0.41
1:C:857:ALA:O	1:C:860:LEU:HB2	2.21	0.41
1:D:1011:LYS:HE2	1:D:1011:LYS:HA	2.02	0.41
1:N:791:LEU:C	1:N:792:LYS:HD3	2.41	0.41
1:J:797:ASP:O	1:J:802:ASN:ND2	2.54	0.41
1:F:762:SER:O	1:F:765:ASN:HB3	2.21	0.41
1:D:705:LEU:N	1:D:705:LEU:HD12	2.35	0.41
1:M:725:HIS:CD2	1:M:727:ASN:HB2	2.56	0.41
2:D:1999:APJ:N1	2:D:1999:APJ:H15	2.36	0.41
1:B:729:ILE:HD12	1:B:745:LEU:HB3	2.01	0.41
1:L:802:ASN:O	1:L:804:LEU:HD22	2.21	0.41
1:M:821:ASN:O	1:M:822:LEU:HB3	2.21	0.41
1:A:978:PRO:HA	1:A:981:TRP:CD1	2.56	0.41
1:A:906:MET:HE3	1:A:906:MET:HB2	1.75	0.41
1:I:758:SER:CB	1:I:768:LEU:HD21	2.51	0.41
1:F:1055:LEU:HD23	1:F:1055:LEU:O	2.21	0.41
1:J:1093:ILE:HG23	1:J:1094:GLY:N	2.36	0.41
1:G:845:ASN:C	1:G:846:LEU:HD22	2.42	0.41
1:B:811:PHE:HB3	1:B:823:ARG:HG3	2.03	0.41
1:K:978:PRO:HA	1:K:981:TRP:CE2	2.56	0.41
1:A:845:ASN:C	1:A:846:LEU:HD22	2.42	0.41
1:L:845:ASN:C	1:L:846:LEU:HD22	2.41	0.41
1:B:860:LEU:HA	1:B:860:LEU:HD23	1.85	0.41
1:I:948:SER:HB3	1:I:1085:THR:HG23	2.02	0.41
1:F:948:SER:HB3	1:F:1085:THR:HG23	2.03	0.41
1:N:898:THR:OG1	1:N:899:ARG:N	2.54	0.41
1:L:1082:ASP:HA	1:L:1085:THR:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1011:LYS:O	1:D:1014:ALA:HB3	2.21	0.41
1:D:948:SER:HB3	1:D:1085:THR:HG23	2.03	0.41
1:H:1106:ASP:O	1:H:1110:ARG:HG3	2.20	0.41
1:D:1003:ASP:HA	1:D:1004:PRO:HA	1.91	0.41
1:N:968:ARG:HA	1:N:969:PRO:HD2	1.91	0.41
1:B:1048:LEU:O	1:B:1049:MET:C	2.59	0.41
1:I:968:ARG:HA	1:I:969:PRO:HD2	1.91	0.41
1:A:712:ALA:O	1:A:716:ILE:HG12	2.21	0.41
1:G:929:SER:O	1:G:933:ARG:HG3	2.21	0.41
1:L:1067:GLU:HG3	1:L:1067:GLU:H	1.74	0.41
1:I:788:LEU:HD13	1:I:788:LEU:HA	1.88	0.41
1:I:719:LEU:HA	1:I:719:LEU:HD23	1.73	0.41
1:M:694:PHE:CG	1:M:695:GLN:N	2.86	0.41
1:A:1034:MET:HE1	1:A:1037:LEU:HD23	2.01	0.41
1:C:906:MET:HE3	1:C:906:MET:HB2	1.76	0.41
1:G:1020:ILE:HB	1:G:1021:PRO:HA	2.02	0.41
1:C:978:PRO:HA	1:C:981:TRP:CD2	2.56	0.41
1:B:1055:LEU:O	1:B:1055:LEU:HD23	2.21	0.41
1:L:740:PHE:HB3	1:L:741:LEU:H	1.64	0.41
1:M:1052:LEU:HD12	1:M:1052:LEU:HA	1.82	0.41
1:H:845:ASN:C	1:H:846:LEU:HD22	2.42	0.41
1:H:977:HIS:CE1	1:H:978:PRO:HG2	2.55	0.41
1:C:919:HIS:CE1	1:C:921:PHE:HD2	2.39	0.41
1:G:797:ASP:O	1:G:802:ASN:ND2	2.54	0.41
1:J:929:SER:O	1:J:933:ARG:HG3	2.21	0.41
1:B:964:ASP:HA	1:B:965:PRO:HD2	1.84	0.41
1:B:1106:ASP:O	1:B:1110:ARG:HG3	2.20	0.41
1:G:712:ALA:O	1:G:716:ILE:HG12	2.21	0.41
1:L:1033:PHE:CE1	1:L:1058:LYS:HE2	2.55	0.41
1:N:919:HIS:ND1	1:N:920:PRO:HD2	2.36	0.41
1:N:705:LEU:N	1:N:705:LEU:HD12	2.35	0.41
1:M:1011:LYS:HE2	1:M:1011:LYS:HA	2.03	0.41
1:A:1033:PHE:CD2	1:A:1034:MET:HE2	2.56	0.40
1:C:906:MET:HG3	1:C:910:PHE:CE1	2.56	0.40
1:L:748:CYS:N	2:L:1999:APJ:HN4	2.12	0.40
1:M:1041:ARG:HG2	1:M:1042:LYS:N	2.36	0.40
1:G:737:THR:HG23	1:G:740:PHE:N	2.35	0.40
1:B:737:THR:HG23	1:B:740:PHE:N	2.37	0.40
1:A:737:THR:HG23	1:A:740:PHE:N	2.36	0.40
1:F:1052:LEU:O	1:F:1055:LEU:HB3	2.22	0.40
1:C:845:ASN:C	1:C:846:LEU:HD22	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:845:ASN:C	1:M:846:LEU:HD22	2.42	0.40
1:H:1093:ILE:HG23	1:H:1094:GLY:N	2.35	0.40
1:D:845:ASN:C	1:D:846:LEU:HD22	2.41	0.40
1:J:978:PRO:HA	1:J:981:TRP:CG	2.56	0.40
1:J:845:ASN:C	1:J:846:LEU:HD22	2.41	0.40
1:E:799:LYS:HB2	1:E:800:PRO:HD2	2.02	0.40
1:N:799:LYS:HB2	1:N:800:PRO:HD2	2.02	0.40
1:N:792:LYS:HE2	1:N:792:LYS:HB2	1.87	0.40
1:G:968:ARG:HA	1:G:969:PRO:HD2	1.93	0.40
1:A:694:PHE:CG	1:A:695:GLN:N	2.88	0.40
1:L:712:ALA:O	1:L:716:ILE:HG12	2.21	0.40
1:C:762:SER:O	1:C:765:ASN:HB3	2.21	0.40
1:H:694:PHE:CG	1:H:695:GLN:N	2.87	0.40
1:D:1048:LEU:O	1:D:1049:MET:C	2.59	0.40
1:G:915:SER:HB2	1:G:918:LYS:HB2	2.03	0.40
1:F:1048:LEU:O	1:F:1049:MET:C	2.59	0.40
1:C:1010:MET:CE	1:C:1010:MET:HA	2.51	0.40
1:I:767:LYS:HB2	1:I:767:LYS:HE2	1.83	0.40
1:G:1067:GLU:H	1:G:1067:GLU:HG3	1.73	0.40
1:G:999:ILE:N	1:G:999:ILE:HD12	2.35	0.40
1:K:1011:LYS:HE2	1:K:1011:LYS:HA	2.03	0.40
1:D:1030:ASP:OD1	1:D:1030:ASP:N	2.53	0.40
1:N:810:ARG:H	1:N:810:ARG:HG3	1.71	0.40
1:L:767:LYS:HB2	1:L:767:LYS:HE2	1.83	0.40
1:K:668:GLN:NE2	1:K:668:GLN:N	2.69	0.40
1:N:1020:ILE:HB	1:N:1021:PRO:HA	2.03	0.40
1:F:895:ARG:HH12	1:F:964:ASP:CG	2.25	0.40
1:J:1055:LEU:O	1:J:1055:LEU:HD23	2.21	0.40
1:K:1093:ILE:HG23	1:K:1094:GLY:N	2.37	0.40
1:F:811:PHE:HB3	1:F:823:ARG:HG3	2.03	0.40
1:L:811:PHE:HB3	1:L:823:ARG:HG3	2.02	0.40
1:E:811:PHE:HB3	1:E:823:ARG:HG3	2.03	0.40
1:G:811:PHE:HB3	1:G:823:ARG:HG3	2.03	0.40
1:H:799:LYS:HB2	1:H:800:PRO:HD2	2.03	0.40
1:A:857:ALA:O	1:A:860:LEU:HB2	2.21	0.40
1:B:898:THR:OG1	1:B:899:ARG:N	2.54	0.40
1:I:929:SER:O	1:I:933:ARG:HG3	2.21	0.40
1:M:1033:PHE:CE1	1:M:1058:LYS:HE2	2.56	0.40
1:E:898:THR:HG23	1:E:900:SER:OG	2.21	0.40
1:F:797:ASP:O	1:F:802:ASN:ND2	2.54	0.40
1:I:857:ALA:O	1:I:860:LEU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:791:LEU:C	1:I:792:LYS:HD3	2.42	0.40
1:J:1067:GLU:H	1:J:1067:GLU:HG3	1.72	0.40
1:J:785:VAL:HG21	1:J:906:MET:HE3	2.01	0.40
1:J:1020:ILE:HB	1:J:1021:PRO:HA	2.02	0.40
2:F:1999:APJ:H15	2:F:1999:APJ:N1	2.36	0.40
2:B:1999:APJ:H15	2:B:1999:APJ:N1	2.36	0.40
1:B:821:ASN:O	1:B:822:LEU:HB3	2.22	0.40
1:A:674:VAL:HG13	1:A:675:VAL:N	2.37	0.40
1:N:1052:LEU:O	1:N:1055:LEU:HB3	2.22	0.40
1:I:799:LYS:HB2	1:I:800:PRO:HD2	2.04	0.40
1:J:762:SER:O	1:J:765:ASN:HB3	2.22	0.40
1:N:915:SER:HB2	1:N:918:LYS:HB2	2.03	0.40
1:I:712:ALA:O	1:I:716:ILE:HG12	2.21	0.40
1:F:773:ASN:O	1:F:776:SER:HB3	2.22	0.40
1:I:915:SER:HB2	1:I:918:LYS:HB2	2.02	0.40
1:F:719:LEU:HA	1:F:719:LEU:HD23	1.68	0.40
1:M:907:GLY:HA2	1:M:960:MET:HE1	2.03	0.40
1:B:1020:ILE:HB	1:B:1021:PRO:HA	2.03	0.40
1:E:895:ARG:HH12	1:E:964:ASP:CG	2.25	0.40
1:D:822:LEU:HD23	1:D:822:LEU:N	2.36	0.40
1:B:785:VAL:CG2	1:B:906:MET:HE1	2.51	0.40
1:H:978:PRO:HA	1:H:981:TRP:CD2	2.56	0.40
1:G:1052:LEU:O	1:G:1055:LEU:HB3	2.21	0.40
1:F:978:PRO:HA	1:F:981:TRP:CD1	2.57	0.40
1:H:836:ASP:HB3	1:H:837:SER:H	1.74	0.40
1:I:845:ASN:C	1:I:846:LEU:HD22	2.41	0.40
1:N:994:SER:HB2	1:N:1052:LEU:HG	2.02	0.40
1:J:977:HIS:CE1	1:J:978:PRO:HG2	2.56	0.40
1:N:799:LYS:HB2	1:N:800:PRO:CD	2.52	0.40
1:J:948:SER:HB3	1:J:1085:THR:HG23	2.03	0.40
1:N:1082:ASP:HA	1:N:1085:THR:HB	2.03	0.40
1:N:694:PHE:CG	1:N:695:GLN:N	2.88	0.40
1:K:937:SER:O	1:K:938:LEU:HD23	2.22	0.40
1:F:929:SER:O	1:F:933:ARG:HG3	2.21	0.40
1:J:787:HIS:O	1:J:790:SER:HB2	2.21	0.40
1:D:1024:ASP:HA	1:D:1045:SER:O	2.21	0.40
1:M:929:SER:O	1:M:933:ARG:HG3	2.22	0.40
1:E:705:LEU:HD12	1:E:705:LEU:N	2.36	0.40
1:M:968:ARG:HA	1:M:969:PRO:HD2	1.90	0.40
1:C:705:LEU:N	1:C:705:LEU:HD12	2.37	0.40
1:K:1048:LEU:O	1:K:1048:LEU:HD23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:906:MET:HG3	1:D:910:PHE:CE1	2.56	0.40
1:A:821:ASN:O	1:A:822:LEU:HB3	2.21	0.40
1:N:785:VAL:HG21	1:N:906:MET:HE1	2.02	0.40
1:A:978:PRO:HA	1:A:981:TRP:CE2	2.56	0.40
1:H:978:PRO:HA	1:H:981:TRP:CE2	2.57	0.40
1:N:1052:LEU:HA	1:N:1052:LEU:HD12	1.84	0.40
1:C:1093:ILE:HG23	1:C:1094:GLY:N	2.36	0.40
1:E:978:PRO:HA	1:E:981:TRP:CD2	2.56	0.40
1:M:978:PRO:HA	1:M:981:TRP:CD2	2.56	0.40
1:C:799:LYS:HB2	1:C:800:PRO:CD	2.51	0.40
1:G:799:LYS:HB2	1:G:800:PRO:CD	2.52	0.40
1:G:964:ASP:HA	1:G:965:PRO:HD2	1.83	0.40
1:J:915:SER:HB2	1:J:918:LYS:HB2	2.03	0.40
1:F:915:SER:HB2	1:F:918:LYS:HB2	2.03	0.40
1:K:762:SER:O	1:K:765:ASN:HB3	2.21	0.40
1:E:670:LEU:O	1:E:735:GLU:OE2	2.39	0.40
1:D:692:GLY:O	1:D:699:VAL:HG22	2.21	0.40
1:K:968:ARG:HA	1:K:969:PRO:HD2	1.91	0.40
1:F:857:ALA:O	1:F:860:LEU:HB2	2.21	0.40
1:C:1011:LYS:HE2	1:C:1011:LYS:HA	2.03	0.40
1:L:719:LEU:HA	1:L:719:LEU:HD23	1.73	0.40
1:G:671:LYS:O	1:G:671:LYS:HD2	2.21	0.40

