



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 05:56 am BST

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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

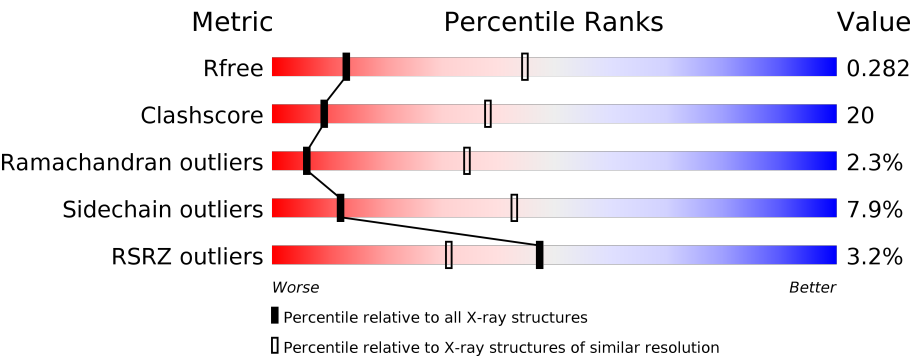
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	448	<div><div>%</div><div><div></div><div>56%</div><div>32%</div><div>• • 7%</div></div></div>
1	B	448	<div><div></div><div>58%</div><div>30%</div><div>5%</div><div>7%</div></div>
1	C	448	<div><div>%</div><div><div></div><div>54%</div><div>34%</div><div>5%</div><div>7%</div></div></div>
1	D	448	<div><div></div><div>55%</div><div>33%</div><div>6%</div><div>5%</div></div>
1	E	448	<div><div>2%</div><div><div></div><div>57%</div><div>31%</div><div>5%</div><div>7%</div></div></div>
1	F	448	<div><div>%</div><div><div></div><div>54%</div><div>33%</div><div>5%</div><div>7%</div></div></div>

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Mol	Chain	Length	Quality of chain
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
1	TPO	I	844	-	-	-	X
1	TPO	L	844	-	-	-	X
2	APJ	J	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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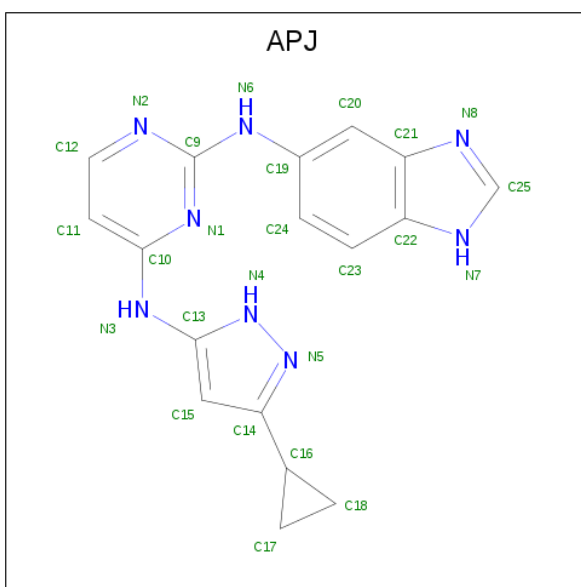
Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	VAL	DELETION	UNP P32361
L	?	-	VAL	DELETION	UNP P32361
L	?	-	SER	DELETION	UNP P32361
L	?	-	SER	DELETION	UNP P32361
L	?	-	ASP	DELETION	UNP P32361
L	?	-	SER	DELETION	UNP P32361
L	?	-	PHE	DELETION	UNP P32361
L	?	-	TYR	DELETION	UNP P32361
L	?	-	ASP	DELETION	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: C₁₇H₁₆N₈).

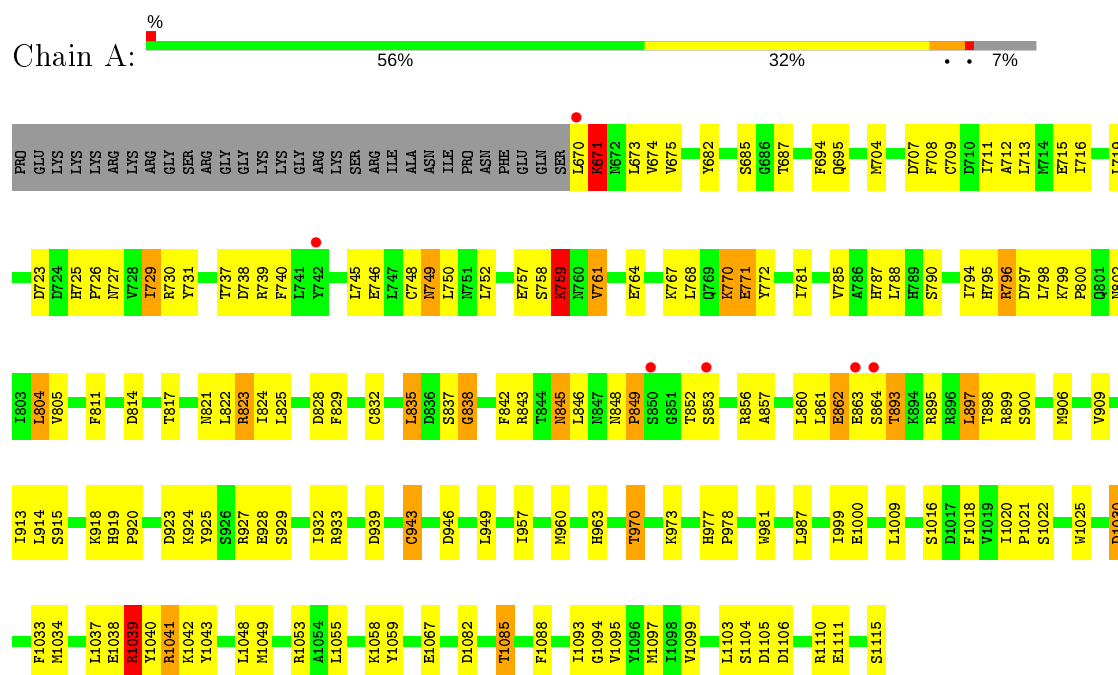


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			25	17	8		
2	B	1	Total	C	N	0	0
			25	17	8		
2	C	1	Total	C	N	0	0
			25	17	8		
2	D	1	Total	C	N	0	0
			25	17	8		
2	E	1	Total	C	N	0	0
			25	17	8		
2	F	1	Total	C	N	0	0
			25	17	8		
2	G	1	Total	C	N	0	0
			25	17	8		
2	H	1	Total	C	N	0	0
			25	17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

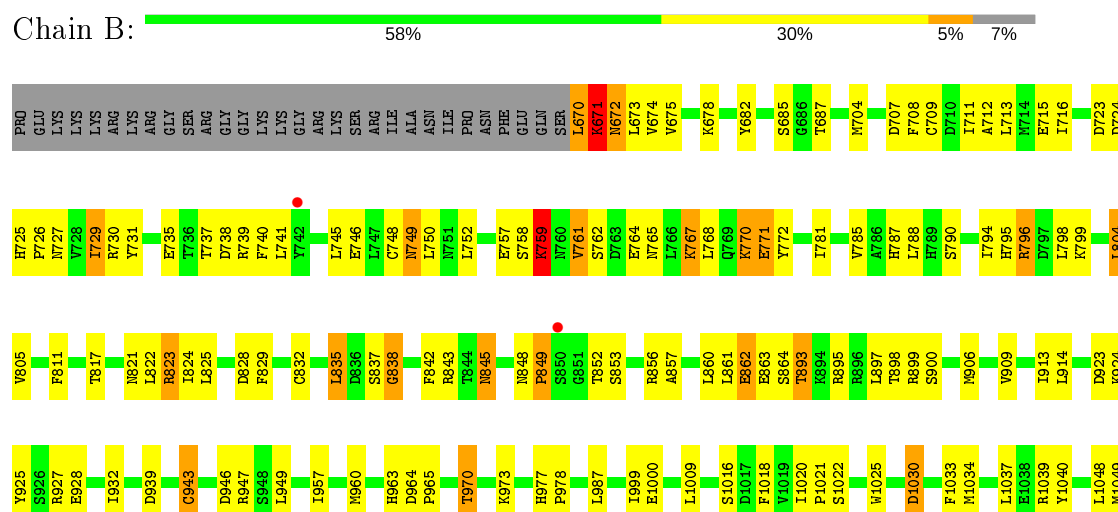
3 Residue-property plots

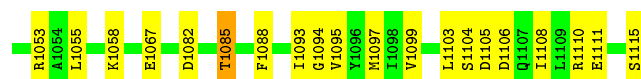
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

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

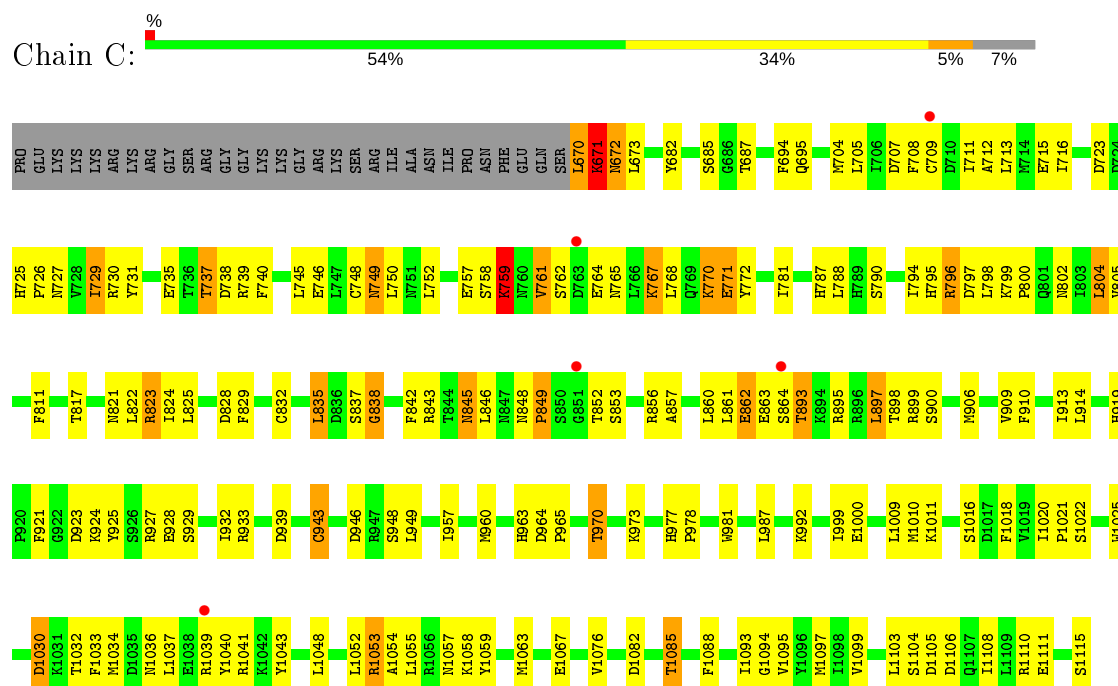


- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

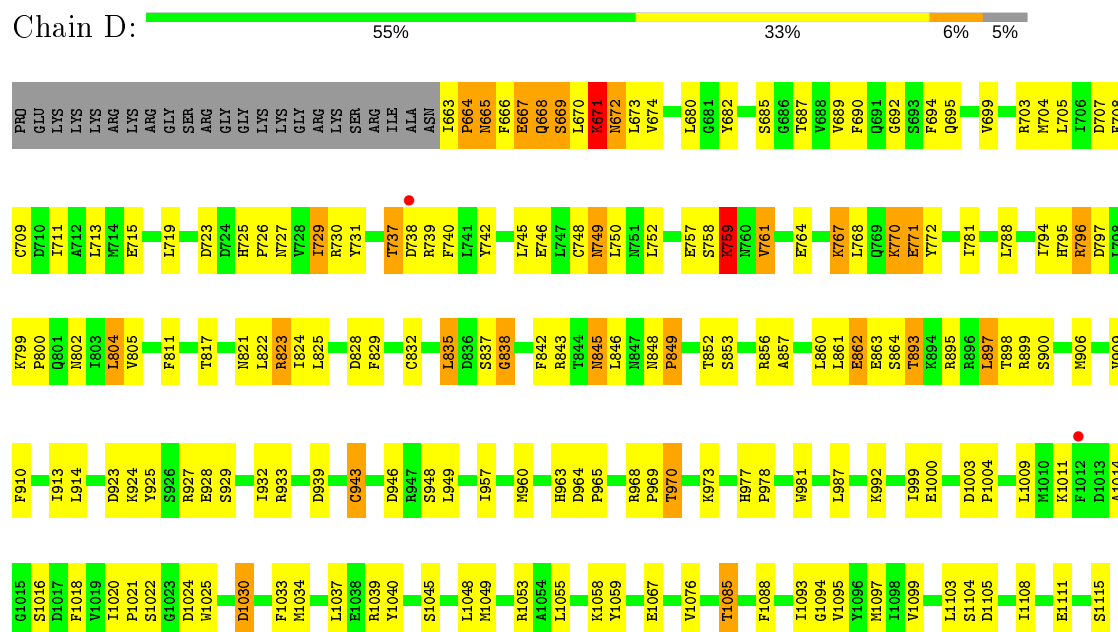




• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

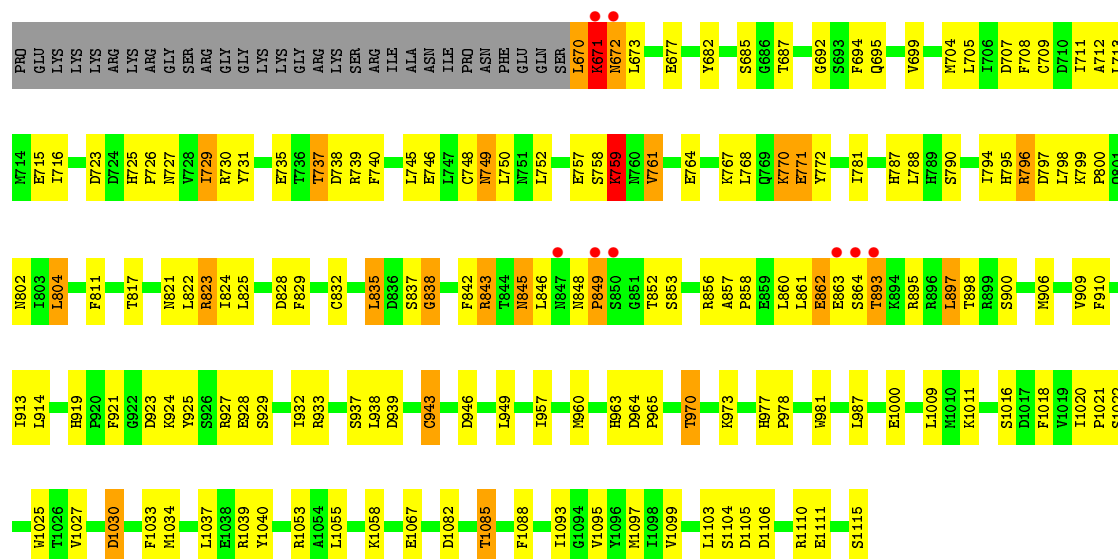


• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

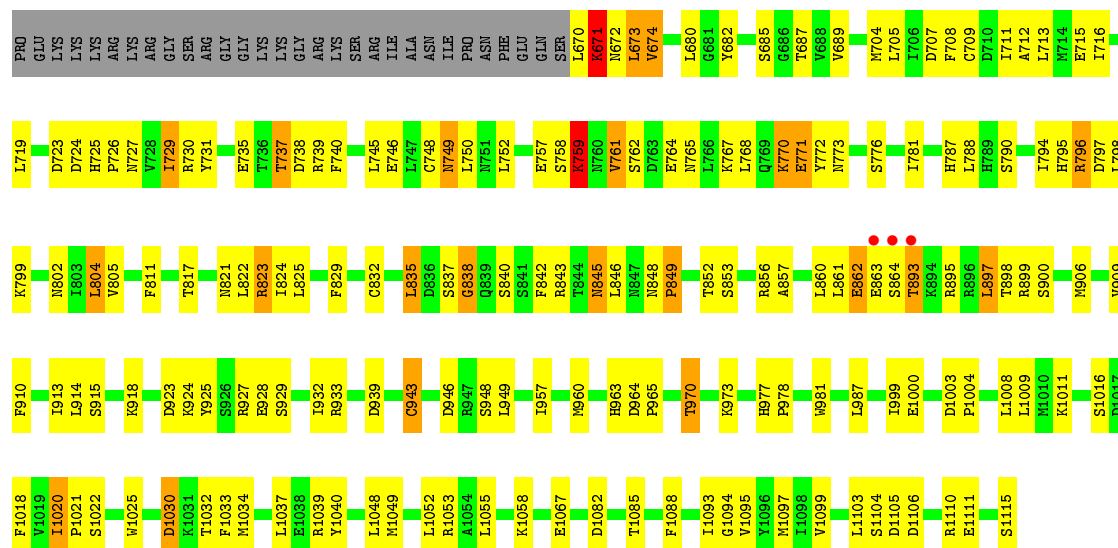


• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

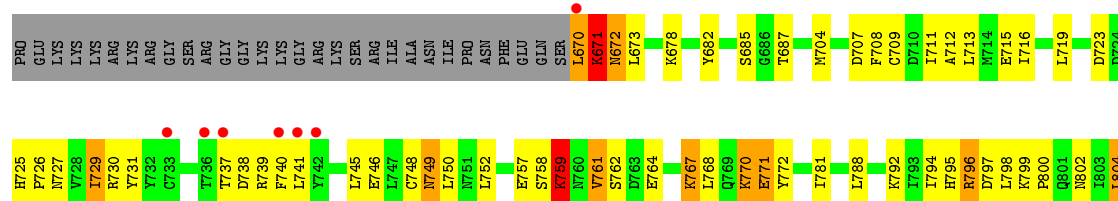


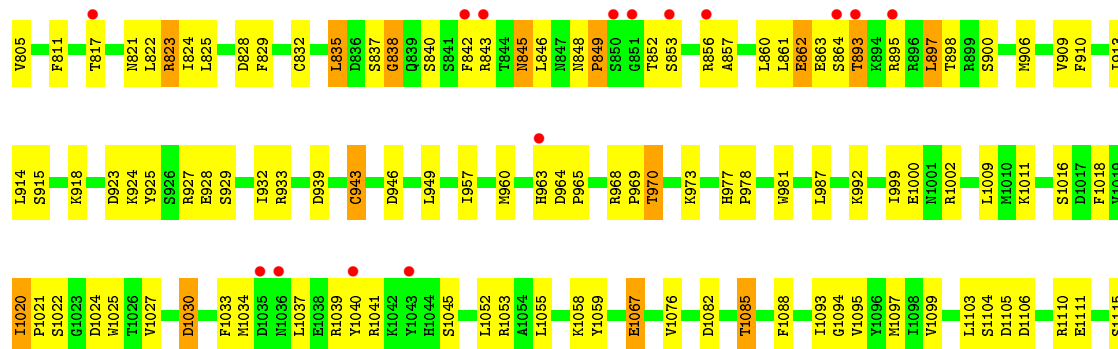


• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

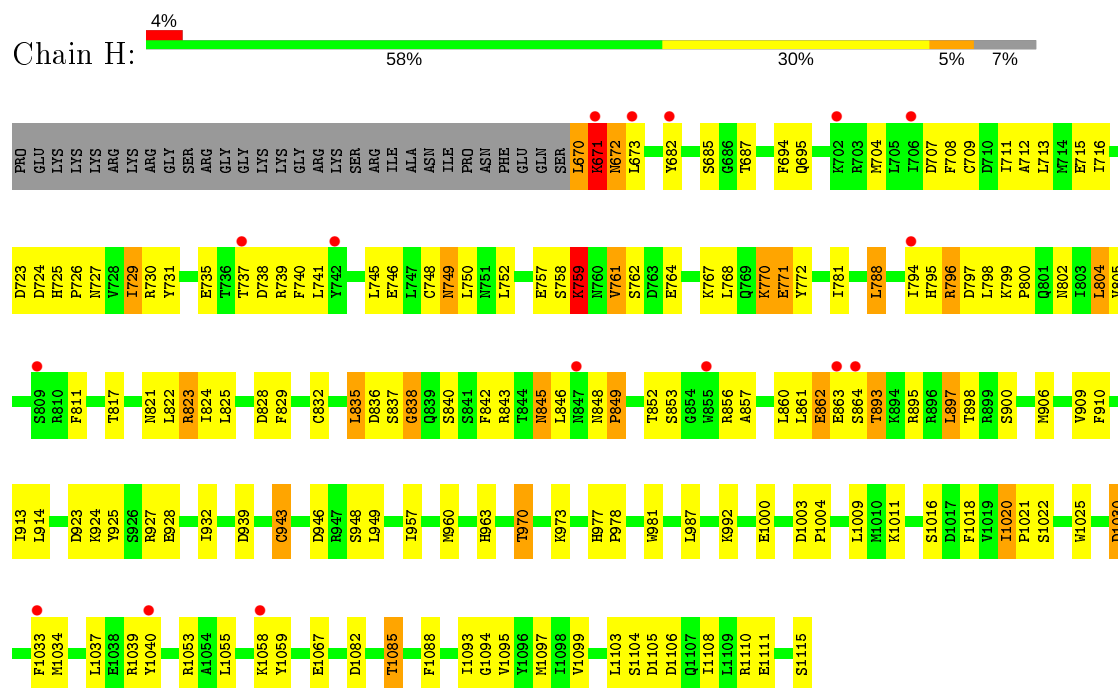


• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

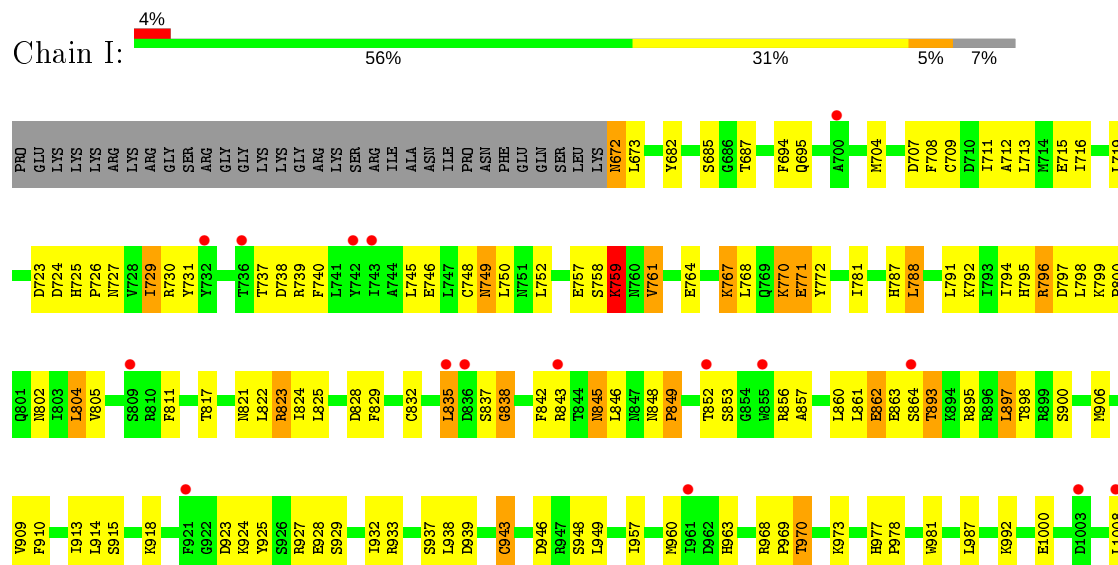


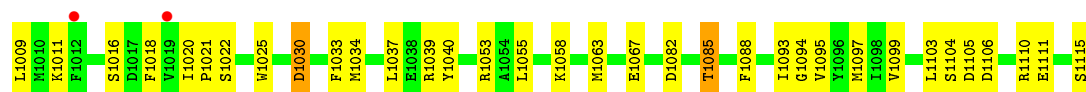


• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

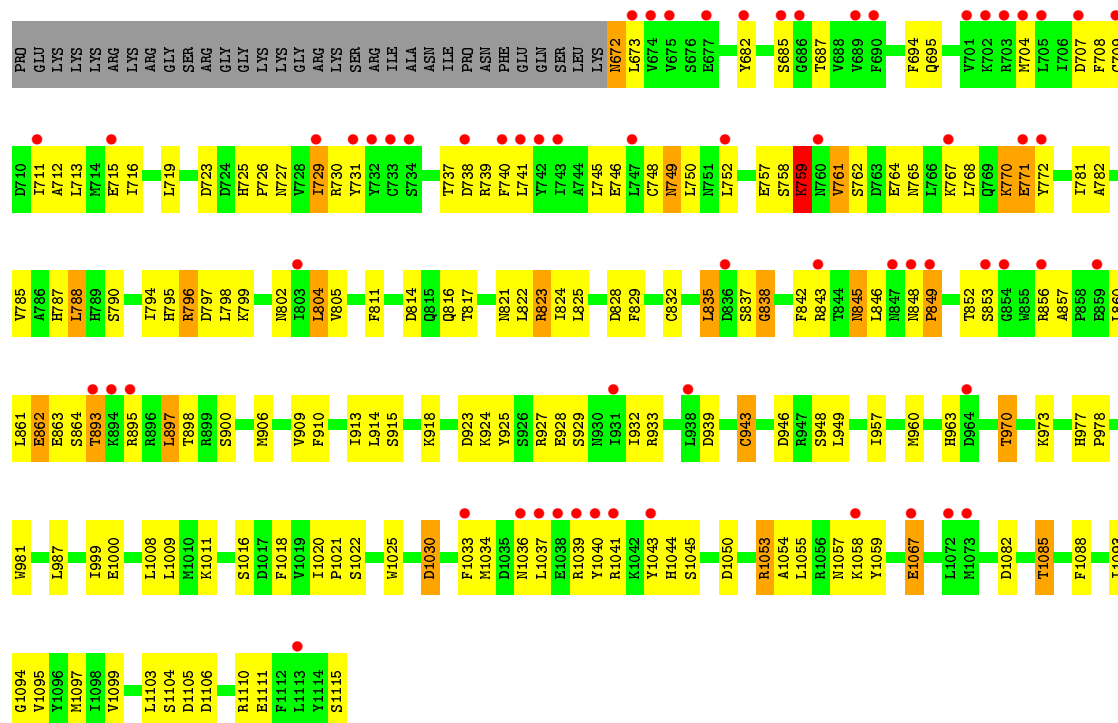


• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

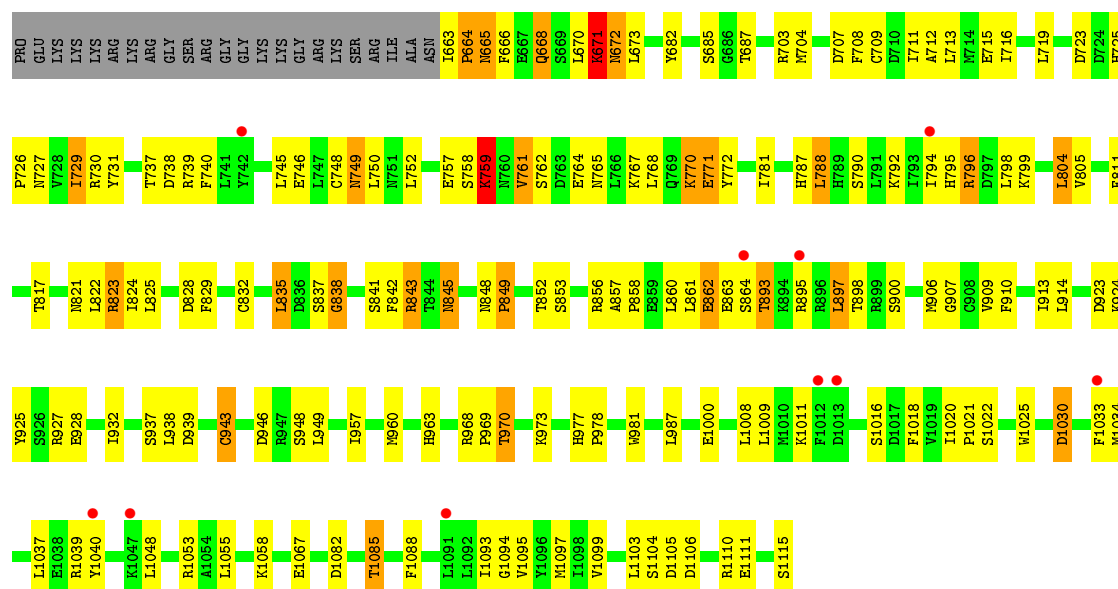




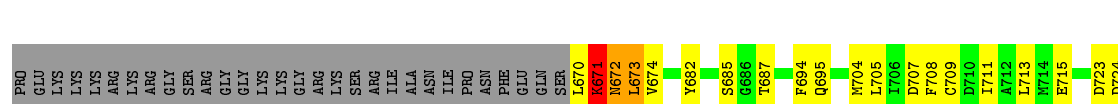
• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1