All (3) 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:I:848:ASN:OD1	1:J:1045:SER:OG[4_457]	1.97	0.23
1:I:848:ASN:CG	1:J:1045:SER:OG[4_457]	2.05	0.15
1:A:1021:PRO:O	1:C:739:ARG:NH1[4_456]	2.10	0.10

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	413/448 (92%)	351 (85%)	50 (12%)	12 (3%)	6	36
1	B	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	8	45
1	C	413/448 (92%)	348 (84%)	56 (14%)	9 (2%)	8	45
1	D	420/448 (94%)	353 (84%)	57 (14%)	10 (2%)	7	43
1	E	413/448 (92%)	354 (86%)	50 (12%)	9 (2%)	8	45
1	F	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	8	45
1	G	413/448 (92%)	351 (85%)	53 (13%)	9 (2%)	8	45
1	H	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	8	45
1	I	411/448 (92%)	353 (86%)	49 (12%)	9 (2%)	8	45
1	J	411/448 (92%)	350 (85%)	52 (13%)	9 (2%)	8	45
1	K	420/448 (94%)	349 (83%)	61 (14%)	10 (2%)	7	43
1	L	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	8	45
1	M	413/448 (92%)	353 (86%)	51 (12%)	9 (2%)	8	45
1	N	413/448 (92%)	353 (86%)	51 (12%)	9 (2%)	8	45
All	All	5792/6272 (92%)	4923 (85%)	738 (13%)	131 (2%)	8	44

All (131) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	759	LYS
1	A	770	LYS
1	A	771	GLU
1	A	862	GLU
1	A	1039	ARG
1	B	759	LYS
1	B	770	LYS
1	B	771	GLU
1	B	862	GLU
1	C	759	LYS
1	C	770	LYS
1	C	771	GLU
1	C	862	GLU
1	D	759	LYS
1	D	770	LYS
1	D	771	GLU
1	D	862	GLU

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Mol	Chain	Res	Type
1	E	759	LYS
1	E	770	LYS
1	E	771	GLU
1	E	862	GLU
1	F	759	LYS
1	F	770	LYS
1	F	771	GLU
1	F	862	GLU
1	G	759	LYS
1	G	770	LYS
1	G	771	GLU
1	G	862	GLU
1	H	759	LYS
1	H	770	LYS
1	H	771	GLU
1	H	862	GLU
1	I	759	LYS
1	I	770	LYS
1	I	771	GLU
1	I	862	GLU
1	J	759	LYS
1	J	770	LYS
1	J	771	GLU
1	J	862	GLU
1	K	759	LYS
1	K	770	LYS
1	K	771	GLU
1	K	862	GLU
1	L	759	LYS
1	L	770	LYS
1	L	771	GLU
1	L	862	GLU
1	M	759	LYS
1	M	770	LYS
1	M	771	GLU
1	M	862	GLU
1	N	759	LYS
1	N	770	LYS
1	N	771	GLU
1	N	862	GLU
1	A	893	THR
1	A	1104	SER

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Mol	Chain	Res	Type
1	B	893	THR
1	C	893	THR
1	D	893	THR
1	D	1104	SER
1	E	893	THR
1	E	1104	SER
1	F	893	THR
1	G	893	THR
1	H	893	THR
1	H	1104	SER
1	I	893	THR
1	I	1104	SER
1	J	893	THR
1	K	893	THR
1	K	1104	SER
1	L	893	THR
1	M	893	THR
1	M	1104	SER
1	N	893	THR
1	N	1104	SER
1	A	1041	ARG
1	A	1042	LYS
1	B	1104	SER
1	C	1104	SER
1	D	664	PRO
1	F	1104	SER
1	G	1104	SER
1	J	1104	SER
1	K	664	PRO
1	L	1104	SER
1	A	738	ASP
1	B	738	ASP
1	C	738	ASP
1	D	738	ASP
1	E	738	ASP
1	G	738	ASP
1	H	738	ASP
1	I	738	ASP
1	J	738	ASP
1	L	738	ASP
1	M	738	ASP
1	F	738	ASP

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Mol	Chain	Res	Type
1	K	738	ASP
1	N	738	ASP
1	A	838	GLY
1	B	838	GLY
1	C	838	GLY
1	D	838	GLY
1	F	838	GLY
1	G	838	GLY
1	H	838	GLY
1	I	838	GLY
1	J	838	GLY
1	K	838	GLY
1	L	838	GLY
1	M	838	GLY
1	N	838	GLY
1	E	838	GLY
1	A	849	PRO
1	B	849	PRO
1	C	849	PRO
1	D	849	PRO
1	F	849	PRO
1	G	849	PRO
1	I	849	PRO
1	J	849	PRO
1	K	849	PRO
1	M	849	PRO
1	N	849	PRO
1	E	849	PRO
1	H	849	PRO
1	L	849	PRO

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	380/405 (94%)	351 (92%)	29 (8%)	16 55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	380/405 (94%)	352 (93%)	28 (7%)	17 56
1	C	380/405 (94%)	350 (92%)	30 (8%)	15 53
1	D	387/405 (96%)	353 (91%)	34 (9%)	12 45
1	E	380/405 (94%)	349 (92%)	31 (8%)	14 50
1	F	380/405 (94%)	349 (92%)	31 (8%)	14 50
1	G	380/405 (94%)	350 (92%)	30 (8%)	15 53
1	H	380/405 (94%)	350 (92%)	30 (8%)	15 53
1	I	378/405 (93%)	351 (93%)	27 (7%)	18 57
1	J	378/405 (93%)	351 (93%)	27 (7%)	18 57
1	K	387/405 (96%)	356 (92%)	31 (8%)	15 52
1	L	380/405 (94%)	350 (92%)	30 (8%)	15 53
1	M	380/405 (94%)	352 (93%)	28 (7%)	17 56
1	N	380/405 (94%)	347 (91%)	33 (9%)	13 45
All	All	5330/5670 (94%)	4911 (92%)	419 (8%)	15 53

All (419) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	670	LEU
1	A	671	LYS
1	A	707	ASP
1	A	711	ILE
1	A	729	ILE
1	A	749	ASN
1	A	750	LEU
1	A	759	LYS
1	A	761	VAL
1	A	767	LYS
1	A	788	LEU
1	A	796	ARG
1	A	804	LEU
1	A	817	THR
1	A	823	ARG
1	A	835	LEU
1	A	843	ARG
1	A	845	ASN
1	A	897	LEU

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Mol	Chain	Res	Type
1	A	939	ASP
1	A	943	CYS
1	A	970	THR
1	A	987	LEU
1	A	1030	ASP
1	A	1040	TYR
1	A	1041	ARG
1	A	1053	ARG
1	A	1067	GLU
1	A	1085	THR
1	B	670	LEU
1	B	671	LYS
1	B	672	ASN
1	B	707	ASP
1	B	711	ILE
1	B	729	ILE
1	B	749	ASN
1	B	750	LEU
1	B	759	LYS
1	B	761	VAL
1	B	767	LYS
1	B	788	LEU
1	B	796	ARG
1	B	804	LEU
1	B	817	THR
1	B	823	ARG
1	B	835	LEU
1	B	843	ARG
1	B	845	ASN
1	B	939	ASP
1	B	943	CYS
1	B	970	THR
1	B	987	LEU
1	B	1030	ASP
1	B	1040	TYR
1	B	1053	ARG
1	B	1067	GLU
1	B	1085	THR
1	C	670	LEU
1	C	671	LYS
1	C	672	ASN
1	C	707	ASP

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Mol	Chain	Res	Type
1	C	711	ILE
1	C	729	ILE
1	C	737	THR
1	C	749	ASN
1	C	750	LEU
1	C	759	LYS
1	C	761	VAL
1	C	767	LYS
1	C	788	LEU
1	C	796	ARG
1	C	804	LEU
1	C	817	THR
1	C	823	ARG
1	C	835	LEU
1	C	843	ARG
1	C	845	ASN
1	C	897	LEU
1	C	939	ASP
1	C	943	CYS
1	C	970	THR
1	C	987	LEU
1	C	1030	ASP
1	C	1040	TYR
1	C	1053	ARG
1	C	1067	GLU
1	C	1085	THR
1	D	665	ASN
1	D	667	GLU
1	D	668	GLN
1	D	669	SER
1	D	671	LYS
1	D	672	ASN
1	D	674	VAL
1	D	707	ASP
1	D	711	ILE
1	D	729	ILE
1	D	737	THR
1	D	749	ASN
1	D	750	LEU
1	D	759	LYS
1	D	761	VAL
1	D	767	LYS

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Mol	Chain	Res	Type
1	D	788	LEU
1	D	796	ARG
1	D	804	LEU
1	D	817	THR
1	D	823	ARG
1	D	835	LEU
1	D	843	ARG
1	D	845	ASN
1	D	897	LEU
1	D	939	ASP
1	D	943	CYS
1	D	970	THR
1	D	987	LEU
1	D	1030	ASP
1	D	1040	TYR
1	D	1053	ARG
1	D	1067	GLU
1	D	1085	THR
1	E	670	LEU
1	E	671	LYS
1	E	672	ASN
1	E	707	ASP
1	E	711	ILE
1	E	729	ILE
1	E	737	THR
1	E	749	ASN
1	E	750	LEU
1	E	759	LYS
1	E	761	VAL
1	E	767	LYS
1	E	788	LEU
1	E	796	ARG
1	E	804	LEU
1	E	817	THR
1	E	823	ARG
1	E	835	LEU
1	E	843	ARG
1	E	845	ASN
1	E	858	PRO
1	E	897	LEU
1	E	939	ASP
1	E	943	CYS

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Mol	Chain	Res	Type
1	E	970	THR
1	E	987	LEU
1	E	1030	ASP
1	E	1040	TYR
1	E	1053	ARG
1	E	1067	GLU
1	E	1085	THR
1	F	671	LYS
1	F	672	ASN
1	F	673	LEU
1	F	674	VAL
1	F	707	ASP
1	F	711	ILE
1	F	729	ILE
1	F	737	THR
1	F	749	ASN
1	F	750	LEU
1	F	759	LYS
1	F	761	VAL
1	F	767	LYS
1	F	788	LEU
1	F	796	ARG
1	F	804	LEU
1	F	817	THR
1	F	823	ARG
1	F	835	LEU
1	F	843	ARG
1	F	845	ASN
1	F	897	LEU
1	F	939	ASP
1	F	943	CYS
1	F	970	THR
1	F	987	LEU
1	F	1020	ILE
1	F	1030	ASP
1	F	1040	TYR
1	F	1053	ARG
1	F	1067	GLU
1	G	670	LEU
1	G	671	LYS
1	G	672	ASN
1	G	707	ASP

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Mol	Chain	Res	Type
1	G	711	ILE
1	G	729	ILE
1	G	749	ASN
1	G	750	LEU
1	G	759	LYS
1	G	761	VAL
1	G	767	LYS
1	G	788	LEU
1	G	796	ARG
1	G	804	LEU
1	G	817	THR
1	G	823	ARG
1	G	835	LEU
1	G	843	ARG
1	G	845	ASN
1	G	897	LEU
1	G	939	ASP
1	G	943	CYS
1	G	970	THR
1	G	987	LEU
1	G	1020	ILE
1	G	1030	ASP
1	G	1040	TYR
1	G	1053	ARG
1	G	1067	GLU
1	G	1085	THR
1	H	670	LEU
1	H	671	LYS
1	H	672	ASN
1	H	707	ASP
1	H	711	ILE
1	H	729	ILE
1	H	749	ASN
1	H	750	LEU
1	H	759	LYS
1	H	761	VAL
1	H	767	LYS
1	H	788	LEU
1	H	796	ARG
1	H	804	LEU
1	H	817	THR
1	H	823	ARG

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Mol	Chain	Res	Type
1	H	835	LEU
1	H	843	ARG
1	H	845	ASN
1	H	897	LEU
1	H	939	ASP
1	H	943	CYS
1	H	970	THR
1	H	987	LEU
1	H	1020	ILE
1	H	1030	ASP
1	H	1040	TYR
1	H	1053	ARG
1	H	1067	GLU
1	H	1085	THR
1	I	672	ASN
1	I	707	ASP
1	I	711	ILE
1	I	729	ILE
1	I	749	ASN
1	I	750	LEU
1	I	759	LYS
1	I	761	VAL
1	I	767	LYS
1	I	788	LEU
1	I	796	ARG
1	I	804	LEU
1	I	817	THR
1	I	823	ARG
1	I	835	LEU
1	I	843	ARG
1	I	845	ASN
1	I	897	LEU
1	I	939	ASP
1	I	943	CYS
1	I	970	THR
1	I	987	LEU
1	I	1030	ASP
1	I	1040	TYR
1	I	1053	ARG
1	I	1067	GLU
1	I	1085	THR
1	J	672	ASN

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Mol	Chain	Res	Type
1	J	707	ASP
1	J	711	ILE
1	J	729	ILE
1	J	749	ASN
1	J	750	LEU
1	J	759	LYS
1	J	761	VAL
1	J	767	LYS
1	J	788	LEU
1	J	796	ARG
1	J	804	LEU
1	J	817	THR
1	J	823	ARG
1	J	835	LEU
1	J	843	ARG
1	J	845	ASN
1	J	897	LEU
1	J	939	ASP
1	J	943	CYS
1	J	970	THR
1	J	987	LEU
1	J	1030	ASP
1	J	1040	TYR
1	J	1053	ARG
1	J	1067	GLU
1	J	1085	THR
1	K	665	ASN
1	K	668	GLN
1	K	671	LYS
1	K	672	ASN
1	K	707	ASP
1	K	711	ILE
1	K	729	ILE
1	K	749	ASN
1	K	750	LEU
1	K	759	LYS
1	K	761	VAL
1	K	767	LYS
1	K	788	LEU
1	K	796	ARG
1	K	804	LEU
1	K	817	THR

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Mol	Chain	Res	Type
1	K	823	ARG
1	K	835	LEU
1	K	843	ARG
1	K	845	ASN
1	K	858	PRO
1	K	897	LEU
1	K	939	ASP
1	K	943	CYS
1	K	970	THR
1	K	987	LEU
1	K	1030	ASP
1	K	1040	TYR
1	K	1053	ARG
1	K	1067	GLU
1	K	1085	THR
1	L	670	LEU
1	L	671	LYS
1	L	672	ASN
1	L	673	LEU
1	L	707	ASP
1	L	711	ILE
1	L	729	ILE
1	L	749	ASN
1	L	750	LEU
1	L	759	LYS
1	L	761	VAL
1	L	767	LYS
1	L	788	LEU
1	L	796	ARG
1	L	804	LEU
1	L	817	THR
1	L	823	ARG
1	L	835	LEU
1	L	843	ARG
1	L	845	ASN
1	L	897	LEU
1	L	939	ASP
1	L	943	CYS
1	L	970	THR
1	L	987	LEU
1	L	1030	ASP
1	L	1040	TYR

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Mol	Chain	Res	Type
1	L	1053	ARG
1	L	1067	GLU
1	L	1085	THR
1	M	671	LYS
1	M	672	ASN
1	M	707	ASP
1	M	711	ILE
1	M	729	ILE
1	M	749	ASN
1	M	750	LEU
1	M	759	LYS
1	M	761	VAL
1	M	767	LYS
1	M	788	LEU
1	M	796	ARG
1	M	804	LEU
1	M	817	THR
1	M	823	ARG
1	M	835	LEU
1	M	843	ARG
1	M	845	ASN
1	M	897	LEU
1	M	939	ASP
1	M	943	CYS
1	M	970	THR
1	M	987	LEU
1	M	1030	ASP
1	M	1040	TYR
1	M	1053	ARG
1	M	1067	GLU
1	M	1085	THR
1	N	670	LEU
1	N	671	LYS
1	N	672	ASN
1	N	673	LEU
1	N	674	VAL
1	N	707	ASP
1	N	711	ILE
1	N	729	ILE
1	N	737	THR
1	N	749	ASN
1	N	750	LEU

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Mol	Chain	Res	Type
1	N	759	LYS
1	N	761	VAL
1	N	767	LYS
1	N	788	LEU
1	N	796	ARG
1	N	804	LEU
1	N	817	THR
1	N	823	ARG
1	N	835	LEU
1	N	843	ARG
1	N	845	ASN
1	N	858	PRO
1	N	897	LEU
1	N	939	ASP
1	N	943	CYS
1	N	970	THR
1	N	987	LEU
1	N	1030	ASP
1	N	1040	TYR
1	N	1053	ARG
1	N	1067	GLU
1	N	1085	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (150) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	672	ASN
1	A	691	GLN
1	A	725	HIS
1	A	727	ASN
1	A	753	GLN
1	A	802	ASN
1	A	839	GLN
1	A	845	ASN
1	A	1001	ASN
1	A	1090	ASN
1	B	672	ASN
1	B	691	GLN
1	B	725	HIS
1	B	753	GLN
1	B	787	HIS
1	B	802	ASN

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Mol	Chain	Res	Type
1	B	839	GLN
1	B	845	ASN
1	B	1001	ASN
1	B	1090	ASN
1	C	672	ASN
1	C	691	GLN
1	C	725	HIS
1	C	753	GLN
1	C	787	HIS
1	C	802	ASN
1	C	839	GLN
1	C	845	ASN
1	C	847	ASN
1	C	1001	ASN
1	C	1057	ASN
1	C	1090	ASN
1	D	665	ASN
1	D	668	GLN
1	D	672	ASN
1	D	691	GLN
1	D	725	HIS
1	D	727	ASN
1	D	753	GLN
1	D	802	ASN
1	D	839	GLN
1	D	845	ASN
1	D	1001	ASN
1	D	1090	ASN
1	E	672	ASN
1	E	691	GLN
1	E	725	HIS
1	E	727	ASN
1	E	753	GLN
1	E	802	ASN
1	E	839	GLN
1	E	845	ASN
1	E	1001	ASN
1	E	1090	ASN
1	F	672	ASN
1	F	691	GLN
1	F	725	HIS
1	F	727	ASN