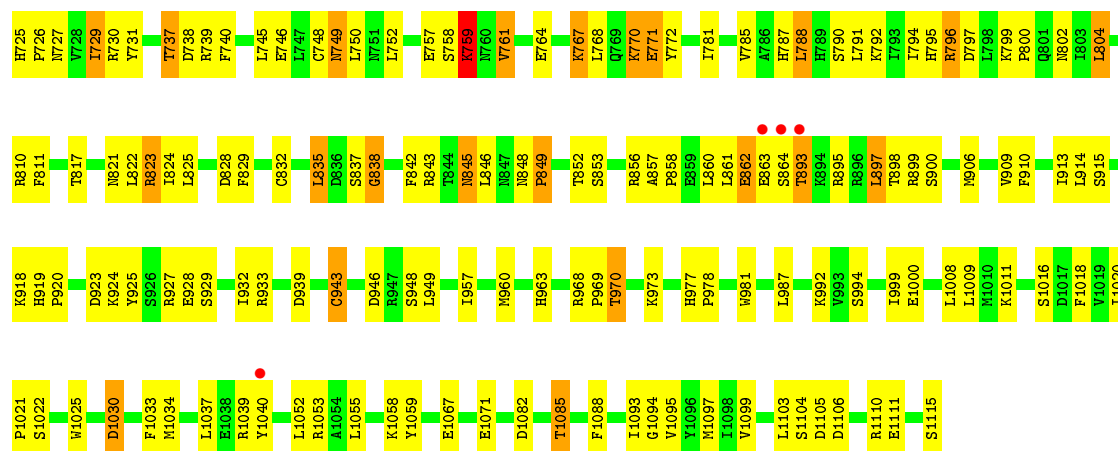


• Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1



Chain L:





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.12Å)	Xtriage
Refinement program	ELVES, PHENIX	Depositor
R, R_{free}	0.235 , 0.283 0.239 , 0.282	Depositor DCC
R_{free} test set	6993 reflections (5.20%)	wwPDB-VP
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 , 81.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.075 for k,h,-l	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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(°)	Ideal(°)
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 ⓘ

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:F:862:GLU:HG3	1:F:863:GLU:H	1.43	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: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: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:668:GLN:CG	1:K:739:ARG:HE	1.91	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:L:715:GLU:HG3	1:L:829:PHE:HB2	1.71	0.73
1:M:715:GLU:HG3	1:M: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:F:730:ARG:HB3	1:F:746:GLU:HG2	1.74	0.70
1:L:848:ASN:HB3	1:L:849:PRO:CA	2.21	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:D:725:HIS:CD2	1:D:727:ASN:H	2.09	0.70
1:M:862:GLU:HG3	1:M:863:GLU:N	2.07	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:D:957:ILE:HA	1:D:960:MET:HE3	1.75	0.69
1:K:862:GLU:HG3	1:K:863:GLU:N	2.08	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:N:862:GLU:HG3	1:N:863:GLU:N	2.08	0.69
1:G:848:ASN:HB3	1:G:849:PRO:CA	2.21	0.69
1:M:795:HIS:HA	1:M:832:CYS:HB3	1.75	0.69
1:B:725:HIS:CD2	1:B:727:ASN:H	2.10	0.69

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

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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:G:957:ILE:HA	1:G:960:MET:HE3	1.77	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: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:C:795:HIS:HA	1:C:832:CYS:HB3	1.78	0.66
1:D:665:ASN:O	1:D:666:PHE:HB2	1.96	0.66
1:A:795:HIS:HA	1:A:832:CYS:HB3	1.78	0.66
1:D:730:ARG:HB3	1:D:746:GLU:HG2	1.77	0.66
1:H:795:HIS:HA	1:H:832:CYS:HB3	1.77	0.66
1:D:666:PHE:HE1	1:D:703:ARG:HD3	1.61	0.66
1:K:848:ASN:HB3	1:K:849:PRO:CA	2.21	0.66
1:B:897:LEU:H	1:B:897:LEU:HD12	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:A:897:LEU:H	1:A: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:F:673:LEU:HD23	1:F:673:LEU:C	2.16	0.65
1:H:725:HIS:CD2	1:H:727:ASN:H	2.14	0.65
1:I:795:HIS:HA	1:I:832:CYS:HB3	1.77	0.65
1:A:673:LEU:O	1:A:673:LEU:HD23	1.95	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:923:ASP:O	1:A:927:ARG:HB2	1.97	0.65
1:E:672:ASN:ND2	1:E:672:ASN:H	1.93	0.65
1:E:897:LEU:H	1:E:897:LEU:HD12	1.61	0.65
1:K:794:ILE:HD11	1:K:835:LEU:HD12	1.78	0.65
1:N:897:LEU:HD12	1:N:897:LEU:H	1.61	0.65
1:F:1020:ILE:HG22	1:F:1022:SER:N	2.11	0.65
1:I:1034:MET:HE2	1:I:1037:LEU:HD23	1.78	0.65
1:C:897:LEU:HD12	1:C:897:LEU:H	1.61	0.65
1:G:923:ASP:O	1:G:927:ARG:HB2	1.96	0.65
1:B:1020:ILE:HG22	1:B:1022:SER:N	2.11	0.65

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:748:CYS:H	2:M:1999:APJ:HN4	1.45	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:748:CYS:H	2:J:1999:APJ:HN4	1.46	0.64
1:J:923:ASP:O	1:J:927:ARG:HB2	1.97	0.64
1:G:795:HIS:HA	1:G:832:CYS:HB3	1.79	0.64
1:E:923:ASP:O	1:E:927:ARG:HB2	1.98	0.63
1:I:897:LEU:H	1:I:897:LEU:HD12	1.64	0.63
1:M:864:SER:HB3	1:M:963:HIS:NE2	2.12	0.63
1:F:897:LEU:HD12	1:F:897:LEU:H	1.63	0.63
1:B:923:ASP:O	1:B:927:ARG:HB2	1.99	0.63
1:C:864:SER:HB3	1:C:963:HIS:NE2	2.13	0.63
1:H:897:LEU:H	1:H:897:LEU:HD12	1.63	0.63
1:K:864:SER:HB3	1:K:963:HIS:NE2	2.12	0.63
1:B:748:CYS:H	2:B:1999:APJ:HN4	1.45	0.63
1:C:992:LYS:HE3	1:D:1059:TYR:OH	1.98	0.63
1:D:1020:ILE:HG22	1:D:1022:SER:N	2.14	0.63
1:D:864:SER:HB3	1:D:963:HIS:NE2	2.13	0.63
1:E:796:ARG:HD3	1:E:832:CYS:HA	1.78	0.63
1:H:923:ASP:O	1:H:927:ARG:HB2	1.97	0.63
1:K:923:ASP:O	1:K:927:ARG:HB2	1.98	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:K:781:ILE:HG22	1:K:906:MET:HE2	1.79	0.63
1:N:1034:MET:HE1	1:N:1037:LEU:HD23	1.81	0.63
1:A:823:ARG:NH2	1:B:724:ASP:OD2	2.32	0.62
1:G:794:ILE:HD11	1:G:835:LEU:HD12	1.81	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:C:794:ILE:HD11	1:C:835:LEU:HD12	1.80	0.62
1:N:848:ASN:HB3	1:N:849:PRO:CA	2.21	0.62
1:J:897:LEU:H	1:J:897:LEU:HD12	1.64	0.62
1:N:923:ASP:O	1:N:927:ARG:HB2	1.99	0.62
1:A:748:CYS:H	2:A:1999:APJ:HN4	1.47	0.62
1:A:771:GLU:HB2	1:A:821:ASN:HD21	1.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:923:ASP:O	1:F:927:ARG:HB2	1.98	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:D:666:PHE:HE1	1:D:703:ARG:CD	2.13	0.61
1:D:897:LEU:HD12	1:D:897:LEU:H	1.65	0.61
1:E:970:THR:HG21	1:G:762:SER:HB2	1.81	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:C:970:THR:HG23	1:C:973:LYS:HB2	1.83	0.61
1:D:771:GLU:HB2	1:D:821:ASN:ND2	2.16	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:K:771:GLU:HB2	1:K:821:ASN:ND2	2.15	0.61
1:M:796:ARG:HD3	1:M:832:CYS:HA	1.81	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: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:K:796:ARG:HD3	1:K:832:CYS:HA	1.83	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:G:771:GLU:HB2	1:G:821:ASN:ND2	2.16	0.60
1:J:796:ARG:HD3	1:J:832:CYS:HA	1.82	0.60
1:L:796:ARG:HD3	1:L:832:CYS:HA	1.81	0.60
1:E:761:VAL:HG21	1:E:764:GLU:HG3	1.83	0.60
1:J:771:GLU:HB2	1:J:821:ASN:ND2	2.17	0.60
1:N:796:ARG:HD3	1:N:832:CYS:HA	1.82	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:A:1038:GLU:O	1:A:1039:ARG:HG3	2.01	0.60
1:J:1043:TYR:OH	1:J:1057:ASN:ND2	2.34	0.60
1:L:771:GLU:HB2	1:L:821:ASN:ND2	2.17	0.60
1:L:970:THR:HG23	1:L:973:LYS:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:970:THR:HG23	1:M:973:LYS:HB2	1.82	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:A:772:TYR:O	1:A:772:TYR:CG	2.54	0.59
1:N:795:HIS:HA	1:N:832:CYS:CB	2.32	0.59
1:B:970:THR:HG23	1:B:973:LYS:HB2	1.83	0.59
1:C:670:LEU:O	1:C:735:GLU:OE2	2.21	0.59
1:K:771:GLU:HB2	1:K:821:ASN:HD21	1.67	0.59
1:K:761:VAL:HG21	1:K:764:GLU:HG3	1.84	0.59
1:F:771:GLU:HB2	1:F:821:ASN:ND2	2.17	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:B:795:HIS:HA	1:B:832:CYS:CB	2.32	0.59
1:E:772:TYR:CG	1:E:772:TYR:O	2.56	0.59
1:M:772:TYR:CG	1:M:772:TYR:O	2.55	0.59
1:C:752:LEU:HD21	1:C:913:ILE:HD11	1.85	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: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:A:761:VAL:HG21	1:A:764:GLU:HG3	1.85	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:C:1037:LEU:HB2	1:C:1058:LYS:NZ	2.18	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:F:970:THR:HG23	1:F:973:LYS:HB2	1.86	0.58
1:A:970:THR:HG23	1:A:973:LYS:HB2	1.86	0.58
1:B:761:VAL:HG21	1:B:764:GLU:HG3	1.85	0.58
1:E:771:GLU:HB2	1:E:821:ASN:HD21	1.67	0.58
1:F:1034:MET:HE2	1:F:1037:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:668:GLN:CD	1:K:739:ARG:HH21	2.05	0.58
1:K:752:LEU:HD21	1:K:913:ILE:HD11	1.85	0.58
1:N:771:GLU:HB2	1:N:821:ASN:ND2	2.18	0.58
1:D:761:VAL:HG21	1:D:764:GLU:HG3	1.86	0.58
1:D:772:TYR:O	1:D:772:TYR:CG	2.56	0.58
1:D:970:THR:HG23	1:D:973:LYS:HB2	1.83	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:N:761:VAL:HG21	1:N:764:GLU:HG3	1.86	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:B:772:TYR:CG	1:B:772:TYR:O	2.56	0.58
1:C:796:ARG:HD3	1:C:832:CYS:HA	1.85	0.58
1:C:977:HIS:CG	1:C:978:PRO:HD2	2.38	0.58
1:D:663:ILE:N	1:D:664:PRO:HD3	2.18	0.58
1:E:781:ILE:HG12	1:E:824:ILE:HG21	1.86	0.58
1:H:761:VAL:HG21	1:H:764:GLU:HG3	1.86	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:C:771:GLU:HB2	1:C:821:ASN:ND2	2.18	0.58
1:C:795:HIS:HA	1:C:832:CYS:CB	2.33	0.58
1:F:761:VAL:HG11	1:H:840:SEP:O2P	2.03	0.58
1:F:771:GLU:HB2	1:F:821:ASN:HD21	1.69	0.58
1:A:977:HIS:CG	1:A:978:PRO:HD2	2.39	0.58
1:G:781:ILE:HG12	1:G:824:ILE:HG21	1.85	0.58
1:G:970:THR:HG23	1:G:973:LYS:HB2	1.84	0.58
1:K:1034:MET:HE2	1:K:1037:LEU:HD23	1.85	0.58
1:L:771:GLU:HB2	1:L:821:ASN:HD21	1.69	0.58
1:B:861:LEU:O	1:B:862:GLU:HB3	2.04	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: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:I:725:HIS:CE1	1:J:816:GLN:HE22	2.22	0.57
1:K:665:ASN:HD22	1:K:665:ASN:N	2.00	0.57
1:L:781:ILE:HG12	1:L:824:ILE:HG21	1.86	0.57
1:M:1002:ARG:HH12	1:M:1041:ARG:CZ	2.17	0.57
1:N:781:ILE:HG12	1:N:824:ILE:HG21	1.86	0.57
1:J:771:GLU:HB2	1:J:821:ASN:HD21	1.69	0.57
1:G:772:TYR:O	1:G:772:TYR:CG	2.57	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:I:781:ILE:HG12	1:I:824:ILE:HG21	1.86	0.57
1:M:752:LEU:HD21	1:M:913:ILE:HD11	1.86	0.57
1:N:772:TYR:O	1:N:772:TYR:CG	2.57	0.57
1:A:1093:ILE:O	1:A:1097:MET:HG3	2.04	0.57
1:F:761:VAL:HG21	1:F:764:GLU:HG3	1.87	0.57
1:G:761:VAL:HG21	1:G:764:GLU:HG3	1.87	0.57
1:M:771:GLU:HB2	1:M:821:ASN:HD21	1.69	0.57
1:N:1034:MET:CE	1:N:1037:LEU:HD23	2.33	0.57
1:D:663:ILE:N	1:D:664:PRO:CD	2.68	0.57
1:B:771:GLU:HB2	1:B:821:ASN:HD21	1.68	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: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:G:1034:MET:HE2	1:G:1037:LEU:HD23	1.86	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:L:761:VAL:HG21	1:L:764:GLU:HG3	1.86	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:I:795:HIS:HA	1:I:832:CYS:CB	2.35	0.57
1:L:772:TYR:CG	1:L:772:TYR:O	2.57	0.57
1:L:795:HIS:HA	1:L:832:CYS:CB	2.34	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:M:781:ILE:HG12	1:M:824:ILE:HG21	1.87	0.57
1:A:1038:GLU:OE2	1:A:1043:TYR:HB2	2.05	0.57
1:H:709:CYS:O	1:H:713:LEU:HD13	2.05	0.57
1:M:1002:ARG:HH12	1:M:1041:ARG:NH2	2.03	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:C:1034:MET:HA	1:C:1034:MET:HE2	1.87	0.56
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:D:861:LEU:O	1:D:862:GLU:HB3	2.06	0.56
1:G:672:ASN:H	1:G:672:ASN:ND2	2.03	0.56
1:H:1034:MET:HE3	1:H:1034:MET:HA	1.87	0.56
1:M:745:LEU:HD12	2:M:1999:APJ:H18A	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:745:LEU:HD12	2:N:1999:APJ:H18A	1.87	0.56
1:N:771:GLU:HB2	1:N:821:ASN:HD21	1.70	0.56
1:A:752:LEU:HD21	1:A:913:ILE:HD11	1.88	0.56
1:J:761:VAL:HG21	1:J:764:GLU:HG3	1.86	0.56
1:M:897:LEU:N	1:M:897:LEU:HD12	2.20	0.56
1:N:737:THR:HG23	1:N:740:PHE:H	1.70	0.56
1:C:673:LEU:HD23	1:C:673:LEU:C	2.26	0.56
1:G:745:LEU:HD12	2:G:1999:APJ:H18A	1.87	0.56
1:I:709:CYS:O	1:I:713:LEU:HD13	2.06	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: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:709:CYS:O	1:G:713:LEU:HD13	2.05	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:D:811:PHE:HB3	1:D:823:ARG:NH1	2.20	0.56
1:E:752:LEU:HD21	1:E:913:ILE:HD11	1.86	0.56
1:G:672:ASN:N	1:G:672:ASN:HD22	2.03	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
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:C:861:LEU:O	1:C:862:GLU:HB3	2.06	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:J:745:LEU:CD1	2:J:1999:APJ:H18A	2.36	0.56
1:L:861:LEU:O	1:L:862:GLU:HB3	2.06	0.56
1:C:1055:LEU:C	1:C:1055:LEU:HD23	2.26	0.56
1:E:897:LEU:HD12	1:E:897:LEU:N	2.21	0.56
1:N:861:LEU:O	1:N:862:GLU:HB3	2.06	0.56
1:A:861:LEU:O	1:A:862:GLU:HB3	2.06	0.55
1:B:745:LEU:HD12	2:B:1999:APJ:H18A	1.87	0.55
1:C:772:TYR:O	1:C:772:TYR:CG	2.58	0.55
1:C:824:ILE:O	1:C:825:LEU:HD23	2.05	0.55
1:E:672:ASN:N	1:E:672:ASN:HD22	2.03	0.55
1:F:781:ILE:HG12	1:F:824:ILE:HG21	1.88	0.55
1:K:781:ILE:HG12	1:K:824:ILE:HG21	1.87	0.55
1:B:749:ASN:OD1	1:B:749:ASN:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1999:APJ:H17	2:D:1999:APJ:N8	2.21	0.55
1:D:781:ILE:HG12	1:D:824:ILE:HG21	1.87	0.55
1:L:745:LEU:HD12	2:L:1999:APJ:H18A	1.88	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:G:771:GLU:HB2	1:G:821:ASN:HD21	1.70	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: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:M:861:LEU:O	1:M:862:GLU:HB3	2.06	0.55
1:D:752:LEU:HD21	1:D:913:ILE:HD11	1.87	0.55
1:K:861:LEU:O	1:K:862:GLU:HB3	2.06	0.55
1:K:843:ARG:NH2	1:M:678:LYS:HD3	2.17	0.55
1:N:709:CYS:O	1:N:713:LEU:HD13	2.06	0.55
1:A:781:ILE:HG22	1:A:906:MET:HE2	1.89	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:D:731:TYR:HA	1:D:745:LEU:HD23	1.89	0.55
1:D:729:ILE:CD1	1:D:745:LEU:HB3	2.37	0.55
1:E:861:LEU:O	1:E:862:GLU:HB3	2.07	0.55
1:G:897:LEU:HD12	1:G:897:LEU:N	2.22	0.55
1:N:745:LEU:CD1	2:N:1999:APJ:H18A	2.36	0.55
1:F:723:ASP:HB2	1:F:730:ARG:HA	1.89	0.55
1:G:752:LEU:HD21	1:G:913:ILE:HD11	1.88	0.55
1:I:861:LEU:O	1:I:862:GLU:HB3	2.06	0.55
1:I:970:THR:HG23	1:I:973:LYS:HB2	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:B:709:CYS:O	1:B:713:LEU:HD13	2.06	0.55
1:D:745:LEU:HD12	2:D:1999:APJ:H18A	1.88	0.55
1:G:1034:MET:HA	1:G:1034:MET:HE3	1.89	0.55
1:H:861:LEU:O	1:H:862:GLU:HB3	2.06	0.55
1:F:781:ILE:HG22	1:F:906:MET:HE2	1.88	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:J:861:LEU:O	1:J:862:GLU:HB3	2.06	0.55
1:K:673:LEU:C	1:K:673:LEU:HD23	2.27	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

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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:D:1055:LEU:C	1:D:1055:LEU:HD23	2.27	0.54
1:K:709:CYS:O	1:K:713:LEU:HD13	2.07	0.54
1:C:749:ASN:N	1:C:749:ASN:OD1	2.40	0.54
1:C:897:LEU:HD12	1:C:897:LEU:N	2.21	0.54
1:F:757:GLU:O	1:F:759:LYS:HE3	2.08	0.54
1:G:729:ILE:CD1	1:G:745:LEU:HB3	2.37	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: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:G:1002:ARG:HH12	1:G:1041:ARG:CZ	2.21	0.54
1:M:749:ASN:N	1:M:749:ASN:OD1	2.41	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:L:745:LEU:CD1	2:L:1999:APJ:H18A	2.38	0.54
1:D:749:ASN:OD1	1:D:749:ASN:N	2.40	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:B:745:LEU:CD1	2:B:1999:APJ:H18A	2.38	0.54
1:D:1111:GLU:O	1:D:1115:SER:HB3	2.08	0.54
1:E:745:LEU:CD1	2:E:1999:APJ:H18A	2.38	0.54
1:B:737:THR:HG23	1:B:740:PHE:H	1.73	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:I:1111:GLU:O	1:I:1115:SER:HB3	2.08	0.54
1:J:1037:LEU:HB2	1:J:1058:LYS:HZ3	1.72	0.54
1:K:672:ASN:ND2	1:K:672:ASN:H	2.06	0.54
1:M:709:CYS:O	1:M:713:LEU:HD13	2.07	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
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:L:749:ASN:OD1	1:L:749:ASN:N	2.41	0.54
1:A:749:ASN:N	1:A:749:ASN:OD1	2.40	0.54
1:I:1034:MET:HA	1:I:1034:MET:HE3	1.89	0.54
1:J:737:THR:HG23	1:J:740:PHE:H	1.73	0.54
1:J:897:LEU:N	1:J:897:LEU:HD12	2.23	0.54
1:K:737:THR:HG23	1:K:740:PHE:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:757:GLU:O	1:M:759:LYS:HE3	2.08	0.54
1:B:1055:LEU:C	1:B:1055:LEU:HD23	2.29	0.53
2:B:1999:APJ:N8	2:B:1999:APJ:H17	2.22	0.53
1:B:671:LYS:O	1:B:671:LYS:HD2	2.08	0.53
1:C:1037:LEU:HD21	1:C:1054:ALA:HB1	1.89	0.53
1:H:757:GLU:O	1:H:759:LYS:HE3	2.08	0.53
1:I:897:LEU:HD12	1:I:897:LEU:N	2.23	0.53
1:J:729:ILE:CD1	1:J:745:LEU:HB3	2.38	0.53
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:D:1093:ILE:O	1:D:1097:MET:HG3	2.08	0.53
1:D:667:GLU:C	1:D:668:GLN:NE2	2.62	0.53
1:E:1093:ILE:O	1:E:1097:MET:HG3	2.08	0.53
1:F:752:LEU:HD21	1:F:913:ILE:HD11	1.90	0.53
1:G:731:TYR:HA	1:G:745:LEU:HD23	1.91	0.53
1:H:897:LEU:N	1:H:897:LEU:HD12	2.23	0.53
1:I:757:GLU:O	1:I:759:LYS:HE3	2.08	0.53
1:J:723:ASP:HB2	1:J:730:ARG:HA	1.89	0.53
1:K:1111:GLU:O	1:K:1115:SER:HB3	2.08	0.53
1:M:745:LEU:CD1	2:M:1999:APJ:H18A	2.38	0.53
1:B:1111:GLU:O	1:B:1115:SER:HB3	2.09	0.53
1:B:909:VAL:O	1:B:913:ILE:HG12	2.08	0.53
1:E:1111:GLU:O	1:E:1115:SER:HB3	2.09	0.53
1:E:672:ASN:N	1:E:672:ASN:ND2	2.56	0.53
1:I:1093:ILE:O	1:I:1097:MET:HG3	2.08	0.53
1:I:787:HIS:CD2	1:J:814:ASP:CG	2.77	0.53
1:M:672:ASN:HD22	1:M:672:ASN:H	1.55	0.53
1:M:723:ASP:HB2	1:M:730:ARG:HA	1.90	0.53
1:N:671:LYS:O	1:N:671:LYS:HD2	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: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:H:737:THR:HG23	1:H:740:PHE:H	1.72	0.53
1:L:757:GLU:O	1:L:759:LYS:HE3	2.08	0.53
1:L:824:ILE:O	1:L:825:LEU:HD23	2.09	0.53
1:N:729:ILE:CD1	1:N:745:LEU:HB3	2.39	0.53
1:B:824:ILE:O	1:B:825:LEU:HD23	2.08	0.53
1:J:1025:TRP:CD1	1:J:1045:SER:O	2.61	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:M:729:ILE:CD1	1:M:745:LEU:HB3	2.38	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:731:TYR:HA	1:N:745:LEU:HD23	1.91	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:G:1093:ILE:O	1:G:1097:MET:HG3	2.09	0.53
1:J:757:GLU:O	1:J:759:LYS:HE3	2.08	0.53
1:N:1111:GLU:O	1:N:1115:SER:HB3	2.08	0.53
1:C:737:THR:HG23	1:C:740:PHE:H	1.74	0.53
1:K:757:GLU:O	1:K:759:LYS:HE3	2.09	0.53
1:D:665:ASN:O	1:D:666:PHE:CB	2.57	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:H:745:LEU:CD1	2:H:1999:APJ:H18A	2.38	0.53
2:L:1999:APJ:N8	2:L:1999:APJ:H17	2.24	0.53
1:A:1016:SER:C	1:A:1018:PHE:H	2.12	0.53
1:D:668:GLN:O	1:D:669:SER:C	2.47	0.53
1:G:757:GLU:O	1:G:759:LYS:HE3	2.08	0.53
1:J:1055:LEU:C	1:J:1055:LEU:HD23	2.30	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:A:757:GLU:O	1:A:759:LYS:HE3	2.08	0.52
1:E:723:ASP:HB2	1:E:730:ARG:HA	1.90	0.52
1:E:909:VAL:O	1:E:913:ILE:HG12	2.09	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:B:1093:ILE:O	1:B:1097:MET:HG3	2.09	0.52
1:C:731:TYR:HA	1:C:745:LEU:HD23	1.91	0.52
1:F:680:LEU:HB2	1:F:689:VAL:HG12	1.91	0.52
1:G:1002:ARG:HH12	1:G:1041:ARG:NH2	2.07	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:M:824:ILE:O	1:M:825:LEU:HD23	2.09	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:E:673:LEU:HD23	1:E:673:LEU:C	2.30	0.52
1:E:737:THR:HG23	1:E:740:PHE:H	1.75	0.52
1:F:824:ILE:O	1:F:825:LEU:HD23	2.10	0.52
1:G:723:ASP:HB2	1:G:730:ARG:HA	1.91	0.52
1:I:749:ASN:N	1:I:749:ASN:OD1	2.41	0.52