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Mol	Chain	Res	Type
1	F	753	GLN
1	F	787	HIS
1	F	802	ASN
1	F	839	GLN
1	F	845	ASN
1	F	1001	ASN
1	F	1090	ASN
1	G	672	ASN
1	G	691	GLN
1	G	725	HIS
1	G	727	ASN
1	G	753	GLN
1	G	802	ASN
1	G	845	ASN
1	G	1001	ASN
1	G	1090	ASN
1	H	672	ASN
1	H	691	GLN
1	H	725	HIS
1	H	727	ASN
1	H	753	GLN
1	H	787	HIS
1	H	802	ASN
1	H	815	GLN
1	H	839	GLN
1	H	845	ASN
1	H	1001	ASN
1	H	1090	ASN
1	I	691	GLN
1	I	725	HIS
1	I	727	ASN
1	I	753	GLN
1	I	787	HIS
1	I	802	ASN
1	I	839	GLN
1	I	845	ASN
1	I	847	ASN
1	I	1001	ASN
1	I	1090	ASN
1	J	691	GLN
1	J	725	HIS
1	J	727	ASN

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Mol	Chain	Res	Type
1	J	753	GLN
1	J	802	ASN
1	J	816	GLN
1	J	845	ASN
1	J	1001	ASN
1	J	1057	ASN
1	J	1090	ASN
1	K	665	ASN
1	K	672	ASN
1	K	691	GLN
1	K	725	HIS
1	K	727	ASN
1	K	753	GLN
1	K	802	ASN
1	K	839	GLN
1	K	845	ASN
1	K	1001	ASN
1	K	1090	ASN
1	L	672	ASN
1	L	691	GLN
1	L	725	HIS
1	L	727	ASN
1	L	753	GLN
1	L	787	HIS
1	L	802	ASN
1	L	839	GLN
1	L	845	ASN
1	L	1001	ASN
1	L	1090	ASN
1	M	672	ASN
1	M	691	GLN
1	M	725	HIS
1	M	727	ASN
1	M	753	GLN
1	M	802	ASN
1	M	839	GLN
1	M	845	ASN
1	M	1001	ASN
1	M	1090	ASN
1	N	672	ASN
1	N	691	GLN
1	N	725	HIS

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Mol	Chain	Res	Type
1	N	727	ASN
1	N	753	GLN
1	N	787	HIS
1	N	802	ASN
1	N	839	GLN
1	N	845	ASN
1	N	1001	ASN
1	N	1090	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

42 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	SEP	A	840	1	8,9,10	1.53	1 (12%)	8,12,14	1.56	1 (12%)
1	SEP	A	841	1	8,9,10	1.48	1 (12%)	8,12,14	1.01	0
1	TPO	A	844	1	8,10,11	2.66	4 (50%)	7,14,16	2.16	3 (42%)
1	SEP	B	840	1	8,9,10	1.54	1 (12%)	8,12,14	1.54	1 (12%)
1	SEP	B	841	1	8,9,10	1.47	1 (12%)	8,12,14	0.88	0
1	TPO	B	844	1	8,10,11	2.65	4 (50%)	7,14,16	2.10	3 (42%)
1	SEP	C	840	1	8,9,10	1.54	1 (12%)	8,12,14	1.56	1 (12%)
1	SEP	C	841	1	8,9,10	1.50	1 (12%)	8,12,14	0.97	0
1	TPO	C	844	1	8,10,11	2.64	4 (50%)	7,14,16	2.17	3 (42%)
1	SEP	D	840	1	8,9,10	1.57	1 (12%)	8,12,14	1.66	1 (12%)
1	SEP	D	841	1	8,9,10	1.46	1 (12%)	8,12,14	0.90	0
1	TPO	D	844	1	8,10,11	2.66	4 (50%)	7,14,16	2.18	3 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SEP	E	840	1	8,9,10	1.53	1 (12%)	8,12,14	1.56	1 (12%)
1	SEP	E	841	1	8,9,10	1.48	1 (12%)	8,12,14	1.07	1 (12%)
1	TPO	E	844	1	8,10,11	2.66	4 (50%)	7,14,16	2.17	3 (42%)
1	SEP	F	840	1	8,9,10	1.52	1 (12%)	8,12,14	1.49	1 (12%)
1	SEP	F	841	1	8,9,10	1.58	1 (12%)	8,12,14	0.89	0
1	TPO	F	844	1	8,10,11	2.66	4 (50%)	7,14,16	2.14	3 (42%)
1	SEP	G	840	1	8,9,10	1.55	1 (12%)	8,12,14	1.53	1 (12%)
1	SEP	G	841	1	8,9,10	1.49	1 (12%)	8,12,14	0.98	0
1	TPO	G	844	1	8,10,11	2.66	4 (50%)	7,14,16	2.11	3 (42%)
1	SEP	H	840	1	8,9,10	1.56	1 (12%)	8,12,14	1.44	1 (12%)
1	SEP	H	841	1	8,9,10	1.50	1 (12%)	8,12,14	0.98	0
1	TPO	H	844	1	8,10,11	2.65	4 (50%)	7,14,16	2.14	3 (42%)
1	SEP	I	840	1	8,9,10	1.54	1 (12%)	8,12,14	1.52	1 (12%)
1	SEP	I	841	1	8,9,10	1.51	1 (12%)	8,12,14	0.96	0
1	TPO	I	844	1	8,10,11	2.66	4 (50%)	7,14,16	2.16	3 (42%)
1	SEP	J	840	1	8,9,10	1.54	1 (12%)	8,12,14	1.56	1 (12%)
1	SEP	J	841	1	8,9,10	1.49	1 (12%)	8,12,14	0.96	0
1	TPO	J	844	1	8,10,11	2.65	4 (50%)	7,14,16	2.14	3 (42%)
1	SEP	K	840	1	8,9,10	1.55	1 (12%)	8,12,14	1.60	1 (12%)
1	SEP	K	841	1	8,9,10	1.49	1 (12%)	8,12,14	0.83	0
1	TPO	K	844	1	8,10,11	2.67	4 (50%)	7,14,16	2.16	3 (42%)
1	SEP	L	840	1	8,9,10	1.54	1 (12%)	8,12,14	1.51	1 (12%)
1	SEP	L	841	1	8,9,10	1.51	1 (12%)	8,12,14	0.93	0
1	TPO	L	844	1	8,10,11	2.65	4 (50%)	7,14,16	2.17	3 (42%)
1	SEP	M	840	1	8,9,10	1.53	1 (12%)	8,12,14	1.48	1 (12%)
1	SEP	M	841	1	8,9,10	1.46	1 (12%)	8,12,14	0.92	0
1	TPO	M	844	1	8,10,11	2.66	4 (50%)	7,14,16	2.17	3 (42%)
1	SEP	N	840	1	8,9,10	1.56	1 (12%)	8,12,14	1.53	1 (12%)
1	SEP	N	841	1	8,9,10	1.52	1 (12%)	8,12,14	0.96	0
1	TPO	N	844	1	8,10,11	2.65	4 (50%)	7,14,16	2.18	3 (42%)

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
1	SEP	A	840	1	-	0/6/8/10	0/0/0/0
1	SEP	A	841	1	-	0/6/8/10	0/0/0/0
1	TPO	A	844	1	-	0/8/11/13	0/0/0/0
1	SEP	B	840	1	-	0/6/8/10	0/0/0/0
1	SEP	B	841	1	-	0/6/8/10	0/0/0/0
1	TPO	B	844	1	-	0/8/11/13	0/0/0/0
1	SEP	C	840	1	-	0/6/8/10	0/0/0/0
1	SEP	C	841	1	-	0/6/8/10	0/0/0/0
1	TPO	C	844	1	-	0/8/11/13	0/0/0/0
1	SEP	D	840	1	-	0/6/8/10	0/0/0/0
1	SEP	D	841	1	-	0/6/8/10	0/0/0/0
1	TPO	D	844	1	-	0/8/11/13	0/0/0/0
1	SEP	E	840	1	-	0/6/8/10	0/0/0/0
1	SEP	E	841	1	-	0/6/8/10	0/0/0/0
1	TPO	E	844	1	-	0/8/11/13	0/0/0/0
1	SEP	F	840	1	-	0/6/8/10	0/0/0/0
1	SEP	F	841	1	-	0/6/8/10	0/0/0/0
1	TPO	F	844	1	-	0/8/11/13	0/0/0/0
1	SEP	G	840	1	-	0/6/8/10	0/0/0/0
1	SEP	G	841	1	-	0/6/8/10	0/0/0/0
1	TPO	G	844	1	-	0/8/11/13	0/0/0/0
1	SEP	H	840	1	-	0/6/8/10	0/0/0/0
1	SEP	H	841	1	-	0/6/8/10	0/0/0/0
1	TPO	H	844	1	-	0/8/11/13	0/0/0/0
1	SEP	I	840	1	-	0/6/8/10	0/0/0/0
1	SEP	I	841	1	-	0/6/8/10	0/0/0/0
1	TPO	I	844	1	-	0/8/11/13	0/0/0/0
1	SEP	J	840	1	-	0/6/8/10	0/0/0/0
1	SEP	J	841	1	-	0/6/8/10	0/0/0/0
1	TPO	J	844	1	-	0/8/11/13	0/0/0/0
1	SEP	K	840	1	-	0/6/8/10	0/0/0/0
1	SEP	K	841	1	-	0/6/8/10	0/0/0/0
1	TPO	K	844	1	-	0/8/11/13	0/0/0/0
1	SEP	L	840	1	-	0/6/8/10	0/0/0/0
1	SEP	L	841	1	-	0/6/8/10	0/0/0/0
1	TPO	L	844	1	-	0/8/11/13	0/0/0/0
1	SEP	M	840	1	-	0/6/8/10	0/0/0/0
1	SEP	M	841	1	-	0/6/8/10	0/0/0/0
1	TPO	M	844	1	-	0/8/11/13	0/0/0/0
1	SEP	N	840	1	-	0/6/8/10	0/0/0/0
1	SEP	N	841	1	-	0/6/8/10	0/0/0/0
1	TPO	N	844	1	-	0/8/11/13	0/0/0/0