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:794:ILE:HG22	1:N:795:HIS:O	2.10	0.52
1:N:752:LEU:HD21	1:N:913:ILE:HD11	1.92	0.52
1:B:731:TYR:HA	1:B:745:LEU:HD23	1.92	0.52
1:F:811:PHE:HB3	1:F:823:ARG:NH1	2.25	0.52
1:G:673:LEU:C	1:G:673:LEU:HD23	2.30	0.52
1:I:723:ASP:HB2	1:I:730:ARG:HA	1.91	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:I:787:HIS:CD2	1:J:814:ASP:OD2	2.57	0.52
1:J:824:ILE:O	1:J:825:LEU:HD23	2.10	0.52
1:J:928:GLU:O	1:J:932:ILE:HG13	2.10	0.52
1:L:1034:MET:HE3	1:L:1034:MET:HA	1.92	0.52
1:L:671:LYS:O	1:L:671:LYS:HD2	2.09	0.52
1:M:671:LYS:HD2	1:M:671:LYS:O	2.09	0.52
1:N:924:LYS:HG3	1:N:925:TYR:CD2	2.45	0.52
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
2:F:1999:APJ:N8	2:F:1999:APJ:H17	2.25	0.51
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
1:K:749:ASN:OD1	1:K:749:ASN:N	2.41	0.51
1:M:731:TYR:HA	1:M:745:LEU:HD23	1.92	0.51
1:A:824:ILE:O	1:A:825:LEU:HD23	2.10	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:L:928:GLU:O	1:L:932:ILE:HG13	2.10	0.51
1:C:794:ILE:N	1:C:794:ILE:HD12	2.25	0.51
1:C:848:ASN:CB	1:C:849:PRO:HA	2.29	0.51
1:C:924:LYS:HG3	1:C:925:TYR:CD2	2.45	0.51
1:D:970:THR:HG23	1:D:973:LYS:CB	2.41	0.51
1:F:1093:ILE:O	1:F:1097:MET:HG3	2.11	0.51
1:F:794:ILE:HG22	1:F:795:HIS:O	2.10	0.51
1:H:824:ILE:O	1:H:825:LEU:HD23	2.10	0.51
1:H:928:GLU:O	1:H:932:ILE:HG13	2.09	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:A:723:ASP:HB2	1:A:730:ARG:HA	1.92	0.51
1:B:758:SER:HB3	1:B:768:LEU:HD21	1.93	0.51
1:D:668:GLN:N	1:D:668:GLN:NE2	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:909:VAL:O	1:J:913:ILE:HG12	2.10	0.51
1:M:1111:GLU:O	1:M:1115:SER:HB3	2.10	0.51
1:A:1034:MET:CE	1:A:1034:MET:HA	2.41	0.51
1:B:861:LEU:O	1:B:862:GLU:CB	2.59	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:M:928:GLU:O	1:M:932:ILE:HG13	2.09	0.51
1:F:1034:MET:HA	1:F:1034:MET:CE	2.41	0.51
2:G:1999:APJ:H17	2:G:1999:APJ:N8	2.26	0.51
1:J:731:TYR:HA	1:J:745:LEU:HD23	1.92	0.51
1:L:909:VAL:O	1:L:913:ILE:HG12	2.10	0.51
1:B:762:SER:HB2	1:M:970:THR:HB	1.93	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
2:E:1999:APJ:H17	2:E:1999:APJ:N8	2.25	0.51
1:F:745:LEU:HD12	2:F:1999:APJ:H18A	1.91	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: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:J:811:PHE:HB3	1:J:823:ARG:NH1	2.26	0.51
1:K:1055:LEU:C	1:K:1055:LEU:HD23	2.31	0.51
1:M:1059:TYR:OH	1:N:992:LYS:HE3	2.11	0.51
1:A:745:LEU:HD12	2:A:1999:APJ:H18A	1.93	0.51
1:A:725:HIS:CG	1:A:726:PRO:HD2	2.46	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:H:1055:LEU:C	1:H:1055:LEU:HD23	2.31	0.51
1:J:1093:ILE:O	1:J:1097:MET:HG3	2.10	0.51
1:K:671:LYS:HD2	1:K:671:LYS:O	2.11	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:E:1034:MET:HE3	1:E:1034:MET:HA	1.91	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:K:837:SER:HB3	1:K:838:GLY:HA2	1.93	0.51
1:K:924:LYS:HG3	1:K:925:TYR:CD2	2.46	0.51
1:L:811:PHE:HB3	1:L:823:ARG:NH1	2.26	0.51
2:C:1999:APJ:H17	2:C:1999:APJ:N8	2.26	0.50
1:D:673:LEU:HD23	1:D:673:LEU:C	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:928:GLU:O	1:E:932:ILE:HG13	2.10	0.50
1:H:845:ASN:N	1:H:845:ASN:HD22	2.09	0.50
1:I:685:SER:HB3	1:I:708:PHE:CZ	2.46	0.50
1:L:731:TYR:HA	1:L:745:LEU:HD23	1.91	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:E:1055:LEU:C	1:E:1055:LEU:HD23	2.31	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:B:1000:GLU:HB2	1:B:1009:LEU:HD21	1.93	0.50
1:B:853:SER:HA	1:B:856:ARG:HG3	1.93	0.50
1:D:737:THR:HG23	1:D:740:PHE:H	1.75	0.50
1:E:824:ILE:O	1:E:825:LEU:HD23	2.10	0.50
2:I:1999:APJ:H17	2:I:1999:APJ:N8	2.26	0.50
1:M:845:ASN:N	1:M:845:ASN:HD22	2.09	0.50
1:C:1000:GLU:HB2	1:C:1009:LEU:HD21	1.93	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:G:1055:LEU:C	1:G:1055:LEU:HD23	2.32	0.50
1:B:794:ILE:HG22	1:B:795:HIS:O	2.12	0.50
1:B:845:ASN:N	1:B:845:ASN:HD22	2.08	0.50
1:C:794:ILE:HG22	1:C:795:HIS:O	2.12	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:M:909:VAL:O	1:M:913:ILE:HG12	2.11	0.50
1:M:970:THR:HG23	1:M:973:LYS:CB	2.41	0.50
1:B:864:SER:O	1:B:893:THR:OG1	2.29	0.50
1:E:1000:GLU:HB2	1:E:1009:LEU:HD21	1.94	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:F:924:LYS:HG3	1:F:925:TYR:CD2	2.46	0.50
1:L:1000:GLU:HB2	1:L:1009:LEU:HD21	1.93	0.50
1:M:781:ILE:HG22	1:M:906:MET:CE	2.41	0.50
1:N:758:SER:HB3	1:N:768:LEU:HD21	1.94	0.50
1:D:1034:MET:HE3	1:D:1034:MET:HA	1.92	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:J:864:SER:O	1:J:893:THR:OG1	2.29	0.50
1:L:682:TYR:O	2:L:1999:APJ:H23	2.11	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:A:1059:TYR:OH	1:B:1108:ILE:HD12	2.12	0.50
1:B:811:PHE:HB3	1:B:823:ARG:NH1	2.26	0.50
1:C:1016:SER:C	1:C:1018:PHE:H	2.14	0.50
1:D:758:SER:HB3	1:D:768:LEU:HD21	1.94	0.50
1:G:1034:MET:CE	1:G:1034:MET:HA	2.41	0.50
1:G:845:ASN:HD22	1:G:845:ASN:N	2.09	0.50
1:H:1093:ILE:O	1:H:1097:MET:HG3	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:N:909:VAL:O	1:N:913:ILE:HG12	2.11	0.50
1:A:1111:GLU:O	1:A:1115:SER:HB3	2.10	0.50
1:C:673:LEU:O	1:C:673:LEU:HD23	2.11	0.50
1:D:781:ILE:HG22	1:D:906:MET:CE	2.42	0.50
1:F:1111:GLU:O	1:F:1115:SER:HB3	2.11	0.50
1:K:758:SER:HB3	1:K:768:LEU:HD21	1.94	0.50
1:L:1016:SER:C	1:L:1018:PHE:H	2.16	0.50
1:M:1016:SER:C	1:M:1018:PHE:H	2.15	0.50
1:M:671:LYS:HA	1:M:673:LEU:H	1.76	0.50
1:A:924:LYS:HG3	1:A:925:TYR:CD2	2.47	0.49
1:D:794:ILE:N	1:D:794:ILE:HD12	2.27	0.49
1:D:861:LEU:O	1:D:862:GLU:CB	2.60	0.49
1:F:909:VAL:O	1:F:913:ILE:HG12	2.12	0.49
1:G:781:ILE:HG22	1:G:906:MET:CE	2.41	0.49
1:K:977:HIS:CG	1:K:978:PRO:HD2	2.47	0.49
1:L:794:ILE:N	1:L:794:ILE:HD12	2.27	0.49
1:K:841:SEP:P	1:M:678:LYS:HZ1	2.35	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:B:673:LEU:HD23	1:B:673:LEU:C	2.33	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: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:N:977:HIS:CG	1:N:978:PRO:HD2	2.47	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:G:1000:GLU:HB2	1:G:1009:LEU:HD21	1.95	0.49
1:H:924:LYS:HG3	1:H:925:TYR:CD2	2.47	0.49
1:J:1041:ARG:NH2	1:J:1053:ARG:HG2	2.27	0.49
1:L:794:ILE:HG22	1:L:795:HIS:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:861:LEU:O	1:N:862:GLU:CB	2.60	0.49
1:D:672:ASN:HD22	1:D:672:ASN:H	1.59	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:F:673:LEU:C	1:F:673:LEU:CD2	2.81	0.49
1:H:1034:MET:CE	1:H:1034:MET:HA	2.42	0.49
1:I:924:LYS:HG3	1:I:925:TYR:CD2	2.47	0.49
1:J:1000:GLU:HB2	1:J:1009:LEU:HD21	1.94	0.49
1:K:685:SER:HB3	1:K:708:PHE:CZ	2.47	0.49
1:L:685:SER:HB3	1:L:708:PHE:CZ	2.47	0.49
1:L:837:SER:HB3	1:L:838:GLY:HA2	1.94	0.49
1:M:853:SER:HA	1:M:856:ARG:HG3	1.94	0.49
1:A:1000:GLU:HB2	1:A:1009:LEU:HD21	1.94	0.49
1:B:837:SER:HB3	1:B:838:GLY:HA2	1.93	0.49
1:B:924:LYS:HG3	1:B:925:TYR:CD2	2.47	0.49
1:F:1016:SER:C	1:F:1018:PHE:H	2.16	0.49
1:G:682:TYR:O	2:G:1999:APJ:H23	2.12	0.49
1:G:758:SER:HB3	1:G:768:LEU:HD21	1.94	0.49
1:H:837:SER:HB3	1:H:838:GLY:HA2	1.95	0.49
2:J:1999:APJ:H17	2:J:1999:APJ:N8	2.28	0.49
1:K:723:ASP:HB2	1:K:730:ARG:HA	1.92	0.49
1:M:685:SER:HB3	1:M:708:PHE:CZ	2.48	0.49
1:M:758:SER:HB3	1:M:768:LEU:HD21	1.94	0.49
1:A:1037:LEU:O	1:A:1037:LEU:HD12	2.12	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:I:824:ILE:O	1:I:825:LEU:HD23	2.13	0.49
1:I:992:LYS:HE3	1:J:1059:TYR:OH	2.13	0.49
1:J:685:SER:HB3	1:J:708:PHE:CZ	2.47	0.49
1:A:745:LEU:CD1	2:A:1999:APJ:H18A	2.42	0.49
1:A:845:ASN:HD22	1:A:845:ASN:N	2.09	0.49
1:B:781:ILE:HG22	1:B:906:MET:CE	2.42	0.49
1:D:845:ASN:HD22	1:D:845:ASN:N	2.10	0.49
1:E:864:SER:O	1:E:893:THR:OG1	2.29	0.49
1:F:845:ASN:N	1:F:845:ASN:HD22	2.09	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:I:682:TYR:O	2:I:1999:APJ:H23	2.13	0.49
1:I:794:ILE:HG22	1:I:795:HIS:O	2.13	0.49
1:I:837:SER:HB3	1:I:838:GLY:HA2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:861:LEU:O	1:M:862:GLU:CB	2.61	0.49
1:B:1034:MET:HA	1:B:1034:MET:CE	2.42	0.49
1:E:1034:MET:HA	1:E:1034:MET:CE	2.42	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:I:845:ASN:HD22	1:I:845:ASN:N	2.09	0.49
1:J:758:SER:HB3	1:J:768:LEU:HD21	1.94	0.49
1:J:924:LYS:HG3	1:J:925:TYR:CD2	2.48	0.49
1:K:794:ILE:N	1:K:794:ILE:HD12	2.28	0.49
1:B:1016:SER:C	1:B:1018:PHE:H	2.15	0.49
1:C:1076:VAL:HG11	1:D:1108:ILE:HD11	1.94	0.49
1:D:671:LYS:HA	1:D:673:LEU:H	1.78	0.49
1:G:861:LEU:O	1:G:862:GLU:CB	2.61	0.49
1:G:924:LYS:HG3	1:G:925:TYR:CD2	2.48	0.49
1:I:853:SER:HA	1:I:856:ARG:HG3	1.94	0.49
1:J:770:LYS:HG2	1:J:771:GLU:N	2.28	0.49
1:J:794:ILE:HG22	1:J:795:HIS:O	2.12	0.49
1:A:785:VAL:HG21	1:A:906:MET:HE1	1.94	0.49
1:A:837:SER:HB3	1:A:838:GLY:HA2	1.94	0.49
1:C:745:LEU:HD12	2:C:1999:APJ:H18A	1.94	0.49
1:C:758:SER:HB3	1:C:768:LEU:HD21	1.94	0.49
1:E:794:ILE:HG22	1:E:795:HIS:O	2.12	0.49
1:H:853:SER:HA	1:H:856:ARG:HG3	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:N:824:ILE:O	1:N:825:LEU:HD23	2.12	0.49
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:D:770:LYS:HG2	1:D:771:GLU:N	2.28	0.48
1:F:861:LEU:O	1:F:862:GLU:CB	2.60	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:J:914:LEU:O	1:J:943:CYS:HB2	2.13	0.48
1:L:861:LEU:O	1:L:862:GLU:CB	2.61	0.48
1:M:682:TYR:O	2:M:1999:APJ:H23	2.13	0.48
1:A:674:VAL:CG1	1:A:675:VAL:N	2.76	0.48
1:C:794:ILE:O	1:C:832:CYS:HB2	2.13	0.48
1:E:837:SER:HB3	1:E:838:GLY:HA2	1.94	0.48
1:F:685:SER:HB3	1:F:708:PHE:CZ	2.48	0.48
1:F:794:ILE:N	1:F:794:ILE:HD12	2.29	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:J:853:SER:HA	1:J:856:ARG:HG3	1.94	0.48
1:N:1034:MET:HA	1:N:1034:MET:CE	2.43	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:K:861:LEU:O	1:K:862:GLU:CB	2.61	0.48
1:E:924:LYS:HG3	1:E:925:TYR:CD2	2.48	0.48
1:G:794:ILE:HG22	1:G:795:HIS:O	2.13	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:K:845:ASN:HD22	1:K:845:ASN:N	2.10	0.48
1:N:1055:LEU:C	1:N:1055:LEU:HD23	2.33	0.48
1:N:781:ILE:HG22	1:N:906:MET:CE	2.43	0.48
1:A:682:TYR:O	2:A:1999:APJ:H23	2.13	0.48
1:C:745:LEU:CD1	2:C:1999:APJ:H18A	2.43	0.48
1:D:1016:SER:C	1:D:1018:PHE:H	2.15	0.48
1:D:977:HIS:CG	1:D:978:PRO:HD2	2.48	0.48
1:I:861:LEU:O	1:I:862:GLU:CB	2.61	0.48
1:I:864:SER:O	1:I:893:THR:OG1	2.30	0.48
1:J:837:SER:HB3	1:J:838:GLY:HA2	1.95	0.48
1:K:1016:SER:C	1:K:1018:PHE:H	2.17	0.48
1:K:824:ILE:O	1:K:825:LEU:HD23	2.13	0.48
1:M:804:LEU:HB2	1:M:825:LEU:HB2	1.96	0.48
1:N:1016:SER:C	1:N:1018:PHE:H	2.17	0.48
1:N:837:SER:HB3	1:N:838:GLY:HA2	1.95	0.48
1:A:1055:LEU:C	1:A:1055:LEU:HD23	2.33	0.48
1:A:685:SER:HB3	1:A:708:PHE:CZ	2.49	0.48
1:A:794:ILE:HG22	1:A:795:HIS:O	2.13	0.48
1:A:914:LEU:O	1:A:943:CYS:HB2	2.14	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: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:H:685:SER:HB3	1:H:708:PHE:CZ	2.49	0.48
1:J:1034:MET:CE	1:J:1034:MET:HA	2.42	0.48
1:J:861:LEU:O	1:J:862:GLU:CB	2.61	0.48
1:L:845:ASN:N	1:L:845:ASN:HD22	2.10	0.48
1:B:828:ASP:HB2	2:B:1999:APJ:H25	1.95	0.48
1:C:1093:ILE:O	1:C:1097:MET:HG3	2.12	0.48
1:D:837:SER:HB3	1:D:838:GLY:HA2	1.95	0.48
1:F:848:ASN:CB	1:F:849:PRO:HA	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1016:SER:C	1:G:1018:PHE:H	2.17	0.48
1:G:673:LEU:O	1:G:673:LEU:HD23	2.13	0.48
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:C:1037:LEU:C	1:C:1039:ARG:H	2.17	0.48
1:C:682:TYR:O	2:C:1999:APJ:H23	2.14	0.48
1:D:914:LEU:O	1:D:943:CYS:HB2	2.13	0.48
1:E:804:LEU:HB2	1:E:825:LEU:HB2	1.95	0.48
1:H:1000:GLU:HB2	1:H:1009:LEU:HD21	1.94	0.48
1:H:1025:TRP:HB2	1:H:1088:PHE:CZ	2.48	0.48
1:H:794:ILE:HG22	1:H:795:HIS:O	2.14	0.48
1:H:861:LEU:O	1:H:862:GLU:CB	2.61	0.48
1:H:914:LEU:O	1:H:943:CYS:HB2	2.13	0.48
1:I:1034:MET:HA	1:I:1034:MET:CE	2.43	0.48
1:J:977:HIS:CG	1:J:978:PRO:HD2	2.49	0.48
1:K:663:ILE:O	1:K:664:PRO:C	2.52	0.48
1:K:853:SER:HA	1:K:856:ARG:HG3	1.94	0.48
1:L:758:SER:HB3	1:L:768:LEU:HD21	1.94	0.48
1:M:1000:GLU:HB2	1:M:1009:LEU:HD21	1.95	0.48
1:A:946:ASP:HB3	1:A:949:LEU:HD12	1.94	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:M:794:ILE:O	1:M:832:CYS:HB2	2.13	0.48
1:A:671:LYS:HD2	1:A:671:LYS:O	2.14	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:E:1016:SER:C	1:E:1018:PHE:H	2.16	0.48
1:F:725:HIS:CG	1:F:726:PRO:HD2	2.49	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: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:M:837:SER:HB3	1:M:838:GLY:HA2	1.95	0.48
1:C:861:LEU:O	1:C:862:GLU:CB	2.60	0.47
1:C:946:ASP:HB3	1:C:949:LEU:HD12	1.95	0.47
1:F:794:ILE:O	1:F:832:CYS:HB2	2.14	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:M:673:LEU:C	1:M:673:LEU:HD23	2.34	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:A:828:ASP:HB2	2:A:1999:APJ:H25	1.96	0.47
1:B:1025:TRP:HB2	1:B:1088:PHE:CZ	2.49	0.47
1:B:674:VAL:CG1	1:B:675:VAL:N	2.76	0.47
1:C:770:LYS:HG2	1:C:771:GLU:N	2.29	0.47
1:C:864:SER:O	1:C:893:THR:OG1	2.29	0.47
1:E:906:MET:HB2	1:E:906:MET:HE3	1.78	0.47
1:G:687:THR:HG23	1:G:704:MET:HG2	1.96	0.47
1:H:781:ILE:HG22	1:H:906:MET:CE	2.43	0.47
1:I:1037:LEU:C	1:I:1039:ARG:H	2.18	0.47
1:I:804:LEU:HB2	1:I:825:LEU:HB2	1.96	0.47
1:I:893:THR:O	1:I:895:ARG:HG3	2.14	0.47
1:L:893:THR:O	1:L:895:ARG:HG3	2.14	0.47
1:L:977:HIS:CG	1:L:978:PRO:HD2	2.50	0.47
1:N:1000:GLU:HB2	1:N:1009:LEU:HD21	1.95	0.47
1:A:1059:TYR:OH	1:B:1108:ILE:CD1	2.63	0.47
1:G:770:LYS:HG2	1:G:771:GLU:N	2.29	0.47
1:H:893:THR:O	1:H:895:ARG:HG3	2.14	0.47
1:I:1000:GLU:HB2	1:I:1009:LEU:HD21	1.95	0.47
1:K:970:THR:HG23	1:K:973:LYS:CB	2.44	0.47
1:L:970:THR:HG23	1:L:973:LYS:CB	2.43	0.47
1:M:1095:VAL:O	1:M:1099:VAL:HG23	2.14	0.47
1:B:977:HIS:CG	1:B:978:PRO:HD2	2.49	0.47
1:C:670:LEU:HD23	1:C:735:GLU:OE2	2.14	0.47
1:G:864:SER:O	1:G:893:THR:OG1	2.30	0.47
1:J:1016:SER:C	1:J:1018:PHE:H	2.17	0.47
1:J:1037:LEU:C	1:J:1039:ARG:H	2.16	0.47
1:I:787:HIS:CD2	1:J:814:ASP:HB2	2.50	0.47
1:K:1025:TRP:HB2	1:K:1088:PHE:CZ	2.49	0.47
1:K:804:LEU:HB2	1:K:825:LEU:HB2	1.97	0.47
1:L:864:SER:O	1:L:893:THR:OG1	2.30	0.47
1:A:758:SER:HB3	1:A:768:LEU:HD21	1.96	0.47
1:A:861:LEU:O	1:A:862:GLU:CB	2.61	0.47
1:D:853:SER:HA	1:D:856:ARG:HG3	1.96	0.47
1:E:828:ASP:HB2	2:E:1999:APJ:H25	1.96	0.47
1:F:671:LYS:O	1:F:671:LYS:HD2	2.15	0.47
1:F:837:SER:HB3	1:F:838:GLY:HA2	1.96	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:M:924:LYS:HG3	1:M:925:TYR:CD2	2.49	0.47
1:F:1034:MET:CE	1:F:1037:LEU:HD23	2.44	0.47
1:G:906:MET:HE3	1:G:906:MET:HB2	1.76	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1095:VAL:O	1:H:1099:VAL:HG23	2.14	0.47
1:K:1034:MET:CE	1:K:1034:MET:HA	2.44	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
1:N:673:LEU:HD23	1:N:673:LEU:O	2.14	0.47
1:N:685:SER:HB3	1:N:708:PHE:CZ	2.48	0.47
1:A:1025:TRP:HB2	1:A:1088:PHE:CZ	2.50	0.47
1:A:814:ASP:OD2	1:B:787:HIS:HD2	1.98	0.47
1:B:682:TYR:O	2:B:1999:APJ:H23	2.15	0.47
1:F:804:LEU:HB2	1:F:825:LEU:HB2	1.97	0.47
1:K:794:ILE:HG22	1:K:795:HIS:O	2.14	0.47
1:N:946:ASP:HB3	1:N:949:LEU:HD12	1.96	0.47
1:B:893:THR:O	1:B:895:ARG:HG3	2.14	0.47
1:G:1025:TRP:HB2	1:G:1088:PHE:CZ	2.50	0.47
1:H:682:TYR:O	2:H:1999:APJ:H23	2.13	0.47
1:H:758:SER:HB3	1:H:768:LEU:HD21	1.95	0.47
1:H:970:THR:HG23	1:H:973:LYS:CB	2.45	0.47
1:J:804:LEU:HB2	1:J:825:LEU:HB2	1.96	0.47
1:L:781:ILE:HG22	1:L:906:MET:CE	2.43	0.47
1:M:794:ILE:HG22	1:M:795:HIS:O	2.14	0.47
1:M:893:THR:O	1:M:895:ARG:HG3	2.15	0.47
1:N:893:THR:O	1:N:895:ARG:HG3	2.15	0.47
1:C:737:THR:C	1:C:739:ARG:H	2.17	0.47
1:E:946:ASP:HB3	1:E:949:LEU:HD12	1.97	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:J:970:THR:HG23	1:J:973:LYS:CB	2.45	0.47
1:K:737:THR:C	1:K:739:ARG:H	2.19	0.47
1:K:906:MET:HE3	1:K:906:MET:HB2	1.75	0.47
1:L:1095:VAL:O	1:L:1099:VAL:HG23	2.15	0.47
1:A:814:ASP:HB2	1:B:787:HIS:CD2	2.50	0.47
1:B:725:HIS:CG	1:B:726:PRO:HD2	2.50	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:G:914:LEU:O	1:G:943:CYS:HB2	2.15	0.47
1:I:1016:SER:C	1:I:1018:PHE:H	2.17	0.47
1:L:737:THR:C	1:L:739:ARG:H	2.19	0.47
1:M:864:SER:O	1:M:893:THR:OG1	2.28	0.47
1:N:1008:LEU:HA	1:N:1008:LEU:HD23	1.78	0.47
1:A:687:THR:HG23	1:A:704:MET:HG2	1.97	0.47
1:C:1055:LEU:HD23	1:C:1055:LEU:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:685:SER:HB3	1:C:708:PHE:CZ	2.50	0.47
1:D:725:HIS:CG	1:D:726:PRO:HD2	2.49	0.47
1:E:781:ILE:HG22	1:E:906:MET:CE	2.44	0.47
1:K:893:THR:O	1:K:895:ARG:HG3	2.15	0.47
1:K:970:THR:HB	1:M:762:SER:HB2	1.96	0.47
1:M:906:MET:HG3	1:M:910:PHE:CE1	2.50	0.47
1:N:770:LYS:HG2	1:N:771:GLU:N	2.30	0.47
1:A:864:SER:O	1:A:893:THR:OG1	2.28	0.46
1:D:665:ASN:ND2	1:D:665:ASN:N	2.59	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:E:893:THR:O	1:E:895:ARG:HG3	2.15	0.46
1:F:893:THR:O	1:F:895:ARG:HG3	2.15	0.46
1:H:770:LYS:HG2	1:H:771:GLU:N	2.30	0.46
1:A:729:ILE:HD12	1:A:745:LEU:HB3	1.98	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:H:804:LEU:HB2	1:H:825:LEU:HB2	1.98	0.46
1:I:1095:VAL:O	1:I:1099:VAL:HG23	2.15	0.46
1:J:1044:HIS:ND1	1:J:1050:ASP:OD2	2.47	0.46
1:J:737:THR:C	1:J:739:ARG:H	2.18	0.46
1:L:842:PHE:O	1:L:842:PHE:CG	2.69	0.46
1:M:770:LYS:HG2	1:M:771:GLU:N	2.31	0.46
1:A:725:HIS:HD2	1:A:727:ASN:H	1.61	0.46
1:A:737:THR:C	1:A:739:ARG:H	2.18	0.46
1:A:804:LEU:HB2	1:A:825:LEU:HB2	1.97	0.46
1:B:837:SER:CB	1:B:838:GLY:HA2	2.45	0.46
1:B:842:PHE:CG	1:B:842:PHE:O	2.68	0.46
1:C:687:THR:HG23	1:C:704:MET:HG2	1.98	0.46
1:C:842:PHE:CG	1:C:842:PHE:O	2.68	0.46
1:F:1037:LEU:C	1:F:1039:ARG:H	2.17	0.46
1:K:1000:GLU:HB2	1:K:1009:LEU:HD21	1.96	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:M:794:ILE:N	1:M:794:ILE:HD12	2.29	0.46
1:N:794:ILE:O	1:N:832:CYS:HB2	2.15	0.46
1:A:837:SER:CB	1:A:838:GLY:HA2	2.45	0.46
1:B:687:THR:HG23	1:B:704:MET:HG2	1.98	0.46
1:C:1076:VAL:CG1	1:D:1108:ILE:HD11	2.45	0.46
1:D:748:CYS:N	2:D:1999:APJ:HN4	2.11	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1037:LEU:C	1:E:1039:ARG:H	2.18	0.46
1:I:1025:TRP:HB2	1:I:1088:PHE:CZ	2.50	0.46
1:I:837:SER:CB	1:I:838:GLY:HA2	2.46	0.46
1:J:893:THR:O	1:J:895:ARG:HG3	2.16	0.46
1:K:842:PHE:CG	1:K:842:PHE:O	2.69	0.46
1:K:864:SER:O	1:K:893:THR:OG1	2.29	0.46
1:C:729:ILE:HD12	1:C:745:LEU:HB3	1.98	0.46
1:C:1108:ILE:HD11	1:D:1076:VAL:HG11	1.96	0.46
1:E:861:LEU:O	1:E:862:GLU:CB	2.61	0.46
1:E:964:ASP:HA	1:E:965:PRO:HD2	1.84	0.46
1:E:977:HIS:CG	1:E:978:PRO:HD2	2.49	0.46
1:K:1095:VAL:O	1:K:1099:VAL:HG23	2.16	0.46
1:A:842:PHE:CG	1:A:842:PHE:O	2.68	0.46
1:A:893:THR:O	1:A:895:ARG:HG3	2.16	0.46
1:B:1037:LEU:C	1:B:1039:ARG:H	2.18	0.46
1:B:947:ARG:HB2	1:N:1071:GLU:OE1	2.15	0.46
1:C:837:SER:HB3	1:C:838:GLY:HA2	1.96	0.46
1:D:804:LEU:HB2	1:D:825:LEU:HB2	1.97	0.46
1:E:671:LYS:O	1:E:671:LYS:HD2	2.16	0.46
1:C:761:VAL:CG1	1:F:840:SEP:O2P	2.55	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:J:687:THR:HG23	1:J:704:MET:HG2	1.97	0.46
1:J:837:SER:CB	1:J:838:GLY:HA2	2.46	0.46
1:K:837:SER:CB	1:K:838:GLY:HA2	2.45	0.46
1:L:804:LEU:HB2	1:L:825:LEU:HB2	1.98	0.46
1:M:906:MET:HB2	1:M:906:MET:HE3	1.78	0.46
1:B:737:THR:C	1:B:739:ARG:H	2.19	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: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:F:970:THR:HG23	1:F:973:LYS:CB	2.45	0.46
1:M:1103:LEU:C	1:M:1105:ASP:H	2.19	0.46
1:N:1095:VAL:O	1:N:1099:VAL:HG23	2.16	0.46
1:A:781:ILE:HG22	1:A:906:MET:CE	2.45	0.46
1:C:893:THR:O	1:C:895:ARG:HG3	2.15	0.46
1:D:1025:TRP:HB2	1:D:1088:PHE:CZ	2.51	0.46
1:D:737:THR:C	1:D:739:ARG:H	2.18	0.46
1:C:1063:MET:HE3	1:D:999:ILE:HD11	1.98	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: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:L:725:HIS:CG	1:L:726:PRO:HD2	2.51	0.46
1:M:671:LYS:CA	1:M:673:LEU:H	2.28	0.46
1:M:737:THR:C	1:M:739:ARG:H	2.19	0.46
1:M:914:LEU:O	1:M:943:CYS:HB2	2.16	0.46
1:M:977:HIS:CG	1:M:978:PRO:HD2	2.51	0.46
1:B:672:ASN:ND2	1:B:672:ASN:H	2.13	0.46
1:B:914:LEU:O	1:B:943:CYS:HB2	2.16	0.46
1:G:842:PHE:O	1:G:842:PHE:CG	2.69	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:687:THR:HG23	1:L:704:MET:HG2	1.98	0.46
1:L:837:SER:CB	1:L:838:GLY:HA2	2.45	0.46
1:G:1095:VAL:O	1:G:1099:VAL:HG23	2.16	0.46
1:G:893:THR:O	1:G:895:ARG:HG3	2.16	0.46
1:H:687:THR:HG23	1:H:704:MET:HG2	1.98	0.46
1:I:737:THR:C	1:I:739:ARG:H	2.19	0.46
1:N:929:SER:O	1:N:933:ARG:HG3	2.17	0.46
1:A:1095:VAL:O	1:A:1099:VAL:HG23	2.16	0.45
1:C:725:HIS:CG	1:C:726:PRO:HD2	2.51	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:F:770:LYS:HG2	1:F:771:GLU:N	2.31	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:H:837:SER:CB	1:H:838:GLY:HA2	2.46	0.45
1:N:804:LEU:HB2	1:N:825:LEU:HB2	1.98	0.45
1:A:770:LYS:HG2	1:A:771:GLU:N	2.31	0.45
1:A:970:THR:HG23	1:A:973:LYS:CB	2.46	0.45
1:B:804:LEU:HB2	1:B:825:LEU:HB2	1.97	0.45
1:D:794:ILE:O	1:D:832:CYS:HB2	2.15	0.45
1:E:1025:TRP:HB2	1:E:1088:PHE:CZ	2.51	0.45
1:E:729:ILE:HD12	1:E:745:LEU:HB3	1.97	0.45
1:F:761:VAL:HG11	1:H:840:SEP:P	2.57	0.45
1:F:946:ASP:HB3	1:F:949:LEU:HD12	1.97	0.45
1:I:770:LYS:HG2	1:I:771:GLU:N	2.30	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:L:794:ILE:O	1:L:832:CYS:HB2	2.17	0.45
1:B:1082:ASP:HA	1:B:1085:THR:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:748:CYS:N	2:B:1999:APJ:HN4	2.12	0.45
1:E:837:SER:CB	1:E:838:GLY:HA2	2.46	0.45
1:E:842:PHE:O	1:E:842:PHE:CG	2.69	0.45
1:H:737:THR:C	1:H:739:ARG:H	2.19	0.45
1:I:725:HIS:CG	1:I:726:PRO:HD2	2.51	0.45
1:M:1008:LEU:HA	1:M:1008:LEU:HD23	1.80	0.45
1:M:719:LEU:HA	1:M:719:LEU:HD23	1.72	0.45
1:N:748:CYS:N	2:N:1999:APJ:HN4	2.11	0.45
1:N:794:ILE:HD12	1:N:794:ILE:N	2.31	0.45
1:C:1043:TYR:OH	1:C:1057:ASN:ND2	2.45	0.45
1:D:1093:ILE:HG23	1:D:1094:GLY:N	2.31	0.45
1:D:666:PHE:HD1	1:D:742:TYR:HH	1.60	0.45
1:F:1033:PHE:CE1	1:F:1058:LYS:HE2	2.52	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:I:906:MET:HB2	1:I:906:MET:HE3	1.75	0.45
1:M:729:ILE:HD12	1:M:745:LEU:HB3	1.98	0.45
1:C:828:ASP:HB2	2:C:1999:APJ:H25	1.99	0.45
1:F:748:CYS:N	2:F:1999:APJ:HN4	2.12	0.45
1:I:828:ASP:HB2	2:I:1999:APJ:H25	1.98	0.45
1:N:837:SER:CB	1:N:838:GLY:HA2	2.46	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:F:842:PHE:CG	1:F:842:PHE:O	2.69	0.45
1:G:1034:MET:CE	1:G:1037:LEU:HD23	2.46	0.45
1:H:842:PHE:CG	1:H:842:PHE:O	2.69	0.45
1:K:946:ASP:HB3	1:K:949:LEU:HD12	1.98	0.45
1:L:1037:LEU:C	1:L:1039:ARG:H	2.19	0.45
1:M:823:ARG:NH2	1:N:724:ASP:OD2	2.50	0.45
1:M:946:ASP:HB3	1:M:949:LEU:HD12	1.98	0.45
1:N:828:ASP:HB2	2:N:1999:APJ:H25	1.99	0.45
1:A:785:VAL:CG2	1:A:906:MET:HE1	2.47	0.45
1:B:1095:VAL:O	1:B:1099:VAL:HG23	2.17	0.45
1:B:805:VAL:HA	1:B:823:ARG:O	2.17	0.45
1:B:857:ALA:O	1:B:860:LEU:HB2	2.16	0.45
1:C:837:SER:CB	1:C:838:GLY:HA2	2.47	0.45
1:D:1037:LEU:C	1:D:1039:ARG:H	2.19	0.45
1:D:666:PHE:HZ	1:D:690:PHE:CZ	2.33	0.45
1:F:837:SER:CB	1:F:838:GLY:HA2	2.47	0.45
1:G:837:SER:CB	1:G:838:GLY:HA2	2.46	0.45
1:H:1037:LEU:C	1:H:1039:ARG:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:729:ILE:HD12	1:I:745:LEU:HB3	1.99	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:K:1034:MET:HA	1:K:1034:MET:HE3	1.98	0.45
1:M:748:CYS:N	2:M:1999:APJ:HN4	2.13	0.45
1:M:842:PHE:CG	1:M:842:PHE:O	2.69	0.45
1:N:842:PHE:O	1:N:842:PHE:CG	2.70	0.45
1:N:970:THR:HG23	1:N:973:LYS:CB	2.44	0.45
1:B:794:ILE:HD12	1:B:794:ILE:N	2.32	0.45
1:C:1095:VAL:O	1:C:1099:VAL:HG23	2.17	0.45
1:D:1055:LEU:HD23	1:D:1055:LEU:O	2.15	0.45
1:J:729:ILE:HD12	1:J:745:LEU:HB3	1.98	0.45
1:K:848:ASN:CB	1:K:849:PRO:HA	2.30	0.45
1:M:992:LYS:HE3	1:N:1059:TYR:OH	2.17	0.45
1:B:798:LEU:HA	1:B:798:LEU:HD23	1.80	0.45
1:B:946:ASP:HB3	1:B:949:LEU:HD12	1.99	0.45
1:D:893:THR:O	1:D:895:ARG:HG3	2.17	0.45
1:E:794:ILE:N	1:E:794:ILE:HD12	2.31	0.45
1:F:673:LEU:HD23	1:F:674:VAL:N	2.31	0.45
1:G:798:LEU:HA	1:G:798:LEU:HD23	1.83	0.45
1:G:804:LEU:HB2	1:G:825:LEU:HB2	1.97	0.45
1:I:794:ILE:O	1:I:832:CYS:HB2	2.17	0.45
1:I:799:LYS:NZ	1:I:852:THR:HG23	2.32	0.45
1:J:725:HIS:CG	1:J:726:PRO:HD2	2.52	0.45
1:J:842:PHE:O	1:J:842:PHE:CG	2.69	0.45
1:K:666:PHE:HE1	1:K:703:ARG:HD3	1.82	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:J:1095:VAL:O	1:J:1099:VAL:HG23	2.17	0.45
1:M:1025:TRP:HB2	1:M:1088:PHE:CZ	2.51	0.45
1:M:725:HIS:CG	1:M:726:PRO:HD2	2.52	0.45
1:A:797:ASP:O	1:A:802:ASN:ND2	2.49	0.44
1:B:785:VAL:HG21	1:B:906:MET:HE1	1.99	0.44
1:C:1030:ASP:N	1:C:1030:ASP:OD1	2.50	0.44
1:G:748:CYS:N	2:G:1999:APJ:HN4	2.14	0.44
1:G:758:SER:O	1:G:759:LYS:HB3	2.17	0.44
1:G:992:LYS:HE3	1:H:1059:TYR:OH	2.17	0.44
1:H:1082:ASP:HA	1:H:1085:THR:HB	2.00	0.44
1:N:925:TYR:N	1:N:925:TYR:CD2	2.85	0.44
1:B:685:SER:HB3	1:B:708:PHE:CZ	2.51	0.44
1:D:1095:VAL:O	1:D:1099:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:906:MET:HG3	1:F:910:PHE:CE1	2.53	0.44
1:F:925:TYR:CD2	1:F:925:TYR:N	2.84	0.44
1:H:740:PHE:HB3	1:H:741:LEU:H	1.63	0.44
1:I:970:THR:HG23	1:I:973:LYS:CB	2.48	0.44
1:J:978:PRO:HA	1:J:981:TRP:CD1	2.53	0.44
1:K:687:THR:HG23	1:K:704:MET:HG2	1.99	0.44
1:L:758:SER:O	1:L:759:LYS:HB3	2.18	0.44
1:B:670:LEU:O	1:B:735:GLU:OE2	2.35	0.44
1:E:1103:LEU:C	1:E:1105:ASP:H	2.21	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:1025:TRP:HB2	1:L:1088:PHE:CZ	2.52	0.44
1:L:906:MET:HE3	1:L:906:MET:HB2	1.78	0.44
1:K:841:SEP:P	1:M:678:LYS:NZ	2.91	0.44
1:N:906:MET:HG3	1:N:910:PHE:CE1	2.52	0.44
1:A:925:TYR:N	1:A:925:TYR:CD2	2.85	0.44
1:B:1093:ILE:HG23	1:B:1094:GLY:N	2.33	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:H:946:ASP:HB3	1:H:949:LEU:HD12	1.99	0.44
1:M:1048:LEU:HD23	1:M:1048:LEU:O	2.18	0.44
1:M:837:SER:CB	1:M:838:GLY:HA2	2.47	0.44
1:M:964:ASP:HA	1:M:965:PRO:HD2	1.85	0.44
1:B:1033:PHE:CE1	1:B:1058:LYS:HE2	2.53	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:F:670:LEU:HD23	1:F:735:GLU:OE2	2.18	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:A:1103:LEU:C	1:A:1105:ASP:H	2.20	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: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:1106:ASP:O	1:K:1110:ARG:HG3	2.18	0.44
1:K:672:ASN:ND2	1:K:672:ASN:N	2.65	0.44
1:M:857:ALA:O	1:M:860:LEU:HB2	2.17	0.44
1:A:1106:ASP:O	1:A:1110:ARG:HG3	2.18	0.44
1:C:925:TYR:CD2	1:C:925:TYR:N	2.83	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:F:898:THR:OG1	1:F:899:ARG:N	2.51	0.44
1:F:914:LEU:O	1:F:943:CYS:HB2	2.18	0.44
1:G:906:MET:HG3	1:G:910:PHE:CE1	2.53	0.44
1:I:1030:ASP:N	1:I:1030:ASP:OD1	2.51	0.44
1:I:672:ASN:ND2	1:I:672:ASN:N	2.64	0.44
1:K:1103:LEU:C	1:K:1105:ASP:H	2.21	0.44
1:K:978:PRO:HA	1:K:981:TRP:CD1	2.53	0.44
1:M:828:ASP:HB2	2:M:1999:APJ:H25	2.00	0.44
1:N:1030:ASP:OD1	1:N:1030:ASP:N	2.51	0.44
1:N:1103:LEU:C	1:N:1105:ASP:H	2.21	0.44
1:N:687:THR:HG23	1:N:704:MET:HG2	2.00	0.44
1:A:1082:ASP:HA	1:A:1085:THR:HB	2.00	0.44
1:A:805:VAL:HA	1:A:823:ARG:O	2.18	0.44
1:A:999:ILE:N	1:A:999:ILE:HD12	2.33	0.44
1:C:898:THR:OG1	1:C:899:ARG:N	2.51	0.44
1:D:767:LYS:HE2	1:D:767:LYS:HB2	1.82	0.44
1:H:1020:ILE:HG22	1:H:1021:PRO:C	2.37	0.44
1:I:1033:PHE:CE1	1:I:1058:LYS:HE2	2.53	0.44
1:K:1030:ASP:OD1	1:K:1030:ASP:N	2.51	0.44
1:K:672:ASN:HD22	1:K:672:ASN:N	2.16	0.44
1:K:788:LEU:HD13	1:K:788:LEU:HA	1.87	0.44
1:L:1008:LEU:HA	1:L:1008:LEU:HD23	1.79	0.44
1:L:799:LYS:NZ	1:L:852:THR:HG23	2.33	0.44
1:L:946:ASP:HB3	1:L:949:LEU:HD12	1.99	0.44
1:N:737:THR:C	1:N:739:ARG:H	2.21	0.44
1:D:758:SER:O	1:D:759:LYS:HB3	2.17	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: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:I:842:PHE:O	1:I:842:PHE:CG	2.70	0.44
1:L:828:ASP:HB2	2:L:1999:APJ:H25	2.00	0.44
1:M:937:SER:O	1:M:938:LEU:HD23	2.17	0.44
1:C:1033:PHE:CE1	1:C:1058:LYS:HE2	2.53	0.43
1:C:671:LYS:HD2	1:C:671:LYS:O	2.17	0.43
1:D:842:PHE:O	1:D:842:PHE:CG	2.70	0.43
1:E:1033:PHE:CE1	1:E:1058:LYS:HE2	2.53	0.43
1:F:799:LYS:NZ	1:F:852:THR:HG23	2.33	0.43
1:L:1020:ILE:HG22	1:L:1021:PRO:C	2.37	0.43
1:N:672:ASN:N	1:N:672:ASN:ND2	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:864:SER:O	1:N:893:THR:OG1	2.31	0.43
1:A:719:LEU:HD23	1:A:719:LEU:HA	1.72	0.43
1:B:1103:LEU:C	1:B:1105:ASP:H	2.22	0.43
1:B:758:SER:O	1:B:759:LYS:HB3	2.17	0.43
1:C:1082:ASP:HA	1:C:1085:THR:HB	2.00	0.43
1:C:821:ASN:O	1:C:822:LEU:HB3	2.18	0.43
1:G:1020:ILE:HG22	1:G:1021:PRO:C	2.39	0.43
1:G:740:PHE:HB3	1:G:741:LEU:H	1.64	0.43
1:H:906:MET:HG3	1:H:910:PHE:CE1	2.53	0.43
1:I:758:SER:O	1:I:759:LYS:HB3	2.18	0.43
1:J:1011:LYS:HA	1:J:1011:LYS:HE2	2.00	0.43
1:J:828:ASP:HB2	2:J:1999:APJ:H25	2.00	0.43
1:K:1033:PHE:CE1	1:K:1058:LYS:HE2	2.54	0.43
1:K:925:TYR:N	1:K:925:TYR:CD2	2.86	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:A:725:HIS:CD2	1:A:727:ASN:HB2	2.53	0.43
1:B:845:ASN:N	1:B:845:ASN:ND2	2.66	0.43
1:C:725:HIS:CD2	1:C:727:ASN:HB2	2.54	0.43
1:E:925:TYR:N	1:E:925:TYR:CD2	2.86	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:F:737:THR:C	1:F:739:ARG:H	2.21	0.43
1:J:946:ASP:HB3	1:J:949:LEU:HD12	1.99	0.43
1:K:828:ASP:HB2	2:K:1999:APJ:H25	2.00	0.43
1:K:725:HIS:CG	1:K:726:PRO:HD2	2.53	0.43
1:L:1020:ILE:HB	1:L:1021:PRO:HA	2.00	0.43
1:L:1030:ASP:OD1	1:L:1030:ASP:N	2.52	0.43
1:N:1093:ILE:HG23	1:N:1094:GLY:N	2.34	0.43
1:N:978:PRO:HA	1:N:981:TRP:CD1	2.53	0.43
1:C:1048:LEU:HD23	1:C:1048:LEU:O	2.19	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:1034:MET:CE	1:E:1037:LEU:HD23	2.48	0.43
1:E:857:ALA:O	1:E:860:LEU:HB2	2.19	0.43
1:I:1082:ASP:HA	1:I:1085:THR:HB	2.00	0.43
1:J:719:LEU:HD23	1:J:719:LEU:HA	1.72	0.43
1:J:798:LEU:HD23	1:J:798:LEU:HA	1.81	0.43
1:J:906:MET:HB2	1:J:906:MET:HE3	1.81	0.43
1:N:758:SER:CB	1:N:768:LEU:HD21	2.49	0.43
1:A:787:HIS:O	1:A:790:SER:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1106:ASP:O	1:C:1110:ARG:HG3	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:K:758:SER:O	1:K:759:LYS:HB3	2.18	0.43
1:N:672:ASN:H	1:N:672:ASN:ND2	2.17	0.43
1:N:729:ILE:HD12	1:N:745:LEU:HB3	2.00	0.43
1:N:999:ILE:N	1:N:999:ILE:HD12	2.34	0.43
1:A:845:ASN:ND2	1:A:845:ASN:N	2.66	0.43
1:C:1020:ILE:HG22	1:C:1021:PRO:C	2.38	0.43
1:C:1034:MET:CE	1:C:1037:LEU:HD23	2.48	0.43
1:E:1082:ASP:HA	1:E:1085:THR:HB	1.99	0.43
1:E:843:ARG:NH2	1:G:678:LYS:HB2	2.34	0.43
1:E:937:SER:O	1:E:938:LEU:HD23	2.18	0.43
1:F:1082:ASP:HA	1:F:1085:THR:HB	2.01	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:J:1106:ASP:O	1:J:1110:ARG:HG3	2.18	0.43
1:K:672:ASN:H	1:K:672:ASN:HD22	1.66	0.43
1:K:719:LEU:HD23	1:K:719:LEU:HA	1.72	0.43
1:K:906:MET:HG3	1:K:910:PHE:CE1	2.53	0.43
1:M:1093:ILE:HG23	1:M:1094:GLY:N	2.34	0.43
1:N:799:LYS:NZ	1:N:852:THR:HG23	2.34	0.43
1:N:906:MET:HB2	1:N:906:MET:HE3	1.78	0.43
1:A:1030:ASP:N	1:A:1030:ASP:OD1	2.52	0.43
1:A:748:CYS:N	2:A:1999:APJ:HN4	2.13	0.43
1:C:799:LYS:HB2	1:C:800:PRO:HD2	2.01	0.43
1:E:845:ASN:N	1:E:845:ASN:ND2	2.67	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: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:H:797:ASP:O	1:H:802:ASN:ND2	2.51	0.43
1:I:1008:LEU:HD23	1:I:1008:LEU:HA	1.81	0.43
1:J:1020:ILE:HG22	1:J:1021:PRO:C	2.38	0.43
1:J:673:LEU:HD23	1:J:673:LEU:C	2.39	0.43
1:J:845:ASN:N	1:J:845:ASN:ND2	2.67	0.43
1:L:906:MET:HG3	1:L:910:PHE:CE1	2.53	0.43
1:N:1020:ILE:HG22	1:N:1021:PRO:C	2.39	0.43
1:A:799:LYS:HB2	1:A:800:PRO:HD2	2.01	0.43
1:B:767:LYS:HE2	1:B:767:LYS:HB2	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:797:ASP:O	1:D:802:ASN:ND2	2.52	0.43
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:F:680:LEU:HB2	1:F:689:VAL:CG1	2.48	0.43
1:F:845:ASN:N	1:F:845:ASN:ND2	2.67	0.43
1:G:1093:ILE:HG23	1:G:1094:GLY:N	2.33	0.43
1:I:1011:LYS:HE2	1:I:1011:LYS:HA	2.00	0.43
1:K:729:ILE:HD12	1:K:745:LEU:HB3	1.99	0.43
1:L:1103:LEU:C	1:L:1105:ASP:H	2.22	0.43
1:L:805:VAL:HA	1:L:823:ARG:O	2.19	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:N:848:ASN:CB	1:N:849:PRO:HA	2.30	0.43
1:A:1048:LEU:O	1:A:1049:MET:C	2.57	0.43
1:A:1033:PHE:CE1	1:A:1058:LYS:HE2	2.54	0.43
1:A:798:LEU:HA	1:A:798:LEU:HD23	1.79	0.43
1:A:848:ASN:CB	1:A:849:PRO:HA	2.30	0.43
1:B:740:PHE:HB3	1:B:741:LEU:H	1.63	0.43
1:E:798:LEU:HD23	1:E:798:LEU:HA	1.79	0.43
1:G:1103:LEU:C	1:G:1105:ASP:H	2.22	0.43
1:G:719:LEU:HD23	1:G:719:LEU:HA	1.72	0.43
1:G:925:TYR:N	1:G:925:TYR:CD2	2.87	0.43
1:I:1103:LEU:C	1:I:1105:ASP:H	2.22	0.43
1:J:925:TYR:CD2	1:J:925:TYR:N	2.87	0.43
1:K:857:ALA:O	1:K:860:LEU:HB2	2.19	0.43
1:L:925:TYR:CD2	1:L:925:TYR:N	2.87	0.43
1:M:845:ASN:N	1:M:845:ASN:ND2	2.66	0.43
1:N:1055:LEU:O	1:N:1055:LEU:HD23	2.19	0.43
1:N:787:HIS:O	1:N:790:SER:HB2	2.19	0.43
1:B:925:TYR:N	1:B:925:TYR:CD2	2.87	0.43
1:D:663:ILE:O	1:D:664:PRO:C	2.58	0.43
1:D:719:LEU:HA	1:D:719:LEU:HD23	1.70	0.43
1:D:925:TYR:CD2	1:D:925:TYR:N	2.87	0.43
1:G:1082:ASP:HA	1:G:1085:THR:HB	2.00	0.43
1:G:758:SER:CB	1:G:768:LEU:HD21	2.49	0.43
1:H:798:LEU:HA	1:H:798:LEU:HD23	1.80	0.43
1:H:821:ASN:O	1:H:822:LEU:HB3	2.19	0.43
1:H:845:ASN:ND2	1:H:845:ASN:N	2.67	0.43
1:J:758:SER:O	1:J:759:LYS:HB3	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:712:ALA:O	1:M:716:ILE:HG12	2.19	0.43
1:N:725:HIS:CG	1:N:726:PRO:HD2	2.54	0.43
1:B:1020:ILE:HG22	1:B:1021:PRO:C	2.39	0.42
1:B:906:MET:HE3	1:B:906:MET:HB2	1.76	0.42
1:C:672:ASN:ND2	1:C:672:ASN:H	2.17	0.42
1:D:1033:PHE:CE1	1:D:1058:LYS:HE2	2.54	0.42
1:E:725:HIS:CG	1:E:726:PRO:HD2	2.54	0.42
1:E:978:PRO:HA	1:E:981:TRP:CD1	2.54	0.42
1:G:1030:ASP:N	1:G:1030:ASP:OD1	2.52	0.42
1:H:799:LYS:NZ	1:H:852:THR:HG23	2.34	0.42
1:H:978:PRO:HA	1:H:981:TRP:CD1	2.54	0.42