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	844	TPO	P-O3P	-2.30	1.46	1.54
1	C	844	TPO	P-O3P	-2.30	1.46	1.54
1	N	844	TPO	P-O3P	-2.29	1.46	1.54
1	B	844	TPO	P-O3P	-2.28	1.46	1.54
1	I	844	TPO	P-O3P	-2.28	1.46	1.54
1	L	844	TPO	P-O3P	-2.28	1.46	1.54
1	K	844	TPO	P-O3P	-2.28	1.46	1.54
1	H	844	TPO	P-O3P	-2.27	1.46	1.54
1	A	844	TPO	P-O3P	-2.27	1.46	1.54
1	M	844	TPO	P-O3P	-2.27	1.46	1.54
1	E	844	TPO	P-O3P	-2.26	1.46	1.54
1	G	844	TPO	P-O3P	-2.26	1.46	1.54
1	J	844	TPO	P-O3P	-2.25	1.46	1.54
1	F	844	TPO	P-O3P	-2.24	1.46	1.54
1	B	844	TPO	P-O2P	2.78	1.64	1.54
1	I	844	TPO	P-O2P	2.92	1.65	1.54
1	F	844	TPO	P-O2P	2.93	1.65	1.54
1	E	844	TPO	P-O2P	2.93	1.65	1.54
1	M	844	TPO	P-O2P	2.94	1.65	1.54
1	G	844	TPO	P-O2P	2.94	1.65	1.54
1	K	844	TPO	P-O2P	2.94	1.65	1.54
1	C	844	TPO	P-O2P	2.94	1.65	1.54
1	N	844	TPO	P-O2P	2.95	1.65	1.54
1	H	844	TPO	P-O2P	2.96	1.65	1.54
1	D	844	TPO	P-O2P	2.96	1.65	1.54
1	L	844	TPO	P-O2P	2.98	1.65	1.54
1	J	844	TPO	P-O2P	2.99	1.65	1.54
1	A	844	TPO	P-O2P	2.99	1.65	1.54
1	D	841	SEP	P-O1P	2.99	1.61	1.51
1	M	841	SEP	P-O1P	3.03	1.61	1.51
1	B	841	SEP	P-O1P	3.04	1.61	1.51
1	K	841	SEP	P-O1P	3.05	1.61	1.51
1	E	841	SEP	P-O1P	3.07	1.61	1.51
1	J	841	SEP	P-O1P	3.09	1.61	1.51
1	A	841	SEP	P-O1P	3.10	1.61	1.51
1	L	841	SEP	P-O1P	3.12	1.61	1.51
1	I	841	SEP	P-O1P	3.12	1.61	1.51
1	M	840	SEP	P-O1P	3.12	1.61	1.51
1	C	840	SEP	P-O1P	3.12	1.61	1.51
1	C	841	SEP	P-O1P	3.13	1.61	1.51
1	G	841	SEP	P-O1P	3.14	1.61	1.51
1	F	840	SEP	P-O1P	3.14	1.61	1.51
1	A	840	SEP	P-O1P	3.14	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	840	SEP	P-O1P	3.15	1.61	1.51
1	G	840	SEP	P-O1P	3.16	1.61	1.51
1	H	841	SEP	P-O1P	3.18	1.61	1.51
1	D	840	SEP	P-O1P	3.18	1.61	1.51
1	J	840	SEP	P-O1P	3.18	1.61	1.51
1	N	841	SEP	P-O1P	3.18	1.61	1.51
1	I	840	SEP	P-O1P	3.19	1.61	1.51
1	K	840	SEP	P-O1P	3.19	1.61	1.51
1	B	840	SEP	P-O1P	3.19	1.61	1.51
1	N	840	SEP	P-O1P	3.22	1.61	1.51
1	L	840	SEP	P-O1P	3.23	1.61	1.51
1	H	840	SEP	P-O1P	3.24	1.61	1.51
1	F	841	SEP	P-O1P	3.33	1.62	1.51
1	C	844	TPO	P-O1P	4.22	1.65	1.51
1	L	844	TPO	P-O1P	4.25	1.65	1.51
1	B	844	TPO	P-O1P	4.25	1.65	1.51
1	N	844	TPO	P-O1P	4.26	1.65	1.51
1	I	844	TPO	P-O1P	4.26	1.65	1.51
1	H	844	TPO	P-O1P	4.28	1.65	1.51
1	J	844	TPO	P-O1P	4.29	1.65	1.51
1	D	844	TPO	P-O1P	4.29	1.65	1.51
1	F	844	TPO	P-O1P	4.29	1.65	1.51
1	A	844	TPO	P-O1P	4.29	1.65	1.51
1	M	844	TPO	P-O1P	4.30	1.65	1.51
1	E	844	TPO	P-O1P	4.30	1.65	1.51
1	G	844	TPO	P-O1P	4.33	1.65	1.51
1	K	844	TPO	P-O1P	4.34	1.65	1.51
1	D	844	TPO	O-C	4.46	1.40	1.19
1	J	844	TPO	O-C	4.46	1.40	1.19
1	A	844	TPO	O-C	4.47	1.40	1.19
1	H	844	TPO	O-C	4.47	1.40	1.19
1	L	844	TPO	O-C	4.47	1.40	1.19
1	E	844	TPO	O-C	4.47	1.40	1.19
1	N	844	TPO	O-C	4.47	1.40	1.19
1	G	844	TPO	O-C	4.47	1.40	1.19
1	C	844	TPO	O-C	4.48	1.40	1.19
1	K	844	TPO	O-C	4.49	1.40	1.19
1	M	844	TPO	O-C	4.49	1.40	1.19
1	I	844	TPO	O-C	4.49	1.40	1.19
1	F	844	TPO	O-C	4.50	1.40	1.19
1	B	844	TPO	O-C	4.60	1.41	1.19

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	844	TPO	O-C-CA	-4.35	113.95	125.44
1	N	844	TPO	O-C-CA	-4.33	113.99	125.44
1	E	844	TPO	O-C-CA	-4.33	114.00	125.44
1	M	844	TPO	O-C-CA	-4.33	114.00	125.44
1	J	844	TPO	O-C-CA	-4.32	114.04	125.44
1	D	844	TPO	O-C-CA	-4.30	114.07	125.44
1	H	844	TPO	O-C-CA	-4.29	114.11	125.44
1	L	844	TPO	O-C-CA	-4.29	114.11	125.44
1	A	844	TPO	O-C-CA	-4.29	114.12	125.44
1	F	844	TPO	O-C-CA	-4.26	114.19	125.44
1	G	844	TPO	O-C-CA	-4.25	114.22	125.44
1	K	844	TPO	O-C-CA	-4.24	114.25	125.44
1	I	844	TPO	O-C-CA	-4.23	114.26	125.44
1	B	844	TPO	O-C-CA	-4.17	114.42	125.44
1	F	844	TPO	CG2-CB-CA	-2.17	108.76	113.17
1	D	844	TPO	CG2-CB-CA	-2.15	108.79	113.17
1	L	844	TPO	CG2-CB-CA	-2.15	108.79	113.17
1	B	844	TPO	CG2-CB-CA	-2.13	108.83	113.17
1	N	844	TPO	CG2-CB-CA	-2.13	108.83	113.17
1	A	844	TPO	CG2-CB-CA	-2.13	108.84	113.17
1	E	844	TPO	CG2-CB-CA	-2.13	108.84	113.17
1	K	844	TPO	CG2-CB-CA	-2.12	108.85	113.17
1	M	844	TPO	CG2-CB-CA	-2.12	108.86	113.17
1	H	844	TPO	CG2-CB-CA	-2.11	108.88	113.17
1	I	844	TPO	CG2-CB-CA	-2.11	108.88	113.17
1	C	844	TPO	CG2-CB-CA	-2.10	108.90	113.17
1	G	844	TPO	CG2-CB-CA	-2.02	109.06	113.17
1	J	844	TPO	CG2-CB-CA	-2.02	109.06	113.17
1	E	841	SEP	OG-CB-CA	2.15	110.11	108.27
1	B	844	TPO	C-CA-N	2.58	115.21	109.83
1	G	844	TPO	C-CA-N	2.76	115.61	109.83
1	H	844	TPO	C-CA-N	2.77	115.62	109.83
1	E	844	TPO	C-CA-N	2.78	115.64	109.83
1	C	844	TPO	C-CA-N	2.79	115.66	109.83
1	J	844	TPO	C-CA-N	2.83	115.74	109.83
1	F	844	TPO	C-CA-N	2.83	115.74	109.83
1	M	844	TPO	C-CA-N	2.83	115.75	109.83
1	L	844	TPO	C-CA-N	2.83	115.75	109.83
1	N	844	TPO	C-CA-N	2.85	115.79	109.83
1	D	844	TPO	C-CA-N	2.87	115.82	109.83
1	A	844	TPO	C-CA-N	2.87	115.84	109.83
1	K	844	TPO	C-CA-N	2.91	115.91	109.83
1	I	844	TPO	C-CA-N	2.92	115.93	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	840	SEP	OG-CB-CA	3.25	111.05	108.27
1	M	840	SEP	OG-CB-CA	3.35	111.13	108.27
1	F	840	SEP	OG-CB-CA	3.37	111.15	108.27
1	L	840	SEP	OG-CB-CA	3.50	111.26	108.27
1	G	840	SEP	OG-CB-CA	3.53	111.28	108.27
1	I	840	SEP	OG-CB-CA	3.57	111.32	108.27
1	N	840	SEP	OG-CB-CA	3.57	111.32	108.27
1	C	840	SEP	OG-CB-CA	3.62	111.36	108.27
1	B	840	SEP	OG-CB-CA	3.66	111.39	108.27
1	J	840	SEP	OG-CB-CA	3.66	111.40	108.27
1	A	840	SEP	OG-CB-CA	3.67	111.40	108.27
1	E	840	SEP	OG-CB-CA	3.68	111.41	108.27
1	K	840	SEP	OG-CB-CA	3.82	111.53	108.27
1	D	840	SEP	OG-CB-CA	4.03	111.71	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	840	SEP	3	0
1	G	840	SEP	1	0
1	H	840	SEP	3	0
1	K	841	SEP	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	APJ	A	1999	-	26,29,29	1.90	5 (19%)	29,41,41	2.67	12 (41%)
2	APJ	B	1999	-	26,29,29	1.82	6 (23%)	29,41,41	2.63	11 (37%)
2	APJ	C	1999	-	26,29,29	1.80	5 (19%)	29,41,41	2.73	12 (41%)
2	APJ	D	1999	-	26,29,29	1.80	6 (23%)	29,41,41	2.68	12 (41%)
2	APJ	E	1999	-	26,29,29	1.77	5 (19%)	29,41,41	2.63	11 (37%)
2	APJ	F	1999	-	26,29,29	1.78	6 (23%)	29,41,41	2.64	13 (44%)
2	APJ	G	1999	-	26,29,29	1.86	6 (23%)	29,41,41	2.62	11 (37%)
2	APJ	H	1999	-	26,29,29	1.80	5 (19%)	29,41,41	2.63	11 (37%)
2	APJ	I	1999	-	26,29,29	1.83	6 (23%)	29,41,41	2.65	11 (37%)
2	APJ	J	1999	-	26,29,29	1.84	5 (19%)	29,41,41	2.64	11 (37%)
2	APJ	K	1999	-	26,29,29	1.82	4 (15%)	29,41,41	2.63	12 (41%)
2	APJ	L	1999	-	26,29,29	1.81	5 (19%)	29,41,41	2.66	12 (41%)
2	APJ	M	1999	-	26,29,29	1.82	6 (23%)	29,41,41	2.66	12 (41%)
2	APJ	N	1999	-	26,29,29	1.78	6 (23%)	29,41,41	2.64	12 (41%)