1:J:906:MET:HG3	1:J:910:PHE:CE1	2.53	0.42
1:K:758:SER:CB	1:K:768:LEU:HD21	2.49	0.42
1:K:821:ASN:O	1:K:822:LEU:HB3	2.19	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:A:799:LYS:NZ	1:A:852:THR:HG23	2.34	0.42
1:C:1025:TRP:HB2	1:C:1088:PHE:CZ	2.53	0.42
1:C:797:ASP:O	1:C:802:ASN:ND2	2.52	0.42
1:E:1030:ASP:OD1	1:E:1030:ASP:N	2.52	0.42
1:E:694:PHE:CG	1:E:695:GLN:N	2.86	0.42
1:E:725:HIS:CD2	1:E:727:ASN:HB2	2.55	0.42
1:F:1093:ILE:HG23	1:F:1094:GLY:N	2.34	0.42
1:F:1103:LEU:C	1:F:1105:ASP:H	2.22	0.42
1:F:758:SER:CB	1:F:768:LEU:HD21	2.49	0.42
1:I:798:LEU:HD23	1:I:798:LEU:HA	1.80	0.42
1:J:672:ASN:ND2	1:J:672:ASN:N	2.67	0.42
1:L:898:THR:HG23	1:L:900:SER:OG	2.19	0.42
1:N:1106:ASP:O	1:N:1110:ARG:HG3	2.18	0.42
1:A:1020:ILE:HB	1:A:1021:PRO:HA	2.01	0.42
1:B:999:ILE:HD12	1:B:999:ILE:N	2.35	0.42
1:C:767:LYS:HB2	1:C:767:LYS:HE2	1.84	0.42
1:G:1024:ASP:HA	1:G:1045:SER:O	2.19	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:906:MET:HG3	1:I:910:PHE:CE1	2.53	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:J:1030:ASP:N	1:J:1030:ASP:OD1	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1003:ASP:HA	1:L:1004:PRO:HA	1.91	0.42
1:M:1106:ASP:O	1:M:1110:ARG:HG3	2.19	0.42
1:N:1033:PHE:CE1	1:N:1058:LYS:HE2	2.54	0.42
1:A:860:LEU:HA	1:A:860:LEU:HD23	1.83	0.42
1:C:758:SER:CB	1:C:768:LEU:HD21	2.49	0.42
1:C:798:LEU:HD23	1:C:798:LEU:HA	1.81	0.42
1:E:758:SER:CB	1:E:768:LEU:HD21	2.49	0.42
1:G:828:ASP:HB2	2:G:1999:APJ:H25	2.00	0.42
1:G:845:ASN:ND2	1:G:845:ASN:N	2.67	0.42
1:M:1030:ASP:N	1:M:1030:ASP:OD1	2.52	0.42
1:M:1103:LEU:O	1:M:1105:ASP:N	2.52	0.42
1:C:748:CYS:N	2:C:1999:APJ:HN4	2.12	0.42
1:C:898:THR:HG23	1:C:900:SER:OG	2.19	0.42
1:D:758:SER:CB	1:D:768:LEU:HD21	2.49	0.42
1:D:964:ASP:HA	1:D:965:PRO:HD2	1.82	0.42
1:F:680:LEU:HD23	1:F:680:LEU:HA	1.87	0.42
1:F:705:LEU:N	1:F:705:LEU:HD12	2.34	0.42
1:I:805:VAL:HA	1:I:823:ARG:O	2.19	0.42
1:J:1041:ARG:HH22	1:J:1053:ARG:HG2	1.84	0.42
1:J:758:SER:CB	1:J:768:LEU:HD21	2.50	0.42
1:J:788:LEU:HA	1:J:788:LEU:HD13	1.88	0.42
1:K:1020:ILE:HB	1:K:1021:PRO:HA	2.02	0.42
1:L:758:SER:CB	1:L:768:LEU:HD21	2.50	0.42
1:N:758:SER:O	1:N:759:LYS:HB3	2.18	0.42
1:N:797:ASP:O	1:N:802:ASN:ND2	2.52	0.42
1:N:845:ASN:C	1:N:846:LEU:HD22	2.40	0.42
1:F:1020:ILE:HG22	1:F:1021:PRO:C	2.39	0.42
1:F:798:LEU:HA	1:F:798:LEU:HD23	1.80	0.42
1:H:1003:ASP:HA	1:H:1004:PRO:HA	1.91	0.42
1:H:857:ALA:O	1:H:860:LEU:HB2	2.19	0.42
1:L:821:ASN:O	1:L:822:LEU:HB3	2.19	0.42
1:L:857:ALA:O	1:L:860:LEU:HB2	2.19	0.42
1:M:773:ASN:O	1:M:776:SER:HB3	2.19	0.42
1:B:762:SER:O	1:B:765:ASN:HB3	2.20	0.42
1:D:1020:ILE:HB	1:D:1021:PRO:HA	2.02	0.42
1:E:919:HIS:CE1	1:E:921:PHE:HD2	2.38	0.42
1:E:970:THR:HG21	1:G:762:SER:CB	2.49	0.42
1:F:687:THR:HG23	1:F:704:MET:HG2	2.01	0.42
1:G:1106:ASP:O	1:G:1110:ARG:HG3	2.20	0.42
1:G:799:LYS:NZ	1:G:852:THR:HG23	2.35	0.42
1:G:978:PRO:HA	1:G:981:TRP:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1103:LEU:C	1:H:1105:ASP:H	2.22	0.42
1:G:1076:VAL:HG11	1:H:1108:ILE:HD11	2.02	0.42
1:I:946:ASP:HB3	1:I:949:LEU:HD12	2.00	0.42
1:J:740:PHE:HB3	1:J:741:LEU:H	1.64	0.42
1:L:694:PHE:CG	1:L:695:GLN:N	2.87	0.42
1:N:725:HIS:CD2	1:N:727:ASN:HB2	2.55	0.42
1:N:898:THR:HG23	1:N:900:SER:OG	2.20	0.42
1:A:929:SER:O	1:A:933:ARG:HG3	2.20	0.42
1:B:758:SER:CB	1:B:768:LEU:HD21	2.49	0.42
1:C:805:VAL:HA	1:C:823:ARG:O	2.20	0.42
1:D:860:LEU:HD23	1:D:860:LEU:HA	1.84	0.42
1:D:898:THR:OG1	1:D:899:ARG:N	2.52	0.42
1:E:1020:ILE:HB	1:E:1021:PRO:HA	2.01	0.42
1:F:1030:ASP:OD1	1:F:1030:ASP:N	2.53	0.42
1:F:821:ASN:O	1:F:822:LEU:HB3	2.19	0.42
1:H:1020:ILE:HB	1:H:1021:PRO:HA	2.02	0.42
1:H:898:THR:HG23	1:H:900:SER:OG	2.20	0.42
1:I:898:THR:HG23	1:I:900:SER:OG	2.20	0.42
1:J:805:VAL:HA	1:J:823:ARG:O	2.19	0.42
1:K:1008:LEU:HA	1:K:1008:LEU:HD23	1.79	0.42
1:K:978:PRO:HA	1:K:981:TRP:CD2	2.55	0.42
1:M:1055:LEU:O	1:M:1055:LEU:HD23	2.20	0.42
1:M:948:SER:HB3	1:M:1085:THR:HG23	2.02	0.42
1:C:1020:ILE:HB	1:C:1021:PRO:HA	2.02	0.42
1:C:999:ILE:HD12	1:C:999:ILE:N	2.35	0.42
1:D:1020:ILE:HG22	1:D:1021:PRO:C	2.40	0.42
1:F:729:ILE:HD12	1:F:745:LEU:HB3	2.02	0.42
1:F:845:ASN:C	1:F:846:LEU:HD22	2.41	0.42
1:G:1011:LYS:HE2	1:G:1011:LYS:HA	2.02	0.42
1:G:792:LYS:HE2	1:G:792:LYS:HB2	1.88	0.42
1:H:1030:ASP:OD1	1:H:1030:ASP:N	2.51	0.42
1:I:1093:ILE:HG23	1:I:1094:GLY:N	2.35	0.42
1:I:1106:ASP:O	1:I:1110:ARG:HG3	2.20	0.42
1:J:1033:PHE:CE1	1:J:1058:LYS:HE2	2.55	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:K:1082:ASP:HA	1:K:1085:THR:HB	2.01	0.42
1:K:805:VAL:HA	1:K:823:ARG:O	2.20	0.42
1:M:758:SER:O	1:M:759:LYS:HB3	2.19	0.42
1:N:737:THR:HG23	1:N:740:PHE:N	2.35	0.42
1:N:821:ASN:O	1:N:822:LEU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:PHE:HB3	1:A:823:ARG:HG3	2.01	0.42
1:A:898:THR:OG1	1:A:899:ARG:N	2.53	0.42
1:B:1030:ASP:N	1:B:1030:ASP:OD1	2.53	0.42
1:C:845:ASN:ND2	1:C:845:ASN:N	2.67	0.42
1:C:929:SER:O	1:C:933:ARG:HG3	2.20	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:692:GLY:O	1:E:699:VAL:HG22	2.20	0.42
1:E:712:ALA:O	1:E:716:ILE:HG12	2.20	0.42
1:E:821:ASN:O	1:E:822:LEU:HB3	2.20	0.42
1:F:787:HIS:O	1:F:790:SER:HB2	2.20	0.42
1:F:999:ILE:HD12	1:F:999:ILE:N	2.35	0.42
1:H:788:LEU:HA	1:H:788:LEU:HD13	1.84	0.42
1:H:811:PHE:HB3	1:H:823:ARG:HG3	2.02	0.42
1:J:1082:ASP:HA	1:J:1085:THR:HB	2.01	0.42
1:J:794:ILE:O	1:J:832:CYS:HB2	2.20	0.42
1:L:1106:ASP:O	1:L:1110:ARG:HG3	2.20	0.42
1:M:811:PHE:HB3	1:M:823:ARG:HG3	2.02	0.42
1:N:1037:LEU:C	1:N:1039:ARG:H	2.24	0.42
1:N:860:LEU:HD23	1:N:860:LEU:HA	1.83	0.42
1:A:799:LYS:HB2	1:A:800:PRO:CD	2.50	0.41
1:A:814:ASP:CG	1:B:787:HIS:HD2	2.23	0.41
1:B:799:LYS:NZ	1:B:852:THR:HG23	2.35	0.41
1:C:739:ARG:CG	1:C:739:ARG:HH11	2.33	0.41
1:C:761:VAL:HG12	1:F:840:SEP:P	2.59	0.41
1:C:978:PRO:HA	1:C:981:TRP:CD1	2.55	0.41
1:D:929:SER:O	1:D:933:ARG:HG3	2.20	0.41
1:E:1106:ASP:O	1:E:1110:ARG:HG3	2.19	0.41
1:H:805:VAL:HA	1:H:823:ARG:O	2.20	0.41
1:I:797:ASP:O	1:I:802:ASN:ND2	2.53	0.41
1:K:1020:ILE:HG22	1:K:1021:PRO:C	2.39	0.41
1:K:798:LEU:HD23	1:K:798:LEU:HA	1.82	0.41
1:L:898:THR:OG1	1:L:899:ARG:N	2.53	0.41
1:L:929:SER:O	1:L:933:ARG:HG3	2.20	0.41
1:B:725:HIS:CD2	1:B:727:ASN:HB2	2.56	0.41
1:B:787:HIS:O	1:B:790:SER:HB2	2.20	0.41
1:C:712:ALA:O	1:C:716:ILE:HG12	2.19	0.41
1:C:924:LYS:HG3	1:C:925:TYR:HD2	1.84	0.41
1:D:823:ARG:HH11	1:D:823:ARG:CG	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:761:VAL:CG1	1:H:840:SEP:O2P	2.69	0.41
1:I:1020:ILE:HG22	1:I:1021:PRO:C	2.40	0.41
1:I:811:PHE:HB3	1:I:823:ARG:HG3	2.01	0.41
1:J:857:ALA:O	1:J:860:LEU:HB2	2.20	0.41
1:J:999:ILE:N	1:J:999:ILE:HD12	2.34	0.41
1:K:712:ALA:O	1:K:716:ILE:HG12	2.20	0.41
1:K:792:LYS:HE2	1:K:792:LYS:HB2	1.88	0.41
1:K:978:PRO:HA	1:K:981:TRP:CG	2.55	0.41
1:M:1020:ILE:HG22	1:M:1021:PRO:C	2.39	0.41
1:M:1052:LEU:O	1:M:1055:LEU:HB3	2.20	0.41
1:M:797:ASP:O	1:M:802:ASN:ND2	2.53	0.41
1:M:805:VAL:HA	1:M:823:ARG:O	2.20	0.41
1:A:919:HIS:ND1	1:A:920:PRO:HD2	2.35	0.41
1:B:712:ALA:O	1:B:716:ILE:HG12	2.20	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:F:1020:ILE:HB	1:F:1021:PRO:HA	2.02	0.41
1:G:767:LYS:HB2	1:G:767:LYS:HE2	1.84	0.41
1:H:748:CYS:N	2:H:1999:APJ:HN4	2.13	0.41
1:H:948:SER:HB3	1:H:1085:THR:HG23	2.03	0.41
1:J:1008:LEU:HA	1:J:1008:LEU:HD23	1.79	0.41
1:J:811:PHE:HB3	1:J:823:ARG:HG3	2.01	0.41
2:K:1999:APJ:N1	2:K:1999:APJ:H15	2.36	0.41
1:L:1093:ILE:HG23	1:L:1094:GLY:N	2.34	0.41
1:N:948:SER:HB3	1:N:1085:THR:HG23	2.02	0.41
1:C:978:PRO:HA	1:C:981:TRP:CE2	2.55	0.41
1:D:680:LEU:HB2	1:D:689:VAL:HG12	2.01	0.41
1:D:666:PHE:CZ	1:D:690:PHE:CZ	3.07	0.41
1:D:968:ARG:HA	1:D:969:PRO:HD2	1.91	0.41
1:G:805:VAL:HA	1:G:823:ARG:O	2.20	0.41
1:H:1011:LYS:HE2	1:H:1011:LYS:HA	2.02	0.41
1:I:1063:MET:HB2	1:I:1063:MET:HE2	1.90	0.41
1:I:694:PHE:CG	1:I:695:GLN:N	2.87	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:J:821:ASN:O	1:J:822:LEU:HB3	2.20	0.41
1:J:978:PRO:HA	1:J:981:TRP:CE2	2.55	0.41
1:L:1055:LEU:O	1:L:1055:LEU:HD23	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:898:THR:HG23	1:A:900:SER:OG	2.20	0.41
1:B:898:THR:HG23	1:B:900:SER:OG	2.20	0.41
1:E:787:HIS:O	1:E:790:SER:HB2	2.20	0.41
1:E:845:ASN:C	1:E:846:LEU:HD22	2.41	0.41
1:E:929:SER:O	1:E:933:ARG:HG3	2.21	0.41
1:E:970:THR:CB	1:G:762:SER:CB	2.84	0.41
1:F:1003:ASP:HA	1:F:1004:PRO:HA	1.91	0.41
1:F:1033:PHE:CD2	1:F:1034:MET:HE3	2.56	0.41
1:F:805:VAL:HA	1:F:823:ARG:O	2.20	0.41
1:H:906:MET:HE3	1:H:906:MET:HB2	1.78	0.41
1:I:748:CYS:N	2:I:1999:APJ:HN4	2.13	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:M:767:LYS:HB2	1:M:767:LYS:HE2	1.83	0.41
1:N:767:LYS:HB2	1:N:767:LYS:HE2	1.83	0.41
1:N:845:ASN:N	1:N:845:ASN:ND2	2.67	0.41
1:C:1052:LEU:O	1:C:1055:LEU:HB3	2.20	0.41
1:C:694:PHE:CG	1:C:695:GLN:N	2.88	0.41
1:D:799:LYS:HB2	1:D:800:PRO:CD	2.51	0.41
1:D:895:ARG:HH12	1:D:964:ASP:CG	2.24	0.41
1:E:797:ASP:O	1:E:802:ASN:ND2	2.53	0.41
1:G:857:ALA:O	1:G:860:LEU:HB2	2.19	0.41
1:H:712:ALA:O	1:H:716:ILE:HG12	2.20	0.41
1:H:758:SER:CB	1:H:768:LEU:HD21	2.51	0.41
1:K:907:GLY:HA2	1:K:960:MET:HE1	2.02	0.41
1:L:1011:LYS:HE2	1:L:1011:LYS:HA	2.01	0.41
1:N:788:LEU:HD13	1:N:788:LEU:HA	1.89	0.41
1:N:857:ALA:O	1:N:860:LEU:HB2	2.20	0.41
1:A:915:SER:HB2	1:A:918:LYS:HB2	2.02	0.41
1:C:1103:LEU:C	1:C:1105:ASP:H	2.24	0.41
1:C:787:HIS:O	1:C:790:SER:HB2	2.21	0.41
1:C:811:PHE:HB3	1:C:823:ARG:HG3	2.02	0.41
1:D:978:PRO:HA	1:D:981:TRP:CD1	2.55	0.41
1:E:1011:LYS:HA	1:E:1011:LYS:HE2	2.03	0.41
1:G:799:LYS:HB2	1:G:800:PRO:HD2	2.03	0.41
1:H:672:ASN:H	1:H:672:ASN:ND2	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1103:LEU:C	1:J:1105:ASP:H	2.24	0.41
1:J:898:THR:HG23	1:J:900:SER:OG	2.21	0.41
1:K:787:HIS:O	1:K:790:SER:HB2	2.20	0.41
1:K:924:LYS:HG3	1:K:925:TYR:HD2	1.86	0.41
1:K:948:SER:HB3	1:K:1085:THR:HG23	2.03	0.41
1:L:948:SER:HB3	1:L:1085:THR:HG23	2.03	0.41
1:N:1011:LYS:HE2	1:N:1011:LYS:HA	2.02	0.41
1:C:1037:LEU:HB2	1:C:1058:LYS:HZ3	1.83	0.41
1:C:857:ALA:O	1:C:860:LEU:HB2	2.21	0.41
1:C:948:SER:HB3	1:C:1085:THR:HG23	2.03	0.41
1:D:1011:LYS:HE2	1:D:1011:LYS:HA	2.02	0.41
1:D:705:LEU:N	1:D:705:LEU:HD12	2.35	0.41
1:D:805:VAL:HA	1:D:823:ARG:O	2.21	0.41
1:F:762:SER:O	1:F:765:ASN:HB3	2.21	0.41
1:F:924:LYS:HG3	1:F:925:TYR:HD2	1.86	0.41
1:H:737:THR:HG23	1:H:740:PHE:N	2.36	0.41
1:H:924:LYS:HG3	1:H:925:TYR:HD2	1.86	0.41
1:J:797:ASP:O	1:J:802:ASN:ND2	2.54	0.41
1:M:1020:ILE:HB	1:M:1021:PRO:HA	2.03	0.41
1:M:978:PRO:HA	1:M:981:TRP:CG	2.56	0.41
1:N:791:LEU:C	1:N:792:LYS:HD3	2.41	0.41
1:A:978:PRO:HA	1:A:981:TRP:CD1	2.56	0.41
1:B:729:ILE:HD12	1:B:745:LEU:HB3	2.01	0.41
1:D:948:SER:HB3	1:D:1085:THR:HG23	2.03	0.41
1:F:948:SER:HB3	1:F:1085:THR:HG23	2.03	0.41
1:G:845:ASN:C	1:G:846:LEU:HD22	2.42	0.41
1:H:1106:ASP:O	1:H:1110:ARG:HG3	2.20	0.41
1:I:948:SER:HB3	1:I:1085:THR:HG23	2.02	0.41
1:J:1093:ILE:HG23	1:J:1094:GLY:N	2.36	0.41
1:K:978:PRO:HA	1:K:981:TRP:CE2	2.56	0.41
1:L:802:ASN:O	1:L:804:LEU:HD22	2.21	0.41
1:N:898:THR:OG1	1:N:899:ARG:N	2.54	0.41
1:A:712:ALA:O	1:A:716:ILE:HG12	2.21	0.41
1:A:845:ASN:C	1:A:846:LEU:HD22	2.42	0.41
1:A:906:MET:HB2	1:A:906:MET:HE3	1.75	0.41
1:B:1048:LEU:O	1:B:1049:MET:C	2.59	0.41
1:B:811:PHE:HB3	1:B:823:ARG:HG3	2.03	0.41
1:B:860:LEU:HA	1:B:860:LEU:HD23	1.85	0.41
1:D:1003:ASP:HA	1:D:1004:PRO:HA	1.91	0.41
1:D:1011:LYS:O	1:D:1014:ALA:HB3	2.21	0.41
2:D:1999:APJ:H15	2:D:1999:APJ:N1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1055:LEU:HD23	1:F:1055:LEU:O	2.21	0.41
1:G:929:SER:O	1:G:933:ARG:HG3	2.21	0.41
1:I:719:LEU:HA	1:I:719:LEU:HD23	1.73	0.41
1:I:758:SER:CB	1:I:768:LEU:HD21	2.51	0.41
1:I:788:LEU:HD13	1:I:788:LEU:HA	1.88	0.41
1:I:968:ARG:HA	1:I:969:PRO:HD2	1.91	0.41
1:L:1067:GLU:HG3	1:L:1067:GLU:H	1.74	0.41
1:L:1082:ASP:HA	1:L:1085:THR:HB	2.01	0.41
1:L:845:ASN:C	1:L:846:LEU:HD22	2.41	0.41
1:M:694:PHE:CG	1:M:695:GLN:N	2.86	0.41
1:M:725:HIS:CD2	1:M:727:ASN:HB2	2.56	0.41
1:M:821:ASN:O	1:M:822:LEU:HB3	2.21	0.41
1:N:968:ARG:HA	1:N:969:PRO:HD2	1.91	0.41
1:A:1034:MET:HE1	1:A:1037:LEU:HD23	2.01	0.41
1:B:1055:LEU:O	1:B:1055:LEU:HD23	2.21	0.41
1:B:1106:ASP:O	1:B:1110:ARG:HG3	2.20	0.41
1:B:964:ASP:HA	1:B:965:PRO:HD2	1.84	0.41
1:C:906:MET:HE3	1:C:906:MET:HB2	1.76	0.41
1:C:919:HIS:CE1	1:C:921:PHE:HD2	2.39	0.41
1:C:978:PRO:HA	1:C:981:TRP:CD2	2.56	0.41
1:G:1020:ILE:HB	1:G:1021:PRO:HA	2.02	0.41
1:G:712:ALA:O	1:G:716:ILE:HG12	2.21	0.41
1:G:797:ASP:O	1:G:802:ASN:ND2	2.54	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:J:929:SER:O	1:J:933:ARG:HG3	2.21	0.41
1:L:1033:PHE:CE1	1:L:1058:LYS:HE2	2.55	0.41
1:L:740:PHE:HB3	1:L:741:LEU:H	1.64	0.41
1:M:1011:LYS:HE2	1:M:1011:LYS:HA	2.03	0.41
1:M:1052:LEU:HD12	1:M:1052:LEU:HA	1.82	0.41
1:N:705:LEU:N	1:N:705:LEU:HD12	2.35	0.41
1:N:919:HIS:ND1	1:N:920:PRO:HD2	2.36	0.41
1:A:1033:PHE:CD2	1:A:1034:MET:HE2	2.56	0.40
1:A:694:PHE:CG	1:A:695:GLN:N	2.88	0.40
1:A:737:THR:HG23	1:A:740:PHE:N	2.36	0.40
1:B:737:THR:HG23	1:B:740:PHE:N	2.37	0.40
1:C:1010:MET:CE	1:C:1010:MET:HA	2.51	0.40
1:C:762:SER:O	1:C:765:ASN:HB3	2.21	0.40
1:C:845:ASN:C	1:C:846:LEU:HD22	2.42	0.40
1:C:906:MET:HG3	1:C:910:PHE:CE1	2.56	0.40
1:D:1030:ASP:OD1	1:D:1030:ASP:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1048:LEU:O	1:D:1049:MET:C	2.59	0.40
1:D:845:ASN:C	1:D:846:LEU:HD22	2.41	0.40
1:E:799:LYS:HB2	1:E:800:PRO:HD2	2.02	0.40
1:F:1048:LEU:O	1:F:1049:MET:C	2.59	0.40
1:F:1052:LEU:O	1:F:1055:LEU:HB3	2.22	0.40
1:G:1067:GLU:H	1:G:1067:GLU:HG3	1.73	0.40
1:G:737:THR:HG23	1:G:740:PHE:N	2.35	0.40
1:G:915:SER:HB2	1:G:918:LYS:HB2	2.03	0.40
1:G:968:ARG:HA	1:G:969:PRO:HD2	1.93	0.40
1:G:999:ILE:N	1:G:999:ILE:HD12	2.35	0.40
1:H:1093:ILE:HG23	1:H:1094:GLY:N	2.35	0.40
1:H:694:PHE:CG	1:H:695:GLN:N	2.87	0.40
1:I:767:LYS:HB2	1:I:767:LYS:HE2	1.83	0.40
1:J:845:ASN:C	1:J:846:LEU:HD22	2.41	0.40
1:J:978:PRO:HA	1:J:981:TRP:CG	2.56	0.40
1:K:1011:LYS:HE2	1:K:1011:LYS:HA	2.03	0.40
1:L:748:CYS:N	2:L:1999:APJ:HN4	2.12	0.40
1:L:712:ALA:O	1:L:716:ILE:HG12	2.21	0.40
1:L:767:LYS:HB2	1:L:767:LYS:HE2	1.83	0.40
1:M:1041:ARG:HG2	1:M:1042:LYS:N	2.36	0.40
1:M:845:ASN:C	1:M:846:LEU:HD22	2.42	0.40
1:N:792:LYS:HE2	1:N:792:LYS:HB2	1.87	0.40
1:N:799:LYS:HB2	1:N:800:PRO:HD2	2.02	0.40
1:N:810:ARG:H	1:N:810:ARG:HG3	1.71	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:E:811:PHE:HB3	1:E:823:ARG:HG3	2.03	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:F:811:PHE:HB3	1:F:823:ARG:HG3	2.03	0.40
1:F:895:ARG:HH12	1:F:964:ASP:CG	2.25	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:I:791:LEU:C	1:I:792:LYS:HD3	2.42	0.40
1:I:857:ALA:O	1:I:860:LEU:HB2	2.21	0.40
1:I:929:SER:O	1:I:933:ARG:HG3	2.21	0.40
1:J:1055:LEU:O	1:J:1055:LEU:HD23	2.21	0.40
1:J:1067:GLU:H	1:J:1067:GLU:HG3	1.72	0.40
1:K:1093:ILE:HG23	1:K:1094:GLY:N	2.37	0.40
1:K:668:GLN:NE2	1:K:668:GLN:N	2.69	0.40
1:L:811:PHE:HB3	1:L:823:ARG:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1033:PHE:CE1	1:M:1058:LYS:HE2	2.56	0.40
1:N:1020:ILE:HB	1:N:1021:PRO:HA	2.03	0.40
1:A:674:VAL:HG13	1:A:675:VAL:N	2.37	0.40
2:B:1999:APJ:N1	2:B:1999:APJ:H15	2.36	0.40
1:B:821:ASN:O	1:B:822:LEU:HB3	2.22	0.40
2:F:1999:APJ:H15	2:F:1999:APJ:N1	2.36	0.40
1:F:719:LEU:HA	1:F:719:LEU:HD23	1.68	0.40
1:F:773:ASN:O	1:F:776:SER:HB3	2.22	0.40
1:I:712:ALA:O	1:I:716:ILE:HG12	2.21	0.40
1:I:799:LYS:HB2	1:I:800:PRO:HD2	2.04	0.40
1:I:915:SER:HB2	1:I:918:LYS:HB2	2.02	0.40
1:J:1020:ILE:HB	1:J:1021:PRO:HA	2.02	0.40
1:J:762:SER:O	1:J:765:ASN:HB3	2.22	0.40
1:J:785:VAL:HG21	1:J:906:MET:HE3	2.01	0.40
1:N:1052:LEU:O	1:N:1055:LEU:HB3	2.22	0.40
1:N:915:SER:HB2	1:N:918:LYS:HB2	2.03	0.40
1:B:1020:ILE:HB	1:B:1021:PRO:HA	2.03	0.40
1:B:785:VAL:CG2	1:B:906:MET:HE1	2.51	0.40
1:C:705:LEU:N	1:C:705:LEU:HD12	2.37	0.40
1:D:1024:ASP:HA	1:D:1045:SER:O	2.21	0.40
1:D:822:LEU:N	1:D:822:LEU:HD23	2.36	0.40
1:E:705:LEU:HD12	1:E:705:LEU:N	2.36	0.40
1:E:895:ARG:HH12	1:E:964:ASP:CG	2.25	0.40
1:F:929:SER:O	1:F:933:ARG:HG3	2.21	0.40
1:F:978:PRO:HA	1:F:981:TRP:CD1	2.57	0.40
1:G:1052:LEU:O	1:G:1055:LEU:HB3	2.21	0.40
1:H:836:ASP:HB3	1:H:837:SER:H	1.74	0.40
1:H:978:PRO:HA	1:H:981:TRP:CD2	2.56	0.40
1:I:845:ASN:C	1:I:846:LEU:HD22	2.41	0.40
1:J:787:HIS:O	1:J:790:SER:HB2	2.21	0.40
1:J:948:SER:HB3	1:J:1085:THR:HG23	2.03	0.40
1:J:977:HIS:CE1	1:J:978:PRO:HG2	2.56	0.40
1:K:1048:LEU:O	1:K:1048:LEU:HD23	2.22	0.40
1:K:937:SER:O	1:K:938:LEU:HD23	2.22	0.40
1:M:907:GLY:HA2	1:M:960:MET:HE1	2.03	0.40
1:M:929:SER:O	1:M:933:ARG:HG3	2.22	0.40
1:M:968:ARG:HA	1:M:969:PRO:HD2	1.90	0.40
1:N:994:SER:HB2	1:N:1052:LEU:HG	2.02	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:N:799:LYS:HB2	1:N:800:PRO:CD	2.52	0.40

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

5.3.1 Protein backbone ⓘ

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

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

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	413/448 (92%)	351 (85%)	50 (12%)	12 (3%)	4	28
1	B	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	6	35
1	C	413/448 (92%)	348 (84%)	56 (14%)	9 (2%)	6	35
1	D	420/448 (94%)	353 (84%)	57 (14%)	10 (2%)	6	34
1	E	413/448 (92%)	354 (86%)	50 (12%)	9 (2%)	6	35
1	F	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	6	35
1	G	413/448 (92%)	351 (85%)	53 (13%)	9 (2%)	6	35
1	H	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	6	35
1	I	411/448 (92%)	353 (86%)	49 (12%)	9 (2%)	6	35
1	J	411/448 (92%)	350 (85%)	52 (13%)	9 (2%)	6	35
1	K	420/448 (94%)	349 (83%)	61 (14%)	10 (2%)	6	34
1	L	413/448 (92%)	352 (85%)	52 (13%)	9 (2%)	6	35
1	M	413/448 (92%)	353 (86%)	51 (12%)	9 (2%)	6	35
1	N	413/448 (92%)	353 (86%)	51 (12%)	9 (2%)	6	35
All	All	5792/6272 (92%)	4923 (85%)	738 (13%)	131 (2%)	6	34

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%)	13 45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	380/405 (94%)	352 (93%)	28 (7%)	13	46
1	C	380/405 (94%)	350 (92%)	30 (8%)	12	43
1	D	387/405 (96%)	353 (91%)	34 (9%)	10	36
1	E	380/405 (94%)	349 (92%)	31 (8%)	11	41
1	F	380/405 (94%)	349 (92%)	31 (8%)	11	41
1	G	380/405 (94%)	350 (92%)	30 (8%)	12	43
1	H	380/405 (94%)	350 (92%)	30 (8%)	12	43
1	I	378/405 (93%)	351 (93%)	27 (7%)	14	47
1	J	378/405 (93%)	351 (93%)	27 (7%)	14	47
1	K	387/405 (96%)	356 (92%)	31 (8%)	12	42
1	L	380/405 (94%)	350 (92%)	30 (8%)	12	43
1	M	380/405 (94%)	352 (93%)	28 (7%)	13	46
1	N	380/405 (94%)	347 (91%)	33 (9%)	10	37
All	All	5330/5670 (94%)	4911 (92%)	419 (8%)	12	43

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	C	841	1	8,9,10	1.54	1 (12%)	8,12,14	1.47	1 (12%)
1	SEP	H	840	1	8,9,10	1.60	1 (12%)	8,12,14	1.77	2 (25%)
1	TPO	M	844	1	8,10,11	3.00	5 (62%)	10,14,16	1.60	2 (20%)
1	SEP	K	841	1	8,9,10	1.53	1 (12%)	8,12,14	1.41	1 (12%)
1	SEP	H	841	1	8,9,10	1.54	1 (12%)	8,12,14	1.47	1 (12%)
1	TPO	E	844	1	8,10,11	2.98	5 (62%)	10,14,16	1.61	2 (20%)
1	SEP	I	840	1	8,9,10	1.58	1 (12%)	8,12,14	1.81	2 (25%)
1	TPO	N	844	1	8,10,11	2.97	5 (62%)	10,14,16	1.59	2 (20%)
1	SEP	F	840	1	8,9,10	1.56	1 (12%)	8,12,14	1.79	2 (25%)
1	TPO	L	844	1	8,10,11	2.98	5 (62%)	10,14,16	1.59	2 (20%)
1	SEP	N	840	1	8,9,10	1.60	1 (12%)	8,12,14	1.81	2 (25%)
1	SEP	L	840	1	8,9,10	1.58	1 (12%)	8,12,14	1.79	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TPO	A	844	1	8,10,11	2.99	5 (62%)	10,14,16	1.59	2 (20%)
1	SEP	G	840	1	8,9,10	1.58	1 (12%)	8,12,14	1.82	2 (25%)
1	SEP	E	840	1	8,9,10	1.56	1 (12%)	8,12,14	1.82	2 (25%)
1	SEP	B	841	1	8,9,10	1.51	1 (12%)	8,12,14	1.46	1 (12%)
1	TPO	J	844	1	8,10,11	2.97	5 (62%)	10,14,16	1.59	2 (20%)
1	SEP	J	841	1	8,9,10	1.53	1 (12%)	8,12,14	1.45	1 (12%)
1	TPO	B	844	1	8,10,11	2.98	5 (62%)	10,14,16	1.58	2 (20%)
1	SEP	D	840	1	8,9,10	1.60	1 (12%)	8,12,14	1.83	2 (25%)
1	TPO	F	844	1	8,10,11	3.00	5 (62%)	10,14,16	1.58	2 (20%)
1	SEP	J	840	1	8,9,10	1.58	1 (12%)	8,12,14	1.83	2 (25%)
1	SEP	A	841	1	8,9,10	1.52	1 (12%)	8,12,14	1.43	1 (12%)
1	TPO	K	844	1	8,10,11	3.00	5 (62%)	10,14,16	1.58	2 (20%)
1	SEP	A	840	1	8,9,10	1.57	1 (12%)	8,12,14	1.83	2 (25%)
1	SEP	I	841	1	8,9,10	1.55	1 (12%)	8,12,14	1.44	1 (12%)
1	TPO	C	844	1	8,10,11	2.96	5 (62%)	10,14,16	1.61	2 (20%)
1	TPO	H	844	1	8,10,11	2.98	5 (62%)	10,14,16	1.59	2 (20%)
1	SEP	M	840	1	8,9,10	1.57	1 (12%)	8,12,14	1.78	2 (25%)
1	SEP	B	840	1	8,9,10	1.58	1 (12%)	8,12,14	1.81	2 (25%)
1	TPO	D	844	1	8,10,11	2.99	5 (62%)	10,14,16	1.59	2 (20%)
1	SEP	K	840	1	8,9,10	1.58	1 (12%)	8,12,14	1.85	2 (25%)
1	TPO	G	844	1	8,10,11	2.99	5 (62%)	10,14,16	1.57	2 (20%)
1	TPO	I	844	1	8,10,11	3.00	5 (62%)	10,14,16	1.56	2 (20%)
1	SEP	F	841	1	8,9,10	1.62	1 (12%)	8,12,14	1.47	1 (12%)
1	SEP	G	841	1	8,9,10	1.53	1 (12%)	8,12,14	1.45	1 (12%)
1	SEP	D	841	1	8,9,10	1.50	1 (12%)	8,12,14	1.39	1 (12%)
1	SEP	E	841	1	8,9,10	1.52	1 (12%)	8,12,14	1.48	2 (25%)
1	SEP	N	841	1	8,9,10	1.56	1 (12%)	8,12,14	1.48	1 (12%)
1	SEP	L	841	1	8,9,10	1.54	1 (12%)	8,12,14	1.44	1 (12%)
1	SEP	M	841	1	8,9,10	1.49	1 (12%)	8,12,14	1.40	1 (12%)
1	SEP	C	840	1	8,9,10	1.58	1 (12%)	8,12,14	1.81	2 (25%)

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	C	841	1	-	1/5/8/10	-
1	SEP	H	840	1	-	4/5/8/10	-
1	TPO	M	844	1	-	4/9/11/13	-
1	SEP	K	841	1	-	1/5/8/10	-
1	SEP	H	841	1	-	1/5/8/10	-
1	TPO	E	844	1	-	4/9/11/13	-
1	SEP	I	840	1	-	4/5/8/10	-
1	TPO	N	844	1	-	4/9/11/13	-
1	SEP	F	840	1	-	4/5/8/10	-
1	TPO	L	844	1	-	4/9/11/13	-
1	SEP	N	840	1	-	4/5/8/10	-
1	SEP	L	840	1	-	4/5/8/10	-
1	TPO	A	844	1	-	4/9/11/13	-
1	SEP	G	840	1	-	4/5/8/10	-
1	SEP	E	840	1	-	3/5/8/10	-
1	SEP	B	841	1	-	1/5/8/10	-
1	TPO	J	844	1	-	4/9/11/13	-
1	SEP	J	841	1	-	1/5/8/10	-
1	TPO	B	844	1	-	4/9/11/13	-
1	SEP	D	840	1	-	4/5/8/10	-
1	TPO	F	844	1	-	4/9/11/13	-
1	SEP	J	840	1	-	4/5/8/10	-
1	SEP	A	841	1	-	1/5/8/10	-
1	TPO	K	844	1	-	4/9/11/13	-
1	SEP	A	840	1	-	4/5/8/10	-
1	SEP	I	841	1	-	1/5/8/10	-
1	TPO	C	844	1	-	4/9/11/13	-
1	TPO	H	844	1	-	4/9/11/13	-
1	SEP	M	840	1	-	4/5/8/10	-
1	SEP	B	840	1	-	4/5/8/10	-
1	TPO	D	844	1	-	4/9/11/13	-
1	SEP	K	840	1	-	4/5/8/10	-
1	TPO	G	844	1	-	4/9/11/13	-
1	TPO	I	844	1	-	4/9/11/13	-
1	SEP	F	841	1	-	1/5/8/10	-
1	SEP	G	841	1	-	1/5/8/10	-
1	SEP	D	841	1	-	1/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	E	841	1	-	1/5/8/10	-
1	SEP	N	841	1	-	1/5/8/10	-
1	SEP	L	841	1	-	1/5/8/10	-
1	SEP	M	841	1	-	1/5/8/10	-
1	SEP	C	840	1	-	4/5/8/10	-

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	844	TPO	O-C	5.30	1.41	1.19
1	F	844	TPO	O-C	5.18	1.40	1.19
1	I	844	TPO	O-C	5.17	1.40	1.19
1	M	844	TPO	O-C	5.17	1.40	1.19
1	K	844	TPO	O-C	5.16	1.40	1.19
1	C	844	TPO	O-C	5.15	1.40	1.19
1	N	844	TPO	O-C	5.15	1.40	1.19
1	G	844	TPO	O-C	5.15	1.40	1.19
1	E	844	TPO	O-C	5.15	1.40	1.19
1	L	844	TPO	O-C	5.14	1.40	1.19
1	H	844	TPO	O-C	5.14	1.40	1.19
1	A	844	TPO	O-C	5.14	1.40	1.19
1	J	844	TPO	O-C	5.14	1.40	1.19
1	D	844	TPO	O-C	5.14	1.40	1.19
1	K	844	TPO	P-O1P	4.62	1.65	1.50
1	G	844	TPO	P-O1P	4.61	1.65	1.50
1	E	844	TPO	P-O1P	4.58	1.65	1.50
1	M	844	TPO	P-O1P	4.58	1.65	1.50
1	A	844	TPO	P-O1P	4.57	1.65	1.50
1	F	844	TPO	P-O1P	4.57	1.65	1.50
1	D	844	TPO	P-O1P	4.57	1.65	1.50
1	J	844	TPO	P-O1P	4.57	1.65	1.50
1	H	844	TPO	P-O1P	4.56	1.65	1.50
1	I	844	TPO	P-O1P	4.54	1.65	1.50
1	N	844	TPO	P-O1P	4.53	1.65	1.50
1	B	844	TPO	P-O1P	4.53	1.65	1.50
1	L	844	TPO	P-O1P	4.53	1.65	1.50
1	C	844	TPO	P-O1P	4.50	1.65	1.50
1	F	841	SEP	P-O1P	3.59	1.62	1.50
1	H	840	SEP	P-O1P	3.50	1.61	1.50
1	L	840	SEP	P-O1P	3.49	1.61	1.50
1	N	840	SEP	P-O1P	3.48	1.61	1.50
1	B	840	SEP	P-O1P	3.45	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	840	SEP	P-O1P	3.45	1.61	1.50
1	I	840	SEP	P-O1P	3.45	1.61	1.50
1	N	841	SEP	P-O1P	3.44	1.61	1.50
1	D	840	SEP	P-O1P	3.44	1.61	1.50
1	J	840	SEP	P-O1P	3.44	1.61	1.50
1	F	844	TPO	P-OG1	3.44	1.65	1.59
1	H	841	SEP	P-O1P	3.44	1.61	1.50
1	I	844	TPO	P-OG1	3.43	1.65	1.59
1	G	840	SEP	P-O1P	3.42	1.61	1.50
1	E	840	SEP	P-O1P	3.41	1.61	1.50
1	A	840	SEP	P-O1P	3.40	1.61	1.50
1	F	840	SEP	P-O1P	3.40	1.61	1.50
1	G	841	SEP	P-O1P	3.39	1.61	1.50
1	C	841	SEP	P-O1P	3.38	1.61	1.50
1	C	840	SEP	P-O1P	3.38	1.61	1.50
1	M	840	SEP	P-O1P	3.38	1.61	1.50
1	I	841	SEP	P-O1P	3.38	1.61	1.50
1	L	841	SEP	P-O1P	3.38	1.61	1.50
1	A	841	SEP	P-O1P	3.35	1.61	1.50
1	M	844	TPO	P-OG1	3.35	1.65	1.59
1	D	844	TPO	P-OG1	3.35	1.65	1.59
1	J	841	SEP	P-O1P	3.34	1.61	1.50
1	K	844	TPO	P-OG1	3.34	1.65	1.59
1	A	844	TPO	P-OG1	3.33	1.65	1.59
1	E	841	SEP	P-O1P	3.32	1.61	1.50
1	L	844	TPO	P-OG1	3.31	1.65	1.59
1	K	841	SEP	P-O1P	3.30	1.61	1.50
1	B	841	SEP	P-O1P	3.29	1.61	1.50
1	M	841	SEP	P-O1P	3.28	1.61	1.50
1	G	844	TPO	P-OG1	3.28	1.65	1.59
1	H	844	TPO	P-OG1	3.28	1.65	1.59
1	E	844	TPO	P-OG1	3.26	1.65	1.59
1	D	841	SEP	P-O1P	3.24	1.61	1.50
1	N	844	TPO	P-OG1	3.24	1.65	1.59
1	J	844	TPO	P-OG1	3.24	1.65	1.59
1	C	844	TPO	P-OG1	3.21	1.65	1.59
1	B	844	TPO	P-OG1	3.21	1.65	1.59
1	A	844	TPO	P-O2P	2.75	1.65	1.54
1	J	844	TPO	P-O2P	2.75	1.65	1.54
1	L	844	TPO	P-O2P	2.74	1.65	1.54
1	D	844	TPO	P-O2P	2.72	1.65	1.54
1	H	844	TPO	P-O2P	2.72	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	844	TPO	P-O2P	2.72	1.65	1.54
1	C	844	TPO	P-O2P	2.71	1.65	1.54
1	K	844	TPO	P-O2P	2.70	1.65	1.54
1	G	844	TPO	P-O2P	2.70	1.65	1.54
1	M	844	TPO	P-O2P	2.70	1.65	1.54
1	E	844	TPO	P-O2P	2.70	1.65	1.54
1	F	844	TPO	P-O2P	2.70	1.65	1.54
1	I	844	TPO	P-O2P	2.69	1.65	1.54
1	B	844	TPO	P-O2P	2.56	1.64	1.54
1	D	844	TPO	P-O3P	-2.18	1.46	1.54
1	C	844	TPO	P-O3P	-2.18	1.46	1.54
1	N	844	TPO	P-O3P	-2.17	1.46	1.54
1	B	844	TPO	P-O3P	-2.16	1.46	1.54
1	I	844	TPO	P-O3P	-2.16	1.46	1.54
1	L	844	TPO	P-O3P	-2.16	1.46	1.54
1	K	844	TPO	P-O3P	-2.16	1.46	1.54
1	H	844	TPO	P-O3P	-2.16	1.46	1.54
1	A	844	TPO	P-O3P	-2.16	1.46	1.54
1	M	844	TPO	P-O3P	-2.15	1.46	1.54
1	E	844	TPO	P-O3P	-2.14	1.46	1.54
1	G	844	TPO	P-O3P	-2.14	1.46	1.54
1	J	844	TPO	P-O3P	-2.14	1.46	1.54
1	F	844	TPO	P-O3P	-2.12	1.46	1.54

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	844	TPO	O-C-CA	-4.13	113.95	124.78
1	N	844	TPO	O-C-CA	-4.12	113.99	124.78
1	E	844	TPO	O-C-CA	-4.11	114.00	124.78
1	M	844	TPO	O-C-CA	-4.11	114.00	124.78
1	J	844	TPO	O-C-CA	-4.10	114.04	124.78
1	D	844	TPO	O-C-CA	-4.08	114.07	124.78
1	H	844	TPO	O-C-CA	-4.07	114.11	124.78
1	L	844	TPO	O-C-CA	-4.07	114.11	124.78
1	A	844	TPO	O-C-CA	-4.07	114.12	124.78
1	F	844	TPO	O-C-CA	-4.04	114.19	124.78
1	G	844	TPO	O-C-CA	-4.03	114.22	124.78
1	K	844	TPO	O-C-CA	-4.02	114.25	124.78
1	I	844	TPO	O-C-CA	-4.01	114.26	124.78
1	B	844	TPO	O-C-CA	-3.95	114.42	124.78
1	H	840	SEP	P-OG-CB	-3.68	108.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	841	SEP	P-OG-CB	-3.68	108.17	118.30
1	F	841	SEP	P-OG-CB	-3.67	108.19	118.30
1	D	840	SEP	OG-CB-CA	3.66	111.71	108.14
1	F	840	SEP	P-OG-CB	-3.64	108.28	118.30
1	N	841	SEP	P-OG-CB	-3.62	108.33	118.30
1	G	840	SEP	P-OG-CB	-3.61	108.35	118.30
1	M	840	SEP	P-OG-CB	-3.60	108.36	118.30
1	K	841	SEP	P-OG-CB	-3.60	108.38	118.30
1	C	841	SEP	P-OG-CB	-3.59	108.41	118.30
1	I	840	SEP	P-OG-CB	-3.58	108.44	118.30
1	N	840	SEP	P-OG-CB	-3.58	108.44	118.30
1	J	840	SEP	P-OG-CB	-3.57	108.45	118.30
1	B	840	SEP	P-OG-CB	-3.54	108.53	118.30
1	A	840	SEP	P-OG-CB	-3.54	108.53	118.30
1	L	840	SEP	P-OG-CB	-3.54	108.55	118.30
1	H	841	SEP	P-OG-CB	-3.53	108.56	118.30
1	L	841	SEP	P-OG-CB	-3.53	108.58	118.30
1	E	840	SEP	P-OG-CB	-3.53	108.58	118.30
1	K	840	SEP	P-OG-CB	-3.53	108.58	118.30
1	J	841	SEP	P-OG-CB	-3.49	108.67	118.30
1	D	841	SEP	P-OG-CB	-3.49	108.67	118.30
1	K	840	SEP	OG-CB-CA	3.48	111.53	108.14
1	G	841	SEP	P-OG-CB	-3.48	108.70	118.30
1	C	840	SEP	P-OG-CB	-3.48	108.71	118.30
1	I	841	SEP	P-OG-CB	-3.45	108.80	118.30
1	M	841	SEP	P-OG-CB	-3.42	108.87	118.30
1	E	841	SEP	P-OG-CB	-3.41	108.90	118.30
1	E	840	SEP	OG-CB-CA	3.36	111.41	108.14
1	A	840	SEP	OG-CB-CA	3.35	111.40	108.14
1	J	840	SEP	OG-CB-CA	3.34	111.40	108.14
1	B	840	SEP	OG-CB-CA	3.34	111.39	108.14
1	C	840	SEP	OG-CB-CA	3.31	111.36	108.14
1	A	841	SEP	P-OG-CB	-3.30	109.20	118.30
1	I	840	SEP	OG-CB-CA	3.26	111.32	108.14
1	N	840	SEP	OG-CB-CA	3.26	111.32	108.14
1	D	840	SEP	P-OG-CB	-3.25	109.35	118.30
1	G	840	SEP	OG-CB-CA	3.22	111.28	108.14
1	L	840	SEP	OG-CB-CA	3.20	111.26	108.14
1	F	840	SEP	OG-CB-CA	3.09	111.15	108.14
1	M	840	SEP	OG-CB-CA	3.07	111.13	108.14
1	H	840	SEP	OG-CB-CA	2.98	111.05	108.14
1	F	844	TPO	CG2-CB-CA	-2.23	108.76	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	844	TPO	CG2-CB-CA	-2.22	108.79	113.16
1	L	844	TPO	CG2-CB-CA	-2.22	108.79	113.16
1	B	844	TPO	CG2-CB-CA	-2.20	108.83	113.16
1	N	844	TPO	CG2-CB-CA	-2.20	108.83	113.16
1	A	844	TPO	CG2-CB-CA	-2.19	108.84	113.16
1	E	844	TPO	CG2-CB-CA	-2.19	108.84	113.16
1	K	844	TPO	CG2-CB-CA	-2.19	108.85	113.16
1	M	844	TPO	CG2-CB-CA	-2.18	108.86	113.16
1	H	844	TPO	CG2-CB-CA	-2.17	108.88	113.16
1	I	844	TPO	CG2-CB-CA	-2.17	108.88	113.16
1	C	844	TPO	CG2-CB-CA	-2.16	108.90	113.16
1	G	844	TPO	CG2-CB-CA	-2.08	109.06	113.16
1	J	844	TPO	CG2-CB-CA	-2.08	109.06	113.16
1	E	841	SEP	OG-CB-CA	2.02	110.11	108.14

There are no chirality outliers.

All (125) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	H	840	SEP	CB-OG-P-O2P
1	H	840	SEP	CB-OG-P-O3P
1	M	844	TPO	N-CA-CB-CG2
1	M	844	TPO	N-CA-CB-OG1
1	M	844	TPO	O-C-CA-CB
1	E	844	TPO	N-CA-CB-CG2
1	E	844	TPO	N-CA-CB-OG1
1	E	844	TPO	O-C-CA-CB
1	I	840	SEP	CB-OG-P-O2P
1	I	840	SEP	CB-OG-P-O3P
1	N	844	TPO	N-CA-CB-CG2
1	N	844	TPO	N-CA-CB-OG1
1	N	844	TPO	O-C-CA-CB
1	F	840	SEP	N-CA-CB-OG
1	F	840	SEP	CB-OG-P-O2P
1	F	840	SEP	CB-OG-P-O3P
1	L	844	TPO	N-CA-CB-CG2
1	L	844	TPO	N-CA-CB-OG1
1	L	844	TPO	O-C-CA-CB
1	N	840	SEP	N-CA-CB-OG
1	N	840	SEP	CB-OG-P-O2P
1	N	840	SEP	CB-OG-P-O3P
1	L	840	SEP	N-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
1	L	840	SEP	CB-OG-P-O2P
1	L	840	SEP	CB-OG-P-O3P
1	A	844	TPO	N-CA-CB-CG2
1	A	844	TPO	N-CA-CB-OG1
1	A	844	TPO	O-C-CA-CB
1	G	840	SEP	CB-OG-P-O2P
1	G	840	SEP	CB-OG-P-O3P
1	E	840	SEP	CB-OG-P-O2P
1	E	840	SEP	CB-OG-P-O3P
1	J	844	TPO	N-CA-CB-CG2
1	J	844	TPO	N-CA-CB-OG1
1	J	844	TPO	O-C-CA-CB
1	B	844	TPO	N-CA-CB-CG2
1	B	844	TPO	N-CA-CB-OG1
1	B	844	TPO	O-C-CA-CB
1	D	840	SEP	N-CA-CB-OG
1	D	840	SEP	CB-OG-P-O2P
1	D	840	SEP	CB-OG-P-O3P
1	F	844	TPO	N-CA-CB-CG2
1	F	844	TPO	N-CA-CB-OG1
1	F	844	TPO	O-C-CA-CB
1	J	840	SEP	N-CA-CB-OG
1	J	840	SEP	CB-OG-P-O2P
1	J	840	SEP	CB-OG-P-O3P
1	K	844	TPO	N-CA-CB-CG2
1	K	844	TPO	N-CA-CB-OG1
1	K	844	TPO	O-C-CA-CB
1	A	840	SEP	N-CA-CB-OG
1	A	840	SEP	CB-OG-P-O2P
1	A	840	SEP	CB-OG-P-O3P
1	C	844	TPO	N-CA-CB-CG2
1	C	844	TPO	N-CA-CB-OG1
1	C	844	TPO	O-C-CA-CB
1	H	844	TPO	N-CA-CB-CG2
1	H	844	TPO	N-CA-CB-OG1
1	H	844	TPO	O-C-CA-CB
1	M	840	SEP	CB-OG-P-O2P
1	M	840	SEP	CB-OG-P-O3P
1	B	840	SEP	N-CA-CB-OG
1	B	840	SEP	CB-OG-P-O2P
1	B	840	SEP	CB-OG-P-O3P
1	D	844	TPO	N-CA-CB-CG2

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Mol	Chain	Res	Type	Atoms
1	D	844	TPO	N-CA-CB-OG1
1	D	844	TPO	O-C-CA-CB
1	K	840	SEP	N-CA-CB-OG
1	K	840	SEP	CB-OG-P-O2P
1	K	840	SEP	CB-OG-P-O3P
1	G	844	TPO	N-CA-CB-CG2
1	G	844	TPO	N-CA-CB-OG1
1	G	844	TPO	O-C-CA-CB
1	I	844	TPO	N-CA-CB-CG2
1	I	844	TPO	N-CA-CB-OG1
1	I	844	TPO	O-C-CA-CB
1	F	841	SEP	CB-OG-P-O3P
1	L	841	SEP	CB-OG-P-O3P
1	C	840	SEP	CB-OG-P-O2P
1	C	840	SEP	CB-OG-P-O3P
1	C	841	SEP	CB-OG-P-O3P
1	H	841	SEP	CB-OG-P-O3P
1	B	841	SEP	CB-OG-P-O3P
1	J	841	SEP	CB-OG-P-O3P
1	A	841	SEP	CB-OG-P-O3P
1	I	841	SEP	CB-OG-P-O3P
1	G	841	SEP	CB-OG-P-O3P
1	E	841	SEP	CB-OG-P-O3P
1	N	841	SEP	CB-OG-P-O3P
1	M	841	SEP	CB-OG-P-O3P
1	H	840	SEP	N-CA-CB-OG
1	I	840	SEP	N-CA-CB-OG
1	G	840	SEP	N-CA-CB-OG
1	E	840	SEP	N-CA-CB-OG
1	M	840	SEP	N-CA-CB-OG
1	C	840	SEP	N-CA-CB-OG
1	K	841	SEP	CB-OG-P-O3P
1	D	841	SEP	CB-OG-P-O3P
1	H	840	SEP	CB-OG-P-O1P
1	I	840	SEP	CB-OG-P-O1P
1	F	840	SEP	CB-OG-P-O1P
1	N	840	SEP	CB-OG-P-O1P
1	L	840	SEP	CB-OG-P-O1P
1	G	840	SEP	CB-OG-P-O1P
1	D	840	SEP	CB-OG-P-O1P
1	J	840	SEP	CB-OG-P-O1P
1	A	840	SEP	CB-OG-P-O1P

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Mol	Chain	Res	Type	Atoms
1	M	840	SEP	CB-OG-P-O1P
1	B	840	SEP	CB-OG-P-O1P
1	K	840	SEP	CB-OG-P-O1P
1	C	840	SEP	CB-OG-P-O1P
1	M	844	TPO	CB-OG1-P-O2P
1	E	844	TPO	CB-OG1-P-O2P
1	N	844	TPO	CB-OG1-P-O2P
1	L	844	TPO	CB-OG1-P-O2P
1	A	844	TPO	CB-OG1-P-O2P
1	J	844	TPO	CB-OG1-P-O2P
1	B	844	TPO	CB-OG1-P-O2P
1	F	844	TPO	CB-OG1-P-O2P
1	K	844	TPO	CB-OG1-P-O2P
1	C	844	TPO	CB-OG1-P-O2P
1	H	844	TPO	CB-OG1-P-O2P
1	D	844	TPO	CB-OG1-P-O2P
1	G	844	TPO	CB-OG1-P-O2P
1	I	844	TPO	CB-OG1-P-O2P

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	H	840	SEP	3	0
1	K	841	SEP	2	0
1	F	840	SEP	3	0
1	G	840	SEP	1	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	K	1999	-	26,29,29	1.80	5 (19%)	30,41,41	2.76	11 (36%)
2	APJ	J	1999	-	26,29,29	1.82	6 (23%)	30,41,41	2.74	11 (36%)
2	APJ	I	1999	-	26,29,29	1.81	6 (23%)	30,41,41	2.77	12 (40%)
2	APJ	H	1999	-	26,29,29	1.78	6 (23%)	30,41,41	2.76	12 (40%)
2	APJ	N	1999	-	26,29,29	1.77	5 (19%)	30,41,41	2.79	11 (36%)
2	APJ	M	1999	-	26,29,29	1.80	6 (23%)	30,41,41	2.77	11 (36%)
2	APJ	L	1999	-	26,29,29	1.79	5 (19%)	30,41,41	2.77	11 (36%)
2	APJ	C	1999	-	26,29,29	1.78	6 (23%)	30,41,41	2.88	11 (36%)
2	APJ	B	1999	-	26,29,29	1.80	6 (23%)	30,41,41	2.77	11 (36%)
2	APJ	A	1999	-	26,29,29	1.88	6 (23%)	30,41,41	2.78	12 (40%)
2	APJ	G	1999	-	26,29,29	1.84	6 (23%)	30,41,41	2.77	11 (36%)
2	APJ	F	1999	-	26,29,29	1.77	6 (23%)	30,41,41	2.76	12 (40%)
2	APJ	E	1999	-	26,29,29	1.76	5 (19%)	30,41,41	2.77	11 (36%)
2	APJ	D	1999	-	26,29,29	1.79	5 (19%)	30,41,41	2.77	12 (40%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	APJ	D	1999	-	-	2/10/14/14	0/5/5/5