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
2	APJ	A	1999	-	-	0/10/14/14	0/4/5/5
2	APJ	B	1999	-	-	0/10/14/14	0/4/5/5
2	APJ	C	1999	-	-	0/10/14/14	0/4/5/5
2	APJ	D	1999	-	-	0/10/14/14	0/4/5/5
2	APJ	E	1999	-	-	0/10/14/14	0/4/5/5
2	APJ	F	1999	-	-	0/10/14/14	0/4/5/5
2	APJ	G	1999	-	-	0/10/14/14	0/4/5/5
2	APJ	H	1999	-	-	0/10/14/14	0/4/5/5
2	APJ	I	1999	-	-	0/10/14/14	0/4/5/5
2	APJ	J	1999	-	-	0/10/14/14	0/4/5/5
2	APJ	K	1999	-	-	0/10/14/14	0/4/5/5
2	APJ	L	1999	-	-	0/10/14/14	0/4/5/5
2	APJ	M	1999	-	-	0/10/14/14	0/4/5/5
2	APJ	N	1999	-	-	0/10/14/14	0/4/5/5

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1999	APJ	N4-N5	-5.64	1.26	1.37
2	C	1999	APJ	N4-N5	-5.56	1.26	1.37
2	G	1999	APJ	N4-N5	-5.56	1.26	1.37
2	D	1999	APJ	N4-N5	-5.48	1.26	1.37
2	H	1999	APJ	N4-N5	-5.48	1.26	1.37
2	E	1999	APJ	N4-N5	-5.48	1.26	1.37
2	I	1999	APJ	N4-N5	-5.45	1.26	1.37
2	L	1999	APJ	N4-N5	-5.42	1.26	1.37
2	B	1999	APJ	N4-N5	-5.42	1.26	1.37
2	M	1999	APJ	N4-N5	-5.40	1.26	1.37
2	F	1999	APJ	N4-N5	-5.39	1.26	1.37
2	J	1999	APJ	N4-N5	-5.39	1.26	1.37
2	K	1999	APJ	N4-N5	-5.38	1.26	1.37
2	N	1999	APJ	N4-N5	-5.32	1.26	1.37
2	N	1999	APJ	C23-C22	-2.20	1.37	1.41
2	M	1999	APJ	C23-C22	-2.17	1.37	1.41
2	D	1999	APJ	C23-C22	-2.16	1.37	1.41
2	B	1999	APJ	C23-C22	-2.13	1.38	1.41
2	F	1999	APJ	C23-C22	-2.08	1.38	1.41
2	E	1999	APJ	C23-C22	-2.05	1.38	1.41
2	I	1999	APJ	C23-C22	-2.03	1.38	1.41
2	G	1999	APJ	C23-C22	-2.01	1.38	1.41
2	H	1999	APJ	C10-N3	2.17	1.42	1.38
2	G	1999	APJ	C10-N3	2.17	1.42	1.38
2	F	1999	APJ	C10-N3	2.19	1.42	1.38
2	B	1999	APJ	C10-N3	2.24	1.42	1.38
2	M	1999	APJ	C10-N3	2.24	1.42	1.38
2	L	1999	APJ	C10-N3	2.26	1.42	1.38
2	I	1999	APJ	C10-N3	2.28	1.42	1.38
2	C	1999	APJ	C10-N3	2.31	1.42	1.38
2	J	1999	APJ	C10-N3	2.34	1.42	1.38
2	N	1999	APJ	C9-N6	2.36	1.40	1.36
2	N	1999	APJ	C10-N3	2.42	1.42	1.38
2	E	1999	APJ	C10-N1	2.43	1.38	1.34
2	A	1999	APJ	C10-N3	2.44	1.43	1.38
2	D	1999	APJ	C9-N6	2.47	1.40	1.36
2	D	1999	APJ	C9-N2	2.50	1.37	1.34
2	D	1999	APJ	C10-N3	2.54	1.43	1.38
2	G	1999	APJ	C10-N1	2.57	1.39	1.34
2	K	1999	APJ	C10-N1	2.57	1.39	1.34
2	H	1999	APJ	C10-N1	2.60	1.39	1.34
2	C	1999	APJ	C10-N1	2.61	1.39	1.34
2	F	1999	APJ	C9-N6	2.61	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1999	APJ	C10-N1	2.62	1.39	1.34
2	H	1999	APJ	C9-N2	2.65	1.38	1.34
2	E	1999	APJ	C9-N2	2.67	1.38	1.34
2	I	1999	APJ	C10-N1	2.71	1.39	1.34
2	F	1999	APJ	C10-N1	2.73	1.39	1.34
2	I	1999	APJ	C9-N2	2.74	1.38	1.34
2	J	1999	APJ	C10-N1	2.75	1.39	1.34
2	L	1999	APJ	C10-N1	2.77	1.39	1.34
2	M	1999	APJ	C10-N1	2.78	1.39	1.34
2	J	1999	APJ	C9-N2	2.79	1.38	1.34
2	N	1999	APJ	C10-N1	2.81	1.39	1.34
2	C	1999	APJ	C9-N6	2.86	1.41	1.36
2	M	1999	APJ	C9-N6	2.86	1.41	1.36
2	F	1999	APJ	C9-N2	2.89	1.38	1.34
2	M	1999	APJ	C9-N2	2.90	1.38	1.34
2	L	1999	APJ	C9-N2	2.90	1.38	1.34
2	B	1999	APJ	C9-N6	2.91	1.41	1.36
2	A	1999	APJ	C9-N6	2.94	1.41	1.36
2	E	1999	APJ	C9-N6	2.96	1.41	1.36
2	B	1999	APJ	C9-N2	2.97	1.38	1.34
2	C	1999	APJ	C9-N2	2.99	1.38	1.34
2	L	1999	APJ	C9-N6	3.00	1.41	1.36
2	D	1999	APJ	C10-N1	3.01	1.40	1.34
2	H	1999	APJ	C9-N6	3.04	1.41	1.36
2	N	1999	APJ	C9-N2	3.06	1.38	1.34
2	I	1999	APJ	C9-N6	3.09	1.41	1.36
2	G	1999	APJ	C9-N2	3.11	1.38	1.34
2	K	1999	APJ	C9-N2	3.14	1.38	1.34
2	A	1999	APJ	C10-N1	3.19	1.40	1.34
2	K	1999	APJ	C9-N6	3.24	1.41	1.36
2	A	1999	APJ	C9-N2	3.29	1.38	1.34
2	J	1999	APJ	C9-N6	3.32	1.42	1.36
2	G	1999	APJ	C9-N6	3.36	1.42	1.36