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1999	APJ	N5-N4	-5.81	1.26	1.37
2	C	1999	APJ	N5-N4	-5.72	1.26	1.37
2	G	1999	APJ	N5-N4	-5.72	1.26	1.37
2	D	1999	APJ	N5-N4	-5.64	1.26	1.37
2	H	1999	APJ	N5-N4	-5.64	1.26	1.37
2	E	1999	APJ	N5-N4	-5.64	1.26	1.37
2	I	1999	APJ	N5-N4	-5.60	1.26	1.37
2	L	1999	APJ	N5-N4	-5.58	1.26	1.37
2	B	1999	APJ	N5-N4	-5.57	1.26	1.37
2	M	1999	APJ	N5-N4	-5.55	1.26	1.37
2	F	1999	APJ	N5-N4	-5.55	1.26	1.37
2	J	1999	APJ	N5-N4	-5.54	1.26	1.37
2	K	1999	APJ	N5-N4	-5.53	1.26	1.37
2	N	1999	APJ	N5-N4	-5.47	1.26	1.37
2	A	1999	APJ	C10-N1	3.00	1.40	1.34
2	A	1999	APJ	C9-N2	2.99	1.38	1.34
2	K	1999	APJ	C9-N2	2.86	1.38	1.34
2	D	1999	APJ	C10-N1	2.83	1.40	1.34
2	G	1999	APJ	C9-N2	2.83	1.38	1.34
2	N	1999	APJ	C9-N2	2.78	1.38	1.34
2	G	1999	APJ	C9-N6	2.76	1.42	1.36
2	J	1999	APJ	C9-N6	2.73	1.42	1.36
2	C	1999	APJ	C9-N2	2.71	1.38	1.34
2	B	1999	APJ	C9-N2	2.70	1.38	1.34
2	K	1999	APJ	C9-N6	2.65	1.41	1.36
2	N	1999	APJ	C10-N1	2.64	1.39	1.34
2	L	1999	APJ	C9-N2	2.63	1.38	1.34
2	M	1999	APJ	C9-N2	2.63	1.38	1.34
2	F	1999	APJ	C9-N2	2.62	1.38	1.34
2	M	1999	APJ	C10-N1	2.61	1.39	1.34
2	L	1999	APJ	C10-N1	2.60	1.39	1.34
2	J	1999	APJ	C10-N1	2.58	1.39	1.34
2	F	1999	APJ	C10-N1	2.56	1.39	1.34
2	D	1999	APJ	C10-N3	2.55	1.43	1.38
2	I	1999	APJ	C10-N1	2.54	1.39	1.34
2	J	1999	APJ	C9-N2	2.53	1.38	1.34
2	I	1999	APJ	C9-N6	2.52	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1999	APJ	C9-N6	2.48	1.41	1.36
2	I	1999	APJ	C9-N2	2.48	1.38	1.34
2	B	1999	APJ	C10-N1	2.46	1.39	1.34
2	A	1999	APJ	C10-N3	2.46	1.43	1.38
2	C	1999	APJ	C10-N1	2.45	1.39	1.34
2	H	1999	APJ	C10-N1	2.45	1.39	1.34
2	L	1999	APJ	C9-N6	2.44	1.41	1.36
2	N	1999	APJ	C10-N3	2.44	1.42	1.38
2	K	1999	APJ	C10-N1	2.42	1.39	1.34
2	E	1999	APJ	C9-N2	2.42	1.38	1.34
2	G	1999	APJ	C10-N1	2.41	1.39	1.34
2	E	1999	APJ	C9-N6	2.41	1.41	1.36
2	A	1999	APJ	C9-N6	2.40	1.41	1.36
2	H	1999	APJ	C9-N2	2.40	1.38	1.34
2	B	1999	APJ	C9-N6	2.37	1.41	1.36
2	J	1999	APJ	C10-N3	2.35	1.42	1.38
2	C	1999	APJ	C10-N3	2.33	1.42	1.38
2	M	1999	APJ	C9-N6	2.33	1.41	1.36
2	N	1999	APJ	C23-C22	-2.33	1.37	1.41
2	C	1999	APJ	C9-N6	2.32	1.41	1.36
2	I	1999	APJ	C10-N3	2.30	1.42	1.38
2	M	1999	APJ	C23-C22	-2.29	1.37	1.41
2	E	1999	APJ	C10-N1	2.28	1.38	1.34
2	D	1999	APJ	C23-C22	-2.28	1.37	1.41
2	L	1999	APJ	C10-N3	2.28	1.42	1.38
2	M	1999	APJ	C10-N3	2.26	1.42	1.38
2	D	1999	APJ	C9-N2	2.26	1.37	1.34
2	B	1999	APJ	C10-N3	2.25	1.42	1.38
2	B	1999	APJ	C23-C22	-2.25	1.38	1.41
2	F	1999	APJ	C10-N3	2.20	1.42	1.38
2	F	1999	APJ	C23-C22	-2.20	1.38	1.41
2	G	1999	APJ	C10-N3	2.19	1.42	1.38
2	H	1999	APJ	C10-N3	2.18	1.42	1.38
2	E	1999	APJ	C23-C22	-2.16	1.38	1.41
2	I	1999	APJ	C23-C22	-2.15	1.38	1.41
2	G	1999	APJ	C23-C22	-2.12	1.38	1.41
2	C	1999	APJ	C23-C22	-2.11	1.38	1.41
2	F	1999	APJ	C9-N6	2.11	1.40	1.36
2	K	1999	APJ	C23-C22	-2.10	1.38	1.41
2	J	1999	APJ	C23-C22	-2.09	1.38	1.41
2	H	1999	APJ	C23-C22	-2.08	1.38	1.41
2	A	1999	APJ	C23-C22	-2.02	1.38	1.41

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1999	APJ	N2-C9-N1	-7.48	119.46	126.55
2	I	1999	APJ	N2-C9-N1	-7.18	119.74	126.55
2	M	1999	APJ	N2-C9-N1	-7.11	119.81	126.55
2	G	1999	APJ	N2-C9-N1	-7.10	119.82	126.55
2	L	1999	APJ	N2-C9-N1	-7.09	119.83	126.55
2	K	1999	APJ	N2-C9-N1	-7.05	119.87	126.55
2	H	1999	APJ	N2-C9-N1	-7.00	119.92	126.55
2	A	1999	APJ	N2-C9-N1	-6.98	119.94	126.55
2	C	1999	APJ	N2-C9-N1	-6.69	120.21	126.55
2	E	1999	APJ	N2-C9-N1	-6.68	120.22	126.55
2	B	1999	APJ	N2-C9-N1	-6.67	120.23	126.55
2	D	1999	APJ	N2-C9-N1	-6.58	120.31	126.55
2	C	1999	APJ	C12-N2-C9	6.38	121.11	115.45
2	L	1999	APJ	C12-N2-C9	6.37	121.10	115.45
2	F	1999	APJ	C12-N2-C9	6.34	121.07	115.45
2	D	1999	APJ	C12-N2-C9	6.29	121.03	115.45
2	N	1999	APJ	C12-N2-C9	6.27	121.01	115.45
2	M	1999	APJ	C12-N2-C9	6.27	121.01	115.45
2	B	1999	APJ	C12-N2-C9	6.26	121.00	115.45
2	C	1999	APJ	C17-C16-C14	-6.20	113.05	120.33
2	F	1999	APJ	N2-C9-N1	-6.19	120.68	126.55
2	N	1999	APJ	N2-C9-N1	-6.19	120.69	126.55
2	K	1999	APJ	C12-N2-C9	6.16	120.91	115.45
2	J	1999	APJ	C12-N2-C9	6.15	120.91	115.45
2	A	1999	APJ	C12-N2-C9	6.15	120.90	115.45
2	I	1999	APJ	C12-N2-C9	6.03	120.80	115.45
2	H	1999	APJ	C12-N2-C9	5.99	120.76	115.45
2	E	1999	APJ	C12-N2-C9	5.96	120.74	115.45
2	G	1999	APJ	C12-N2-C9	5.93	120.71	115.45
2	E	1999	APJ	C17-C16-C14	-5.87	113.43	120.33
2	N	1999	APJ	C17-C16-C14	-5.86	113.45	120.33
2	N	1999	APJ	C12-C11-C10	5.76	120.53	116.76
2	C	1999	APJ	C12-C11-C10	5.76	120.53	116.76
2	H	1999	APJ	C17-C16-C14	-5.69	113.64	120.33
2	L	1999	APJ	C17-C16-C14	-5.64	113.71	120.33
2	I	1999	APJ	C17-C16-C14	-5.63	113.72	120.33
2	G	1999	APJ	C17-C16-C14	-5.62	113.72	120.33
2	B	1999	APJ	C12-C11-C10	5.56	120.40	116.76
2	E	1999	APJ	C12-C11-C10	5.55	120.39	116.76
2	D	1999	APJ	C17-C16-C14	-5.50	113.87	120.33
2	G	1999	APJ	C12-C11-C10	5.47	120.34	116.76
2	M	1999	APJ	C17-C16-C14	-5.44	113.93	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1999	APJ	C17-C16-C14	-5.44	113.94	120.33
2	F	1999	APJ	C12-C11-C10	5.44	120.32	116.76
2	F	1999	APJ	C17-C16-C14	-5.43	113.95	120.33
2	A	1999	APJ	C17-C16-C14	-5.42	113.96	120.33
2	J	1999	APJ	C17-C16-C14	-5.42	113.96	120.33
2	H	1999	APJ	C12-C11-C10	5.30	120.23	116.76
2	K	1999	APJ	C12-C11-C10	5.17	120.14	116.76
2	B	1999	APJ	C17-C16-C14	-5.17	114.26	120.33
2	I	1999	APJ	C12-C11-C10	5.07	120.08	116.76
2	L	1999	APJ	C12-C11-C10	4.96	120.01	116.76
2	A	1999	APJ	C12-C11-C10	4.94	119.99	116.76
2	M	1999	APJ	C12-C11-C10	4.91	119.97	116.76
2	J	1999	APJ	C12-C11-C10	4.76	119.87	116.76
2	D	1999	APJ	C12-C11-C10	4.70	119.83	116.76
2	D	1999	APJ	C16-C14-N5	4.15	126.36	120.23
2	N	1999	APJ	C11-C12-N2	-4.09	118.87	123.96
2	C	1999	APJ	C16-C14-N5	4.07	126.24	120.23
2	B	1999	APJ	C16-C14-N5	4.05	126.22	120.23
2	F	1999	APJ	C11-C12-N2	-4.05	118.93	123.96
2	A	1999	APJ	C16-C14-N5	4.02	126.17	120.23
2	H	1999	APJ	C16-C14-N5	4.02	126.17	120.23
2	I	1999	APJ	C16-C14-N5	4.01	126.16	120.23
2	C	1999	APJ	C11-C12-N2	-3.97	119.03	123.96
2	J	1999	APJ	C16-C14-N5	3.97	126.09	120.23
2	L	1999	APJ	C16-C14-N5	3.94	126.04	120.23
2	G	1999	APJ	C16-C14-N5	3.91	126.01	120.23
2	K	1999	APJ	C16-C14-N5	3.90	125.99	120.23
2	M	1999	APJ	C16-C14-N5	3.90	125.99	120.23
2	B	1999	APJ	C11-C12-N2	-3.86	119.16	123.96
2	E	1999	APJ	C16-C14-N5	3.80	125.84	120.23
2	N	1999	APJ	C16-C14-N5	3.76	125.78	120.23
2	F	1999	APJ	C16-C14-N5	3.75	125.76	120.23
2	E	1999	APJ	C11-C12-N2	-3.69	119.38	123.96
2	D	1999	APJ	C19-C20-C21	-3.65	116.51	120.50
2	K	1999	APJ	C11-C12-N2	-3.60	119.49	123.96
2	L	1999	APJ	C11-C12-N2	-3.56	119.53	123.96
2	D	1999	APJ	C11-C12-N2	-3.54	119.56	123.96
2	M	1999	APJ	C11-C12-N2	-3.53	119.58	123.96
2	G	1999	APJ	C11-C12-N2	-3.47	119.65	123.96
2	D	1999	APJ	C24-C23-C22	-3.46	116.49	120.84
2	H	1999	APJ	C11-C12-N2	-3.44	119.69	123.96
2	A	1999	APJ	C11-C12-N2	-3.41	119.72	123.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1999	APJ	C19-C20-C21	-3.36	116.83	120.50
2	I	1999	APJ	C11-C12-N2	-3.36	119.79	123.96
2	F	1999	APJ	C19-C20-C21	-3.31	116.89	120.50
2	C	1999	APJ	C19-C20-C21	-3.27	116.93	120.50
2	A	1999	APJ	C19-C20-C21	-3.24	116.96	120.50
2	J	1999	APJ	C11-C12-N2	-3.23	119.95	123.96
2	B	1999	APJ	C24-C23-C22	-3.16	116.86	120.84
2	F	1999	APJ	C24-C23-C22	-3.15	116.88	120.84
2	M	1999	APJ	C19-C20-C21	-3.11	117.10	120.50
2	M	1999	APJ	C24-C23-C22	-3.06	116.99	120.84
2	E	1999	APJ	C24-C23-C22	-2.96	117.11	120.84
2	B	1999	APJ	C19-C20-C21	-2.89	117.34	120.50
2	K	1999	APJ	C19-C20-C21	-2.89	117.34	120.50
2	L	1999	APJ	C19-C20-C21	-2.87	117.36	120.50
2	E	1999	APJ	C19-C20-C21	-2.87	117.37	120.50
2	A	1999	APJ	C24-C23-C22	-2.87	117.23	120.84
2	I	1999	APJ	C24-C23-C22	-2.83	117.28	120.84
2	K	1999	APJ	C24-C23-C22	-2.83	117.28	120.84
2	N	1999	APJ	C24-C23-C22	-2.82	117.29	120.84
2	C	1999	APJ	C24-C23-C22	-2.82	117.29	120.84
2	J	1999	APJ	C15-C13-N4	-2.77	106.51	110.47
2	H	1999	APJ	C24-C23-C22	-2.73	117.41	120.84
2	L	1999	APJ	C24-C23-C22	-2.70	117.44	120.84
2	I	1999	APJ	C15-C13-N4	-2.67	106.64	110.47
2	G	1999	APJ	C24-C23-C22	-2.66	117.48	120.84
2	G	1999	APJ	C19-C20-C21	-2.66	117.59	120.50
2	I	1999	APJ	C19-C20-C21	-2.66	117.59	120.50
2	M	1999	APJ	C15-C13-N4	-2.66	106.67	110.47
2	A	1999	APJ	C15-C13-N4	-2.64	106.69	110.47
2	E	1999	APJ	C15-C13-N4	-2.63	106.71	110.47
2	H	1999	APJ	C19-C20-C21	-2.61	117.65	120.50
2	H	1999	APJ	C15-C13-N4	-2.59	106.77	110.47
2	C	1999	APJ	C15-C13-N4	-2.57	106.79	110.47
2	G	1999	APJ	C15-C13-N4	-2.54	106.83	110.47
2	J	1999	APJ	C24-C23-C22	-2.51	117.68	120.84
2	A	1999	APJ	C15-C14-C16	-2.51	125.39	129.25
2	F	1999	APJ	C15-C14-C16	-2.50	125.40	129.25
2	L	1999	APJ	C15-C13-N4	-2.50	106.89	110.47
2	D	1999	APJ	C15-C14-C16	-2.46	125.47	129.25
2	B	1999	APJ	C15-C14-C16	-2.43	125.51	129.25
2	K	1999	APJ	C15-C13-N4	-2.42	107.00	110.47
2	C	1999	APJ	C15-C14-C16	-2.41	125.55	129.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1999	APJ	C15-C13-N4	-2.39	107.05	110.47
2	J	1999	APJ	C19-C20-C21	-2.35	117.93	120.50
2	B	1999	APJ	C15-C13-N4	-2.34	107.11	110.47
2	F	1999	APJ	C15-C13-N4	-2.33	107.13	110.47
2	L	1999	APJ	C15-C14-C16	-2.32	125.69	129.25
2	I	1999	APJ	N6-C9-N1	2.27	124.62	116.92
2	D	1999	APJ	C15-C13-N4	-2.27	107.22	110.47
2	J	1999	APJ	N6-C9-N1	2.26	124.59	116.92
2	K	1999	APJ	N6-C9-N1	2.25	124.55	116.92
2	H	1999	APJ	N6-C9-N1	2.24	124.52	116.92
2	N	1999	APJ	C15-C14-C16	-2.23	125.82	129.25
2	G	1999	APJ	N6-C9-N1	2.23	124.48	116.92
2	H	1999	APJ	C15-C14-C16	-2.22	125.84	129.25
2	I	1999	APJ	C15-C14-C16	-2.22	125.84	129.25
2	M	1999	APJ	N6-C9-N1	2.20	124.39	116.92
2	L	1999	APJ	N6-C9-N1	2.18	124.33	116.92
2	E	1999	APJ	C15-C14-C16	-2.18	125.90	129.25
2	E	1999	APJ	N6-C9-N1	2.17	124.30	116.92
2	G	1999	APJ	C15-C14-C16	-2.17	125.91	129.25
2	A	1999	APJ	N6-C9-N1	2.16	124.25	116.92
2	B	1999	APJ	N6-C9-N1	2.15	124.20	116.92
2	M	1999	APJ	C15-C14-C16	-2.14	125.95	129.25
2	K	1999	APJ	C15-C14-C16	-2.14	125.95	129.25
2	C	1999	APJ	N6-C9-N1	2.12	124.12	116.92
2	F	1999	APJ	N6-C9-N1	2.10	124.04	116.92
2	F	1999	APJ	C13-C15-C14	-2.08	104.24	106.07
2	D	1999	APJ	N6-C9-N1	2.08	123.97	116.92
2	J	1999	APJ	C15-C14-C16	-2.06	126.08	129.25
2	I	1999	APJ	N3-C10-N1	2.05	122.74	116.95
2	D	1999	APJ	N3-C10-N1	2.05	122.73	116.95
2	H	1999	APJ	N3-C10-N1	2.04	122.71	116.95
2	N	1999	APJ	N6-C9-N1	2.03	123.82	116.92
2	A	1999	APJ	N3-C10-N1	2.02	122.65	116.95

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	1999	APJ	N5-C14-C16-C18
2	K	1999	APJ	C15-C14-C16-C18
2	J	1999	APJ	N5-C14-C16-C18
2	J	1999	APJ	C15-C14-C16-C18

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Mol	Chain	Res	Type	Atoms
2	I	1999	APJ	N5-C14-C16-C18
2	I	1999	APJ	C15-C14-C16-C18
2	H	1999	APJ	N5-C14-C16-C18
2	H	1999	APJ	C15-C14-C16-C18
2	N	1999	APJ	N5-C14-C16-C18
2	N	1999	APJ	C15-C14-C16-C18
2	M	1999	APJ	N5-C14-C16-C18
2	M	1999	APJ	C15-C14-C16-C18
2	L	1999	APJ	N5-C14-C16-C18
2	L	1999	APJ	C15-C14-C16-C18
2	C	1999	APJ	N5-C14-C16-C18
2	C	1999	APJ	C15-C14-C16-C18
2	B	1999	APJ	N5-C14-C16-C18
2	B	1999	APJ	C15-C14-C16-C18
2	A	1999	APJ	N5-C14-C16-C18
2	A	1999	APJ	C15-C14-C16-C18
2	G	1999	APJ	N5-C14-C16-C18
2	G	1999	APJ	C15-C14-C16-C18
2	F	1999	APJ	N5-C14-C16-C18
2	F	1999	APJ	C15-C14-C16-C18
2	E	1999	APJ	N5-C14-C16-C18
2	E	1999	APJ	C15-C14-C16-C18
2	D	1999	APJ	N5-C14-C16-C18
2	D	1999	APJ	C15-C14-C16-C18

There are no ring outliers.

14 monomers are involved in 101 short contacts:

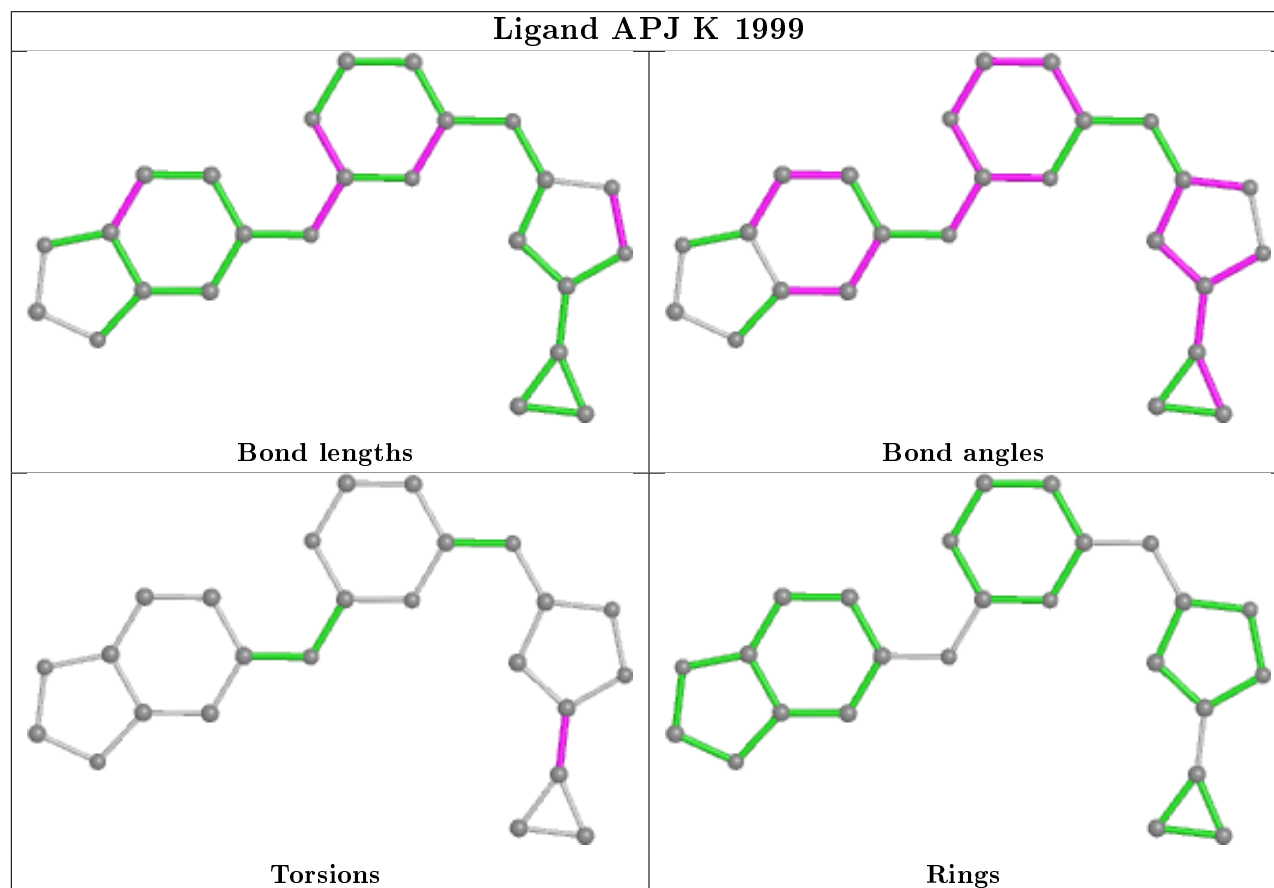
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	1999	APJ	8	0
2	J	1999	APJ	7	0
2	I	1999	APJ	7	0
2	H	1999	APJ	7	0
2	N	1999	APJ	7	0
2	M	1999	APJ	7	0
2	L	1999	APJ	7	0
2	C	1999	APJ	7	0
2	B	1999	APJ	8	0
2	A	1999	APJ	7	0
2	G	1999	APJ	7	0
2	F	1999	APJ	7	0
2	E	1999	APJ	7	0