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	1999	APJ	N2-C9-N1	-6.77	119.46	126.67
2	I	1999	APJ	N2-C9-N1	-6.50	119.74	126.67
2	M	1999	APJ	N2-C9-N1	-6.44	119.81	126.67
2	G	1999	APJ	N2-C9-N1	-6.42	119.82	126.67
2	L	1999	APJ	N2-C9-N1	-6.42	119.83	126.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	1999	APJ	N2-C9-N1	-6.38	119.87	126.67
2	C	1999	APJ	C17-C16-C14	-6.36	113.05	120.09
2	H	1999	APJ	N2-C9-N1	-6.34	119.92	126.67
2	A	1999	APJ	N2-C9-N1	-6.32	119.94	126.67
2	C	1999	APJ	N2-C9-N1	-6.06	120.21	126.67
2	E	1999	APJ	N2-C9-N1	-6.05	120.22	126.67
2	B	1999	APJ	N2-C9-N1	-6.05	120.23	126.67
2	E	1999	APJ	C17-C16-C14	-6.01	113.43	120.09
2	N	1999	APJ	C17-C16-C14	-5.99	113.45	120.09
2	D	1999	APJ	N2-C9-N1	-5.97	120.31	126.67
2	H	1999	APJ	C17-C16-C14	-5.82	113.64	120.09
2	L	1999	APJ	C17-C16-C14	-5.76	113.71	120.09
2	I	1999	APJ	C17-C16-C14	-5.75	113.72	120.09
2	G	1999	APJ	C17-C16-C14	-5.75	113.72	120.09
2	F	1999	APJ	N2-C9-N1	-5.62	120.68	126.67
2	N	1999	APJ	N2-C9-N1	-5.61	120.69	126.67
2	D	1999	APJ	C17-C16-C14	-5.61	113.87	120.09
2	M	1999	APJ	C17-C16-C14	-5.56	113.93	120.09
2	K	1999	APJ	C17-C16-C14	-5.55	113.94	120.09
2	F	1999	APJ	C17-C16-C14	-5.54	113.95	120.09
2	A	1999	APJ	C17-C16-C14	-5.53	113.96	120.09
2	J	1999	APJ	C17-C16-C14	-5.53	113.96	120.09
2	B	1999	APJ	C17-C16-C14	-5.26	114.26	120.09
2	N	1999	APJ	C11-C12-N2	-4.40	118.87	123.90
2	F	1999	APJ	C11-C12-N2	-4.36	118.93	123.90
2	C	1999	APJ	C11-C12-N2	-4.27	119.03	123.90
2	B	1999	APJ	C11-C12-N2	-4.15	119.16	123.90
2	D	1999	APJ	C24-C23-C22	-4.05	116.49	120.88
2	E	1999	APJ	C11-C12-N2	-3.96	119.38	123.90
2	K	1999	APJ	C11-C12-N2	-3.87	119.49	123.90
2	L	1999	APJ	C11-C12-N2	-3.83	119.53	123.90
2	D	1999	APJ	C11-C12-N2	-3.80	119.56	123.90
2	M	1999	APJ	C11-C12-N2	-3.79	119.58	123.90
2	G	1999	APJ	C11-C12-N2	-3.72	119.65	123.90
2	B	1999	APJ	C24-C23-C22	-3.71	116.86	120.88
2	H	1999	APJ	C11-C12-N2	-3.69	119.69	123.90
2	F	1999	APJ	C24-C23-C22	-3.69	116.88	120.88
2	A	1999	APJ	C11-C12-N2	-3.66	119.72	123.90
2	I	1999	APJ	C11-C12-N2	-3.60	119.79	123.90
2	M	1999	APJ	C24-C23-C22	-3.58	116.99	120.88
2	E	1999	APJ	C24-C23-C22	-3.47	117.11	120.88
2	J	1999	APJ	C11-C12-N2	-3.46	119.95	123.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1999	APJ	C24-C23-C22	-3.36	117.23	120.88
2	I	1999	APJ	C24-C23-C22	-3.32	117.28	120.88
2	K	1999	APJ	C24-C23-C22	-3.32	117.28	120.88
2	N	1999	APJ	C24-C23-C22	-3.31	117.29	120.88
2	C	1999	APJ	C24-C23-C22	-3.31	117.29	120.88
2	H	1999	APJ	C24-C23-C22	-3.20	117.41	120.88
2	L	1999	APJ	C24-C23-C22	-3.17	117.44	120.88
2	G	1999	APJ	C24-C23-C22	-3.13	117.48	120.88
2	A	1999	APJ	C18-C17-C16	-3.04	58.91	60.63
2	J	1999	APJ	C24-C23-C22	-2.95	117.68	120.88
2	J	1999	APJ	C15-C13-N4	-2.86	106.51	110.55
2	I	1999	APJ	C15-C13-N4	-2.77	106.64	110.55
2	M	1999	APJ	C15-C13-N4	-2.75	106.67	110.55
2	A	1999	APJ	C15-C13-N4	-2.74	106.69	110.55
2	E	1999	APJ	C15-C13-N4	-2.72	106.71	110.55
2	G	1999	APJ	C18-C17-C16	-2.71	59.10	60.63
2	C	1999	APJ	C18-C17-C16	-2.71	59.10	60.63
2	F	1999	APJ	C18-C17-C16	-2.70	59.10	60.63
2	N	1999	APJ	C18-C17-C16	-2.69	59.11	60.63
2	H	1999	APJ	C15-C13-N4	-2.68	106.77	110.55
2	L	1999	APJ	C18-C17-C16	-2.67	59.12	60.63
2	C	1999	APJ	C15-C13-N4	-2.66	106.79	110.55
2	D	1999	APJ	C18-C17-C16	-2.66	59.13	60.63
2	I	1999	APJ	C18-C17-C16	-2.65	59.13	60.63
2	E	1999	APJ	C18-C17-C16	-2.64	59.14	60.63
2	G	1999	APJ	C15-C13-N4	-2.64	106.83	110.55
2	K	1999	APJ	C18-C17-C16	-2.63	59.14	60.63
2	B	1999	APJ	C18-C17-C16	-2.63	59.14	60.63
2	H	1999	APJ	C18-C17-C16	-2.62	59.15	60.63
2	D	1999	APJ	C19-C20-C21	-2.61	116.51	120.42
2	M	1999	APJ	C18-C17-C16	-2.60	59.16	60.63
2	L	1999	APJ	C15-C13-N4	-2.59	106.89	110.55
2	A	1999	APJ	C15-C14-C16	-2.58	125.39	129.21
2	F	1999	APJ	C15-C14-C16	-2.57	125.40	129.21
2	J	1999	APJ	C18-C17-C16	-2.57	59.18	60.63
2	D	1999	APJ	C15-C14-C16	-2.53	125.47	129.21
2	K	1999	APJ	C15-C13-N4	-2.51	107.00	110.55
2	B	1999	APJ	C15-C14-C16	-2.50	125.51	129.21
2	N	1999	APJ	C15-C13-N4	-2.48	107.05	110.55
2	C	1999	APJ	C15-C14-C16	-2.47	125.55	129.21
2	B	1999	APJ	C15-C13-N4	-2.44	107.11	110.55
2	F	1999	APJ	C15-C13-N4	-2.42	107.13	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	1999	APJ	C19-C20-C21	-2.39	116.83	120.42
2	L	1999	APJ	C15-C14-C16	-2.38	125.69	129.21
2	D	1999	APJ	C15-C13-N4	-2.36	107.22	110.55
2	F	1999	APJ	C19-C20-C21	-2.35	116.89	120.42
2	C	1999	APJ	C19-C20-C21	-2.33	116.93	120.42
2	A	1999	APJ	C19-C20-C21	-2.31	116.96	120.42
2	N	1999	APJ	C15-C14-C16	-2.29	125.82	129.21
2	H	1999	APJ	C15-C14-C16	-2.28	125.84	129.21
2	I	1999	APJ	C15-C14-C16	-2.28	125.84	129.21
2	E	1999	APJ	C15-C14-C16	-2.24	125.90	129.21
2	G	1999	APJ	C15-C14-C16	-2.23	125.91	129.21
2	M	1999	APJ	C19-C20-C21	-2.21	117.10	120.42
2	M	1999	APJ	C15-C14-C16	-2.20	125.95	129.21
2	K	1999	APJ	C15-C14-C16	-2.20	125.95	129.21
2	F	1999	APJ	C13-C15-C14	-2.15	104.24	106.19
2	J	1999	APJ	C15-C14-C16	-2.12	126.08	129.21
2	B	1999	APJ	C19-C20-C21	-2.05	117.34	120.42
2	K	1999	APJ	C19-C20-C21	-2.05	117.34	120.42
2	L	1999	APJ	C19-C20-C21	-2.04	117.36	120.42
2	E	1999	APJ	C19-C20-C21	-2.03	117.37	120.42
2	K	1999	APJ	C17-C18-C16	2.05	61.79	60.63
2	G	1999	APJ	C17-C18-C16	2.05	61.79	60.63
2	L	1999	APJ	C17-C18-C16	2.06	61.80	60.63
2	M	1999	APJ	C17-C18-C16	2.06	61.80	60.63
2	D	1999	APJ	C17-C18-C16	2.07	61.80	60.63
2	H	1999	APJ	C17-C18-C16	2.09	61.81	60.63
2	I	1999	APJ	C17-C18-C16	2.10	61.82	60.63
2	C	1999	APJ	C17-C18-C16	2.11	61.82	60.63
2	J	1999	APJ	C17-C18-C16	2.16	61.85	60.63
2	A	1999	APJ	C17-C18-C16	2.16	61.85	60.63
2	F	1999	APJ	C17-C18-C16	2.17	61.86	60.63
2	N	1999	APJ	N6-C9-N1	2.27	123.82	116.91
2	N	1999	APJ	C17-C18-C16	2.29	61.93	60.63
2	D	1999	APJ	N6-C9-N1	2.32	123.97	116.91
2	F	1999	APJ	N6-C9-N1	2.34	124.04	116.91
2	C	1999	APJ	N6-C9-N1	2.37	124.12	116.91
2	B	1999	APJ	N6-C9-N1	2.40	124.20	116.91
2	A	1999	APJ	N6-C9-N1	2.41	124.25	116.91
2	E	1999	APJ	N6-C9-N1	2.43	124.30	116.91
2	L	1999	APJ	N6-C9-N1	2.44	124.33	116.91
2	M	1999	APJ	N6-C9-N1	2.46	124.39	116.91
2	G	1999	APJ	N6-C9-N1	2.49	124.48	116.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1999	APJ	N6-C9-N1	2.50	124.52	116.91
2	K	1999	APJ	N6-C9-N1	2.51	124.55	116.91
2	J	1999	APJ	N6-C9-N1	2.52	124.59	116.91
2	I	1999	APJ	N6-C9-N1	2.54	124.62	116.91
2	F	1999	APJ	C16-C14-N5	3.38	125.76	120.24
2	N	1999	APJ	C16-C14-N5	3.39	125.78	120.24
2	E	1999	APJ	C16-C14-N5	3.43	125.84	120.24
2	M	1999	APJ	C16-C14-N5	3.52	125.99	120.24
2	K	1999	APJ	C16-C14-N5	3.52	125.99	120.24
2	G	1999	APJ	C16-C14-N5	3.53	126.01	120.24
2	L	1999	APJ	C16-C14-N5	3.55	126.04	120.24
2	J	1999	APJ	C16-C14-N5	3.58	126.09	120.24
2	I	1999	APJ	C16-C14-N5	3.62	126.16	120.24
2	H	1999	APJ	C16-C14-N5	3.63	126.17	120.24
2	A	1999	APJ	C16-C14-N5	3.63	126.17	120.24
2	B	1999	APJ	C16-C14-N5	3.66	126.22	120.24
2	C	1999	APJ	C16-C14-N5	3.68	126.24	120.24
2	D	1999	APJ	C16-C14-N5	3.75	126.36	120.24
2	G	1999	APJ	C12-N2-C9	6.01	120.71	115.49
2	E	1999	APJ	C12-N2-C9	6.04	120.74	115.49
2	H	1999	APJ	C12-N2-C9	6.07	120.76	115.49
2	I	1999	APJ	C12-N2-C9	6.11	120.80	115.49
2	A	1999	APJ	C12-N2-C9	6.23	120.90	115.49
2	J	1999	APJ	C12-N2-C9	6.23	120.91	115.49
2	K	1999	APJ	C12-N2-C9	6.24	120.91	115.49
2	B	1999	APJ	C12-N2-C9	6.34	121.00	115.49
2	M	1999	APJ	C12-N2-C9	6.35	121.01	115.49
2	N	1999	APJ	C12-N2-C9	6.36	121.01	115.49
2	D	1999	APJ	C12-N2-C9	6.38	121.03	115.49
2	F	1999	APJ	C12-N2-C9	6.42	121.07	115.49
2	L	1999	APJ	C12-N2-C9	6.46	121.10	115.49
2	C	1999	APJ	C12-N2-C9	6.47	121.11	115.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 101 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1999	APJ	7	0
2	B	1999	APJ	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1999	APJ	7	0
2	D	1999	APJ	8	0
2	E	1999	APJ	7	0
2	F	1999	APJ	7	0
2	G	1999	APJ	7	0
2	H	1999	APJ	7	0
2	I	1999	APJ	7	0
2	J	1999	APJ	7	0
2	K	1999	APJ	8	0
2	L	1999	APJ	7	0
2	M	1999	APJ	7	0
2	N	1999	APJ	7	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	415/448 (92%)	-0.14	6 (1%) 78 65	53, 111, 203, 287	0
1	B	415/448 (92%)	-0.15	3 (0%) 89 83	53, 108, 202, 287	0
1	C	415/448 (92%)	-0.17	5 (1%) 81 69	41, 102, 208, 268	0
1	D	422/448 (94%)	-0.25	2 (0%) 91 87	44, 99, 190, 261	0
1	E	415/448 (92%)	-0.17	8 (1%) 70 55	70, 119, 208, 308	0
1	F	415/448 (92%)	-0.17	4 (0%) 84 75	65, 107, 200, 259	0
1	G	415/448 (92%)	0.22	23 (5%) 29 16	99, 161, 256, 323	0
1	H	415/448 (92%)	0.19	17 (4%) 41 27	109, 166, 248, 312	0
1	I	413/448 (92%)	0.22	24 (5%) 26 15	123, 185, 259, 322	0
1	J	413/448 (92%)	0.72	66 (15%) 3 2	145, 210, 301, 366	0
1	K	422/448 (94%)	0.12	10 (2%) 62 47	108, 173, 258, 302	0
1	L	415/448 (92%)	0.31	21 (5%) 32 18	122, 177, 242, 319	0
1	M	415/448 (92%)	-0.08	7 (1%) 73 60	74, 123, 209, 271	0
1	N	415/448 (92%)	-0.13	4 (0%) 84 75	70, 106, 198, 296	0
All	All	5820/6272 (92%)	0.04	200 (3%) 49 34	41, 141, 246, 366	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	864	SER	12.6
1	L	863	GLU	8.9
1	N	893	THR	7.7
1	N	864	SER	6.0
1	F	864	SER	5.9
1	F	863	GLU	5.5
1	J	772	TYR	5.2
1	I	742	TYR	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	1039	ARG	4.9
1	B	850	SER	4.9
1	N	863	GLU	4.8
1	L	835	LEU	4.6
1	J	689	VAL	4.5
1	G	850	SER	4.4
1	J	752	LEU	4.3
1	J	742	TYR	4.3
1	I	1003	ASP	4.2
1	J	740	PHE	4.2
1	J	895	ARG	4.1
1	J	677	GLU	4.1
1	J	709	CYS	4.1
1	G	736	THR	4.1
1	J	673	LEU	4.1
1	J	704	MET	4.0
1	I	736	THR	4.0
1	J	701	VAL	4.0
1	J	847	ASN	4.0
1	J	703	ARG	4.0
1	G	1043	TYR	3.9
1	A	864	SER	3.9
1	J	1036	ASN	3.9
1	J	690	PHE	3.9
1	J	1040	TYR	3.8
1	G	740	PHE	3.8
1	J	1043	TYR	3.8
1	H	863	GLU	3.7
1	G	1035	ASP	3.7
1	J	732	TYR	3.7
1	E	864	SER	3.7
1	J	1073	MET	3.7
1	K	1040	TYR	3.7
1	J	743	ILE	3.7
1	J	733	CYS	3.7
1	J	931	ILE	3.7
1	J	675	VAL	3.6
1	G	851	GLY	3.6
1	H	671	LYS	3.6
1	G	893	THR	3.6
1	G	856	ARG	3.5
1	E	671	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	742	TYR	3.5
1	J	731	TYR	3.5
1	J	738	ASP	3.5
1	I	864	SER	3.4
1	G	864	SER	3.4
1	I	1008	LEU	3.4
1	H	855	TRP	3.4
1	G	853	SER	3.4
1	M	709	CYS	3.3
1	L	842	PHE	3.3
1	J	686	GLY	3.3
1	L	893	THR	3.2
1	J	734	SER	3.2
1	L	760	ASN	3.2
1	J	843	ARG	3.1
1	H	1040	TYR	3.1
1	J	938	LEU	3.1
1	A	850	SER	3.1
1	C	851	GLY	3.1
1	J	1037	LEU	3.1
1	F	893	THR	3.0
1	H	864	SER	3.0
1	C	763	ASP	3.0
1	J	682	TYR	3.0
1	J	853	SER	3.0
1	J	705	LEU	3.0
1	L	1012	PHE	3.0
1	E	847	ASN	2.9
1	E	863	GLU	2.9
1	A	742	TYR	2.9
1	J	760	ASN	2.9
1	C	864	SER	2.9
1	B	742	TYR	2.9
1	L	794	ILE	2.9
1	G	741	LEU	2.9
1	J	859	GLU	2.9
1	L	902	ASP	2.9
1	L	729	ILE	2.8
1	J	849	PRO	2.8
1	J	1041	ARG	2.8
1	J	674	VAL	2.8
1	J	856	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	764	GLU	2.8
1	J	729	ILE	2.7
1	L	765	ASN	2.7
1	J	894	LYS	2.7
1	E	850	SER	2.7
1	G	670	LEU	2.7
1	J	1113	LEU	2.7
1	M	1040	TYR	2.6
1	J	1067	GLU	2.6
1	H	1058	LYS	2.6
1	H	1033	PHE	2.6
1	G	1040	TYR	2.6
1	K	1013	ASP	2.6
1	J	964	ASP	2.6
1	J	767	LYS	2.6
1	D	738	ASP	2.5
1	J	702	LYS	2.5
1	K	1033	PHE	2.5
1	L	763	ASP	2.5
1	L	761	VAL	2.5
1	G	843	ARG	2.5
1	J	711	ILE	2.5
1	H	742	TYR	2.5
1	J	1033	PHE	2.5
1	G	963	HIS	2.5
1	K	742	TYR	2.5
1	J	685	SER	2.5
1	G	733	CYS	2.5
1	E	893	THR	2.5
1	J	771	GLU	2.5
1	K	1012	PHE	2.5
1	J	715	GLU	2.5
1	L	858	PRO	2.4
1	I	961	ILE	2.4
1	L	702	LYS	2.4
1	I	1012	PHE	2.4
1	K	1047	LYS	2.4
1	G	817	THR	2.4
1	G	1036	ASN	2.4
1	I	843	ARG	2.4
1	K	794	ILE	2.4
1	G	737	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	732	TYR	2.3
1	L	793	ILE	2.3
1	H	847	ASN	2.3
1	L	852	THR	2.3
1	M	895	ARG	2.3
1	J	1072	LEU	2.3
1	H	702	LYS	2.3
1	E	849	PRO	2.3
1	J	1039	ARG	2.3
1	K	895	ARG	2.3
1	I	809	SER	2.3
1	I	836	ASP	2.3
1	D	1012	PHE	2.3
1	L	682	TYR	2.3
1	E	672	ASN	2.3
1	A	853	SER	2.3
1	H	794	ILE	2.3
1	H	809	SER	2.3
1	K	1091	LEU	2.2
1	J	1038	GLU	2.2
1	J	893	THR	2.2
1	C	709	CYS	2.2
1	L	860	LEU	2.2
1	J	1058	LYS	2.2
1	I	743	ILE	2.2
1	H	737	THR	2.2
1	G	895	ARG	2.2
1	I	700	ALA	2.2
1	G	842	PHE	2.2
1	H	682	TYR	2.2
1	M	742	TYR	2.2
1	K	864	SER	2.2
1	I	835	LEU	2.2
1	M	1030	ASP	2.2
1	I	852	THR	2.1
1	H	706	ILE	2.1
1	J	741	LEU	2.1
1	J	854	GLY	2.1
1	A	863	GLU	2.1
1	N	1040	TYR	2.1
1	M	893	THR	2.1
1	I	855	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	671	LYS	2.1
1	I	1019	VAL	2.1
1	J	707	ASP	2.1
1	H	673	LEU	2.1
1	I	731	TYR	2.1
1	J	803	ILE	2.1
1	I	921	PHE	2.1
1	J	848	ASN	2.1
1	A	670	LEU	2.1
1	I	833	LYS	2.1
1	J	700	ALA	2.1
1	I	707	ASP	2.1
1	J	836	ASP	2.1
1	I	744	ALA	2.1
1	L	920	PRO	2.1
1	F	1043	TYR	2.0
1	I	925	TYR	2.0
1	H	860	LEU	2.0
1	J	708	PHE	2.0
1	B	851	GLY	2.0
1	J	939	ASP	2.0
1	G	682	TYR	2.0
1	J	747	LEU	2.0
1	I	794	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
1	SEP	C	841	10/11	0.92	0.15	-	90,114,135,145	0
1	SEP	H	840	10/11	0.74	0.21	-	179,184,191,192	0
1	TPO	M	844	11/12	0.86	0.22	-	228,257,285,285	0
1	SEP	K	841	10/11	0.85	0.15	-	148,161,173,180	0
1	SEP	H	841	10/11	0.91	0.13	-	145,157,165,172	0
1	TPO	E	844	11/12	0.79	0.23	-	238,260,293,298	0
1	SEP	I	840	10/11	0.84	0.23	-	216,220,226,226	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	TPO	N	844	11/12	0.76	0.22	-	235,252,274,280	0
1	SEP	F	840	10/11	0.84	0.17	-	138,142,146,152	0
1	TPO	L	844	11/12	0.70	0.44	-	306,329,351,352	0
1	SEP	N	840	10/11	0.85	0.15	-	172,174,179,183	0
1	SEP	L	840	10/11	0.51	0.32	-	244,256,269,270	0
1	TPO	A	844	11/12	0.90	0.17	-	256,286,315,317	0
1	SEP	G	840	10/11	0.84	0.22	-	187,192,200,202	0
1	SEP	E	840	10/11	0.89	0.28	-	184,188,196,198	0
1	SEP	B	841	10/11	0.90	0.17	-	111,133,156,162	0
1	TPO	J	844	11/12	0.70	0.22	-	253,261,280,285	0
1	SEP	J	841	10/11	0.92	0.14	-	175,183,188,193	0
1	TPO	B	844	11/12	0.87	0.23	-	166,194,212,216	0
1	SEP	D	840	10/11	0.91	0.22	-	134,138,146,146	0
1	TPO	F	844	11/12	0.73	0.30	-	232,250,267,271	0
1	SEP	J	840	10/11	0.79	0.25	-	210,217,231,232	0
1	SEP	A	841	10/11	0.85	0.13	-	117,131,144,148	0
1	TPO	K	844	11/12	0.82	0.36	-	261,276,304,315	0
1	SEP	A	840	10/11	0.66	0.28	-	202,208,216,216	0
1	SEP	I	841	10/11	0.92	0.12	-	171,181,192,193	0
1	TPO	C	844	11/12	0.86	0.23	-	199,232,261,263	0
1	TPO	H	844	11/12	0.76	0.24	-	260,273,298,309	0
1	SEP	M	840	10/11	0.83	0.27	-	146,150,158,160	0
1	SEP	B	840	10/11	0.87	0.22	-	147,153,162,164	0
1	TPO	D	844	11/12	0.80	0.20	-	216,242,266,272	0
1	SEP	K	840	10/11	0.80	0.27	-	184,186,190,191	0
1	TPO	G	844	11/12	0.80	0.37	-	280,298,330,346	0
1	TPO	I	844	11/12	0.69	0.47	-	258,270,291,301	0
1	SEP	F	841	10/11	0.91	0.13	-	110,119,130,131	0
1	SEP	G	841	10/11	0.90	0.11	-	141,156,172,175	0
1	SEP	D	841	10/11	0.95	0.12	-	82,92,114,119	0
1	SEP	E	841	10/11	0.92	0.12	-	117,136,158,163	0
1	SEP	N	841	10/11	0.93	0.11	-	120,133,149,152	0
1	SEP	L	841	10/11	0.55	0.23	-	213,235,255,263	0
1	SEP	M	841	10/11	0.94	0.10	-	103,112,132,137	0
1	SEP	C	840	10/11	0.87	0.20	-	151,156,164,164	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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, 95^{th} 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	APJ	K	1999	25/25	0.88	0.40	2.13	135,135,135,135	0
2	APJ	H	1999	25/25	0.81	0.49	2.05	170,170,170,170	0
2	APJ	J	1999	25/25	0.76	0.68	2.00	197,197,197,197	0
2	APJ	C	1999	25/25	0.93	0.26	1.09	66,66,66,66	0
2	APJ	D	1999	25/25	0.92	0.24	1.09	78,78,78,78	0
2	APJ	E	1999	25/25	0.95	0.22	0.74	101,101,101,101	0
2	APJ	G	1999	25/25	0.92	0.30	0.64	145,145,145,145	0
2	APJ	M	1999	25/25	0.92	0.24	0.42	113,113,113,113	0
2	APJ	L	1999	25/25	0.84	0.34	0.34	142,142,142,142	0
2	APJ	I	1999	25/25	0.83	0.29	0.32	171,171,171,171	0
2	APJ	F	1999	25/25	0.93	0.22	0.23	93,93,93,93	0
2	APJ	A	1999	25/25	0.93	0.22	-0.04	93,93,93,93	0
2	APJ	N	1999	25/25	0.94	0.21	-0.10	87,87,87,87	0
2	APJ	B	1999	25/25	0.94	0.21	-0.26	96,96,96,96	0

6.5 Other polymers

There are no such residues in this entry.