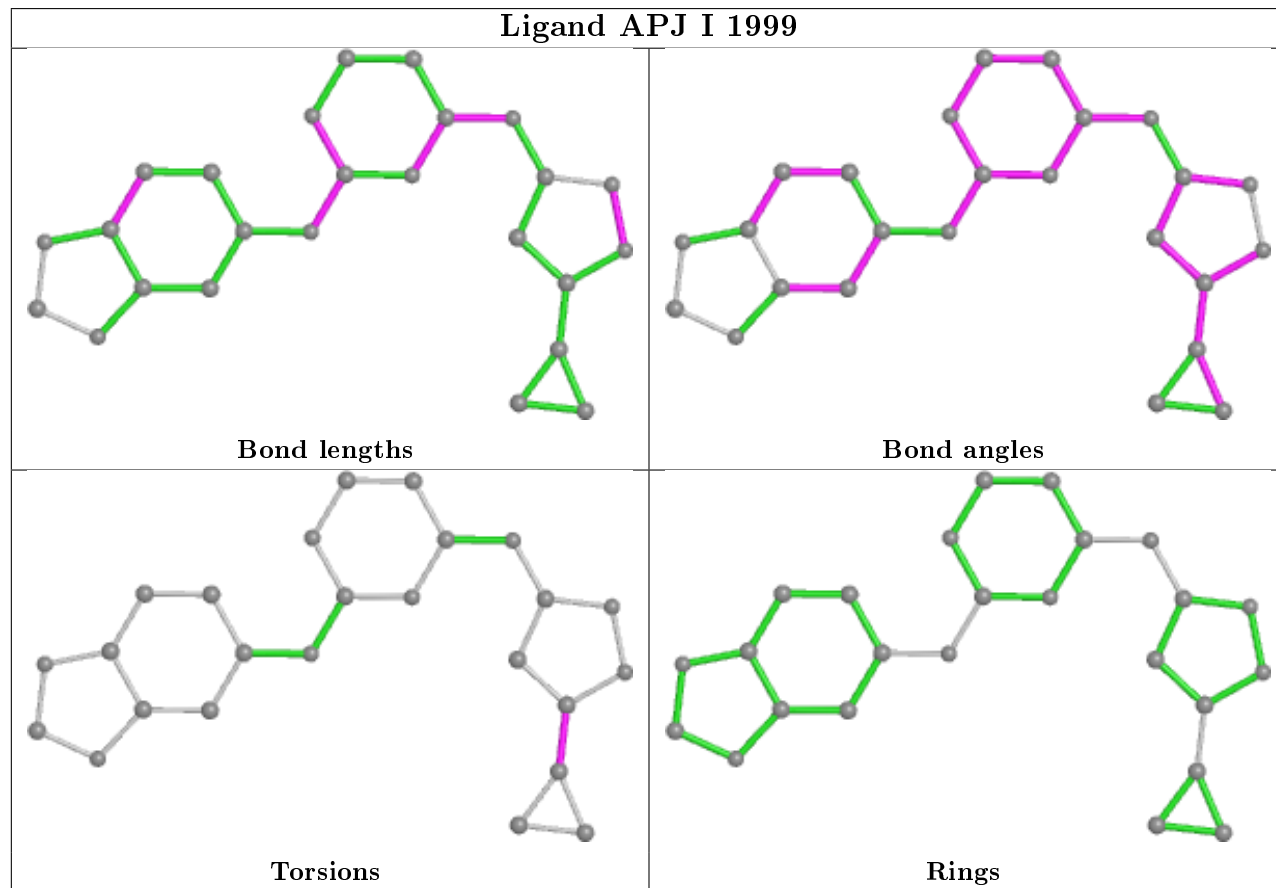
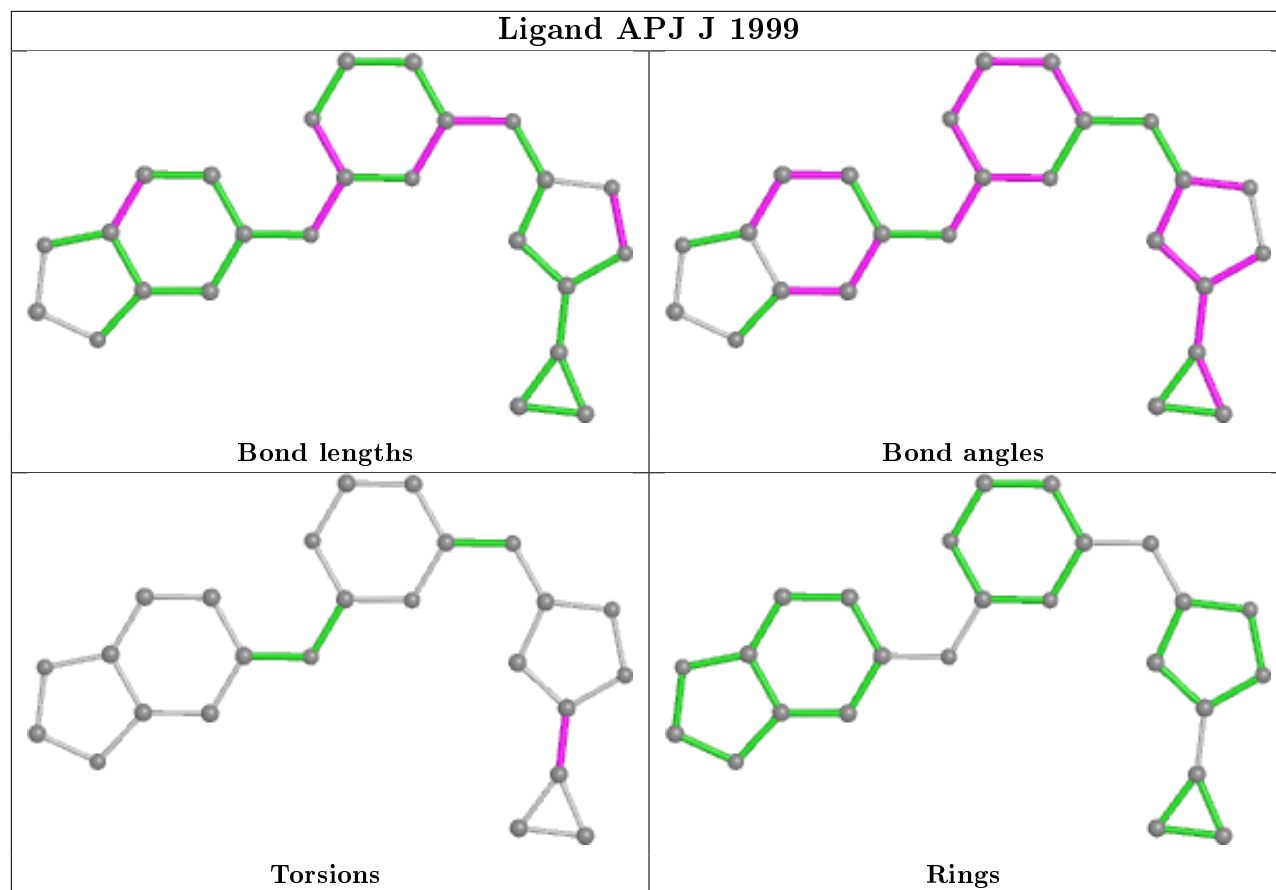
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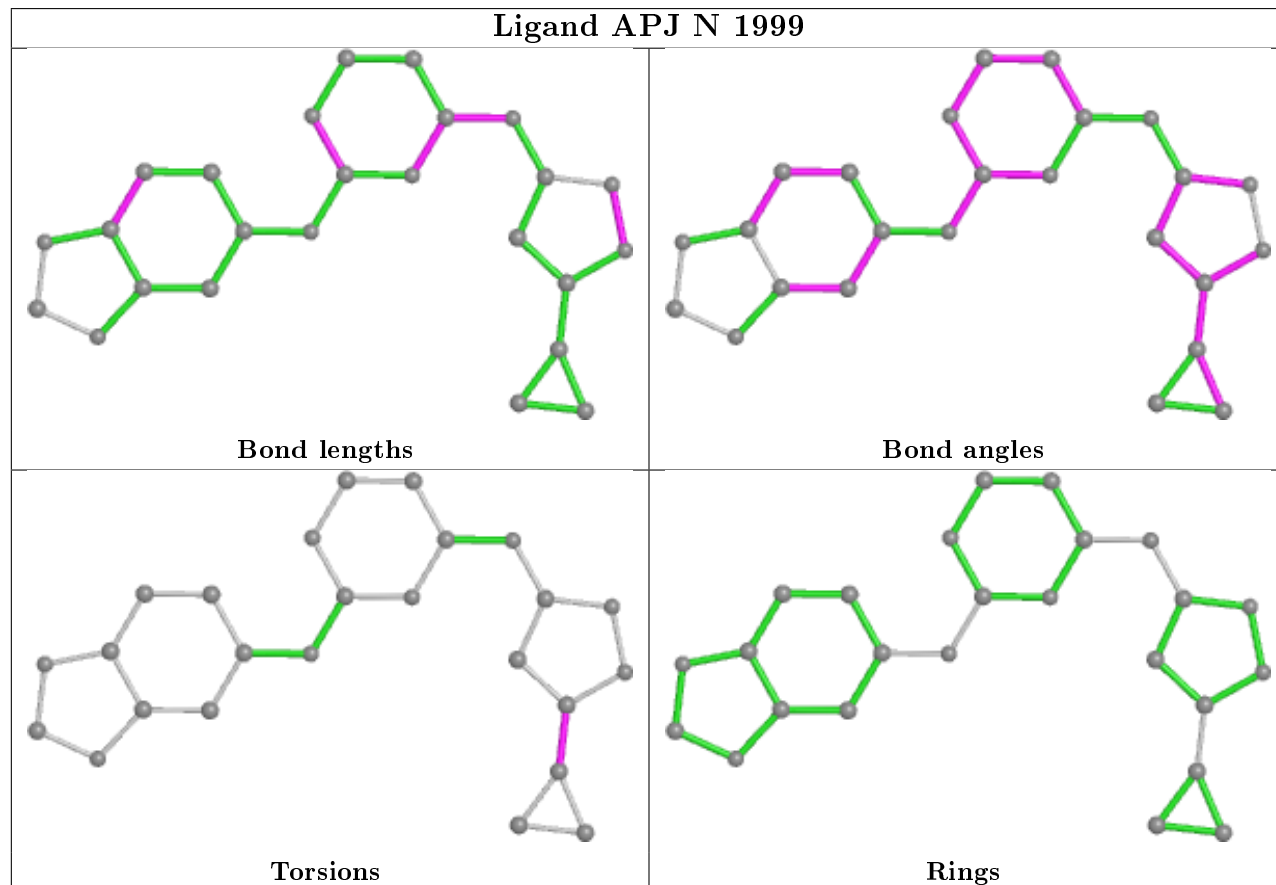
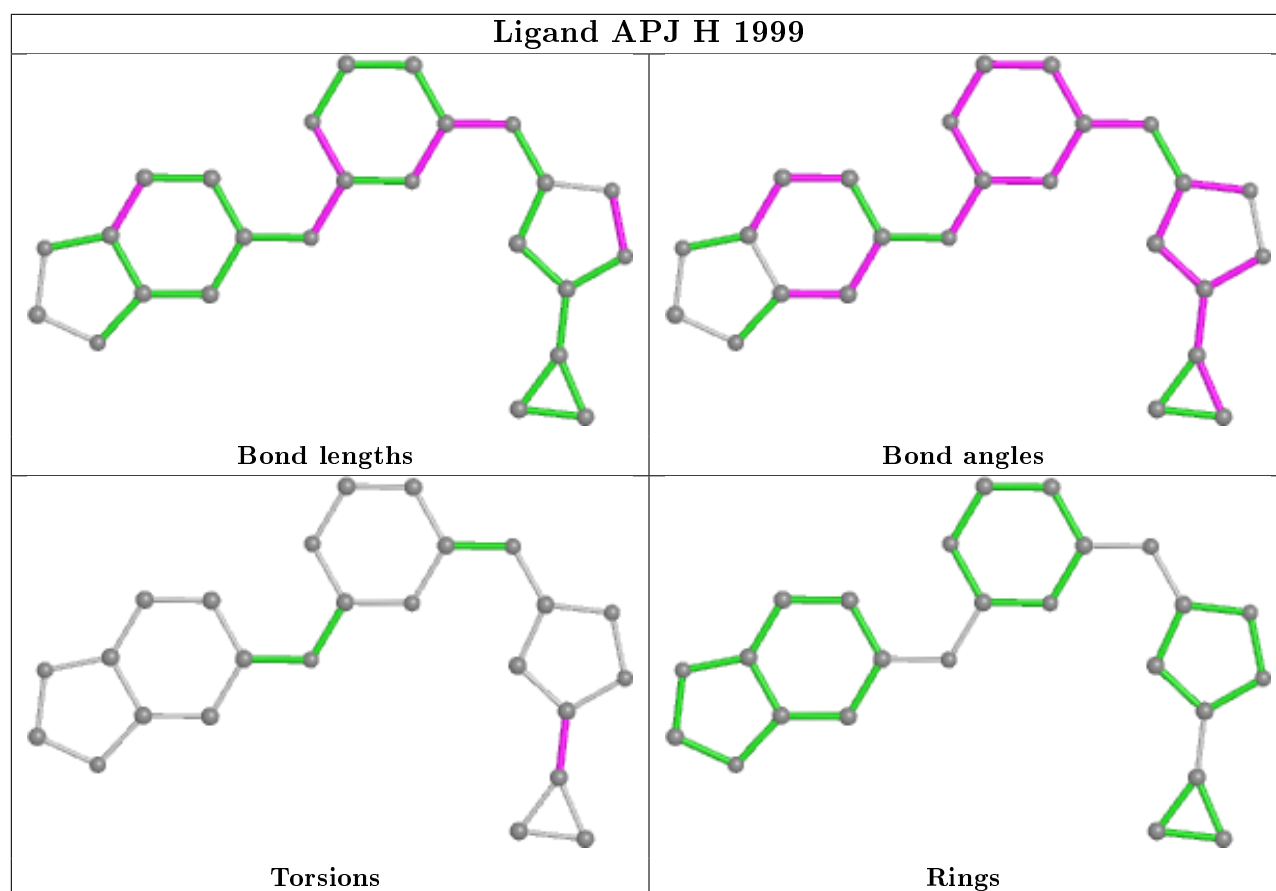
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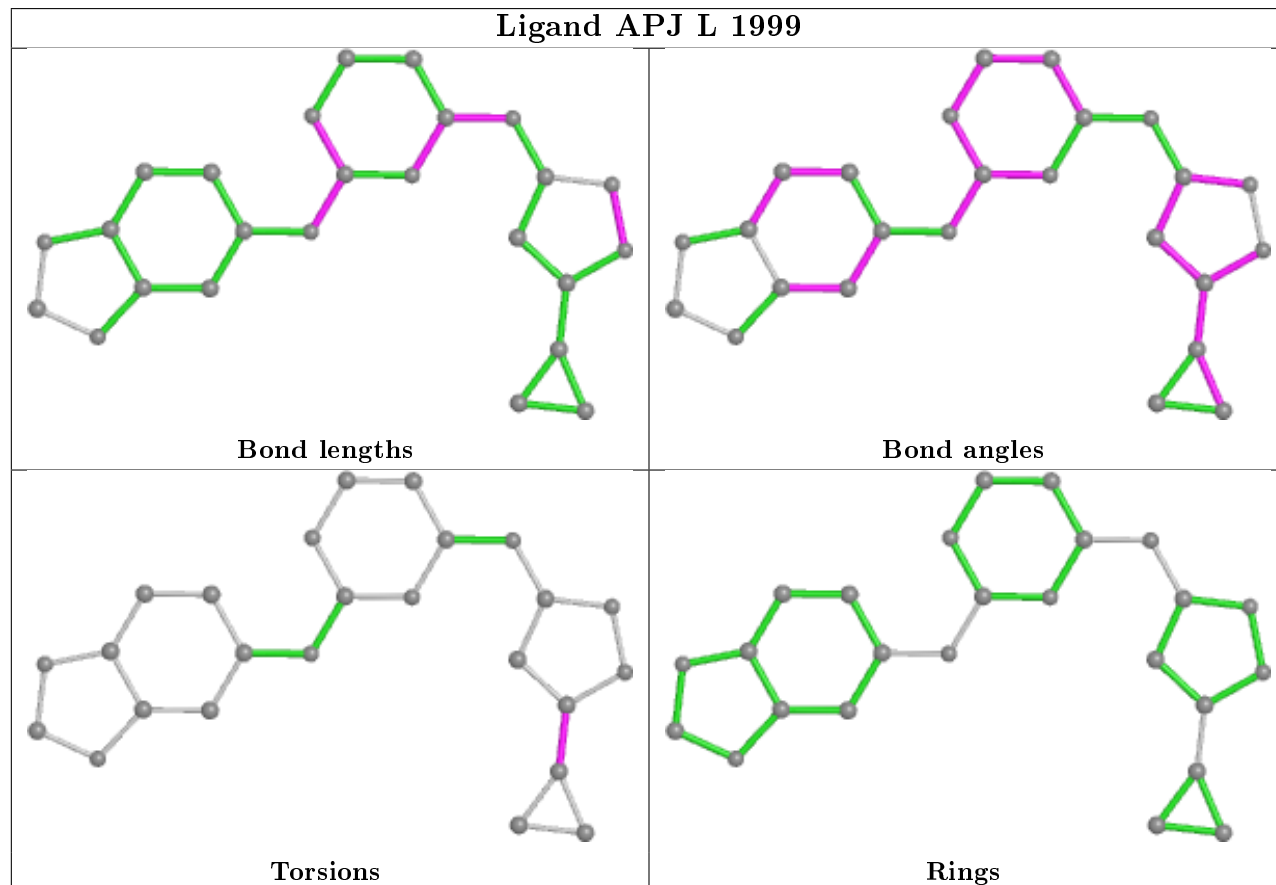
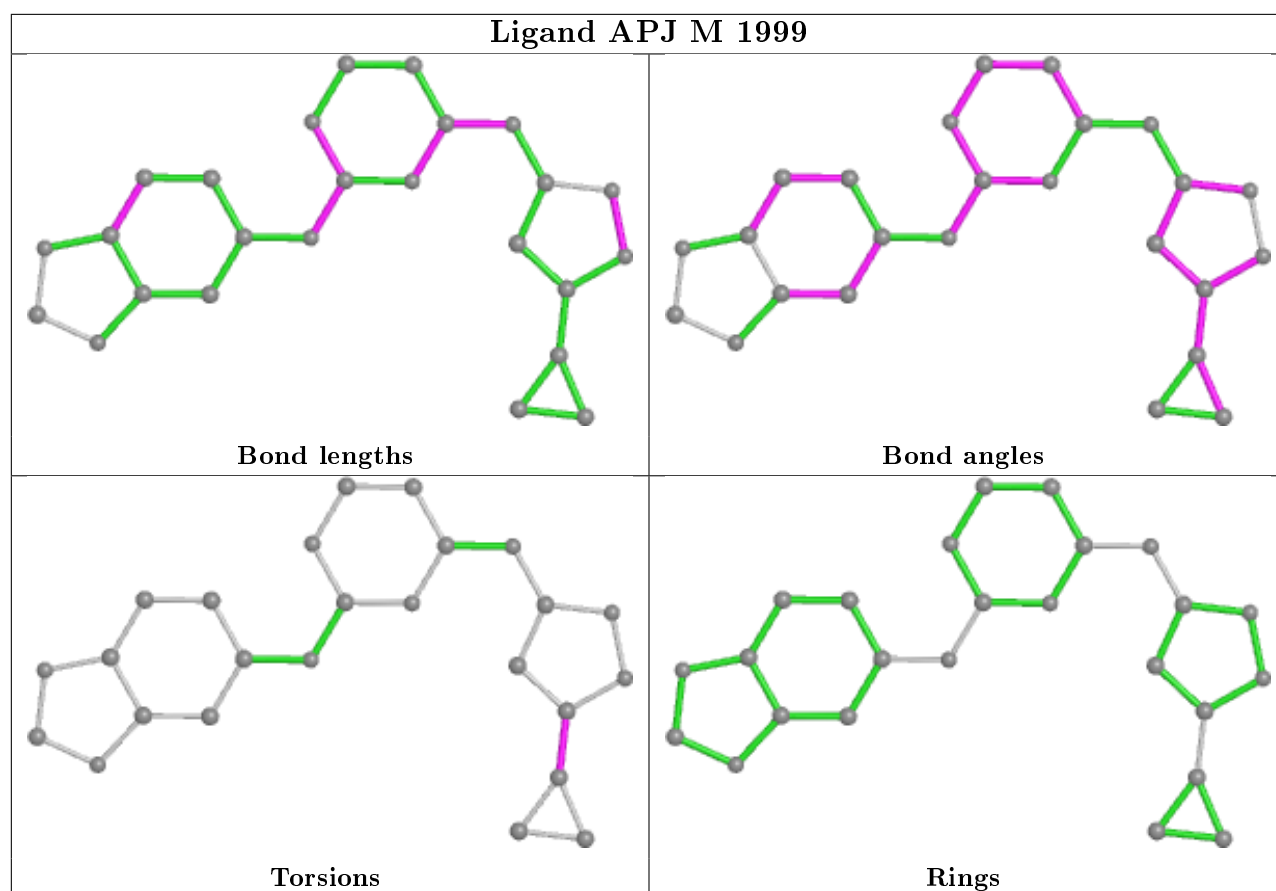
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1999	APJ	8	0

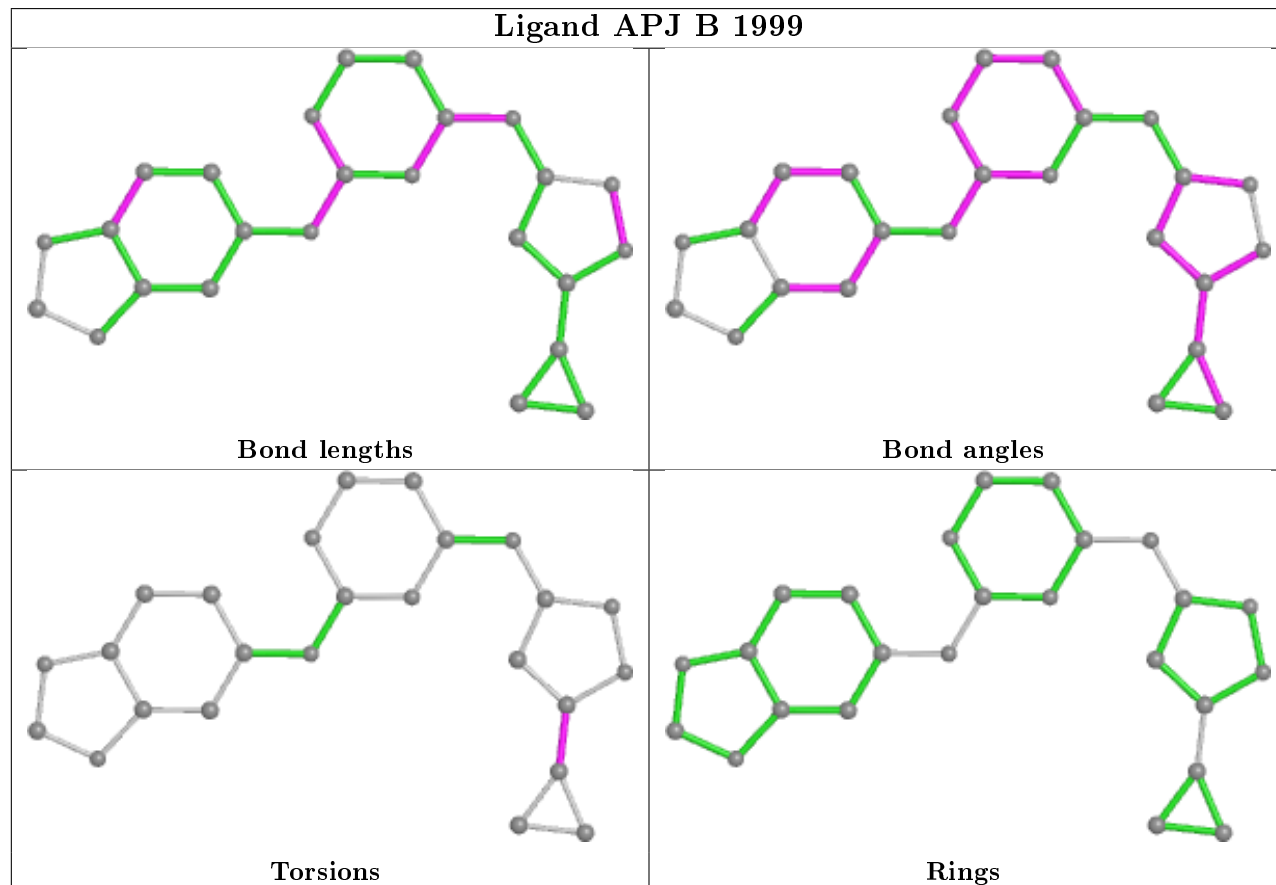
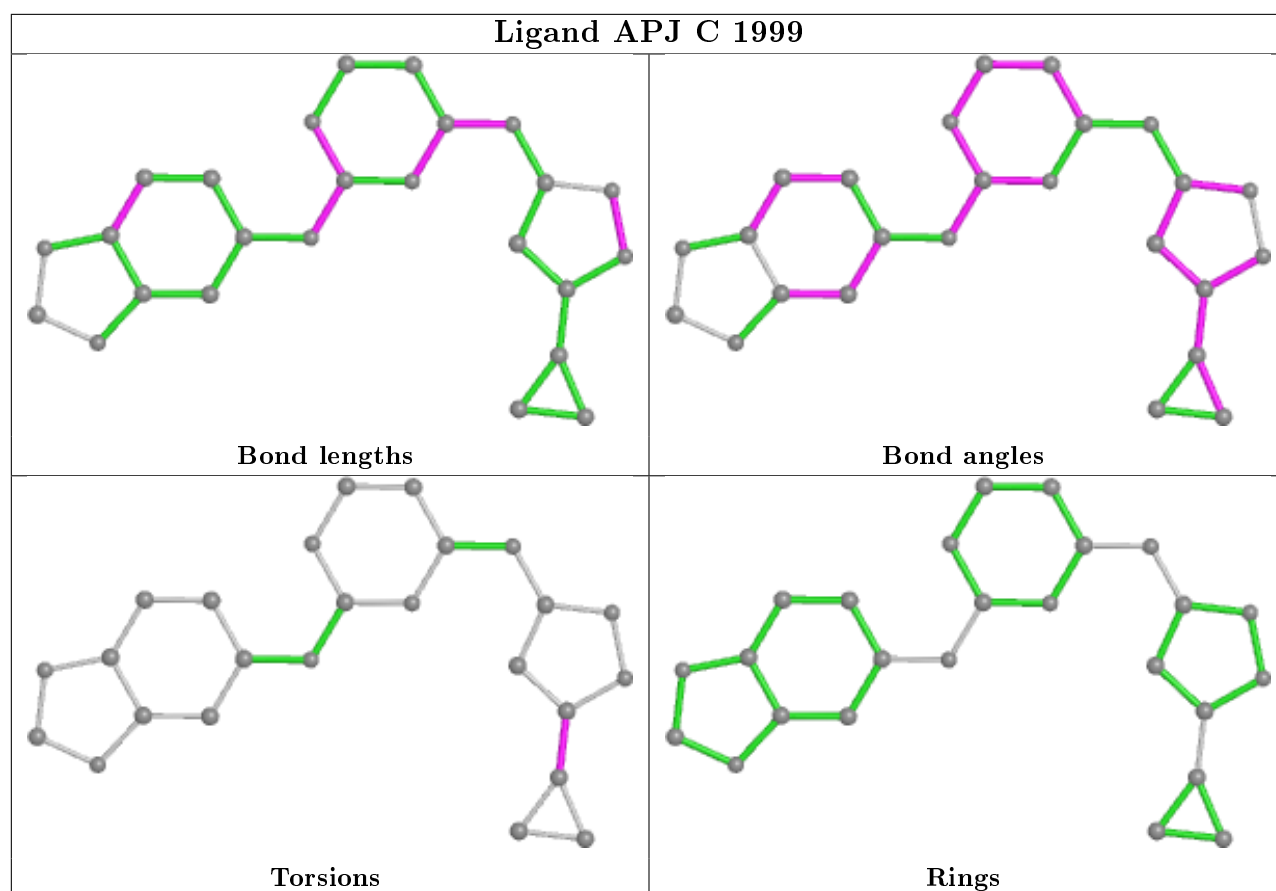
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

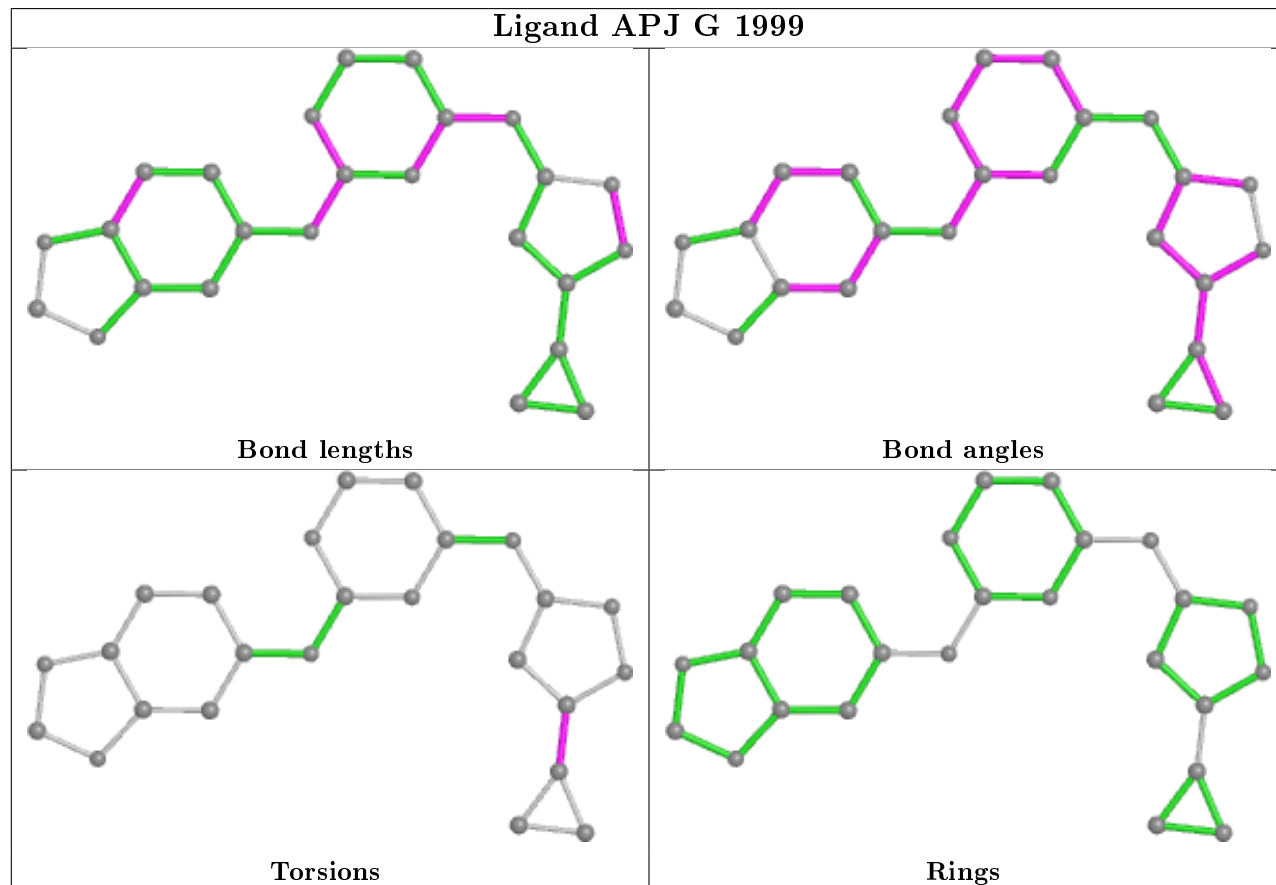
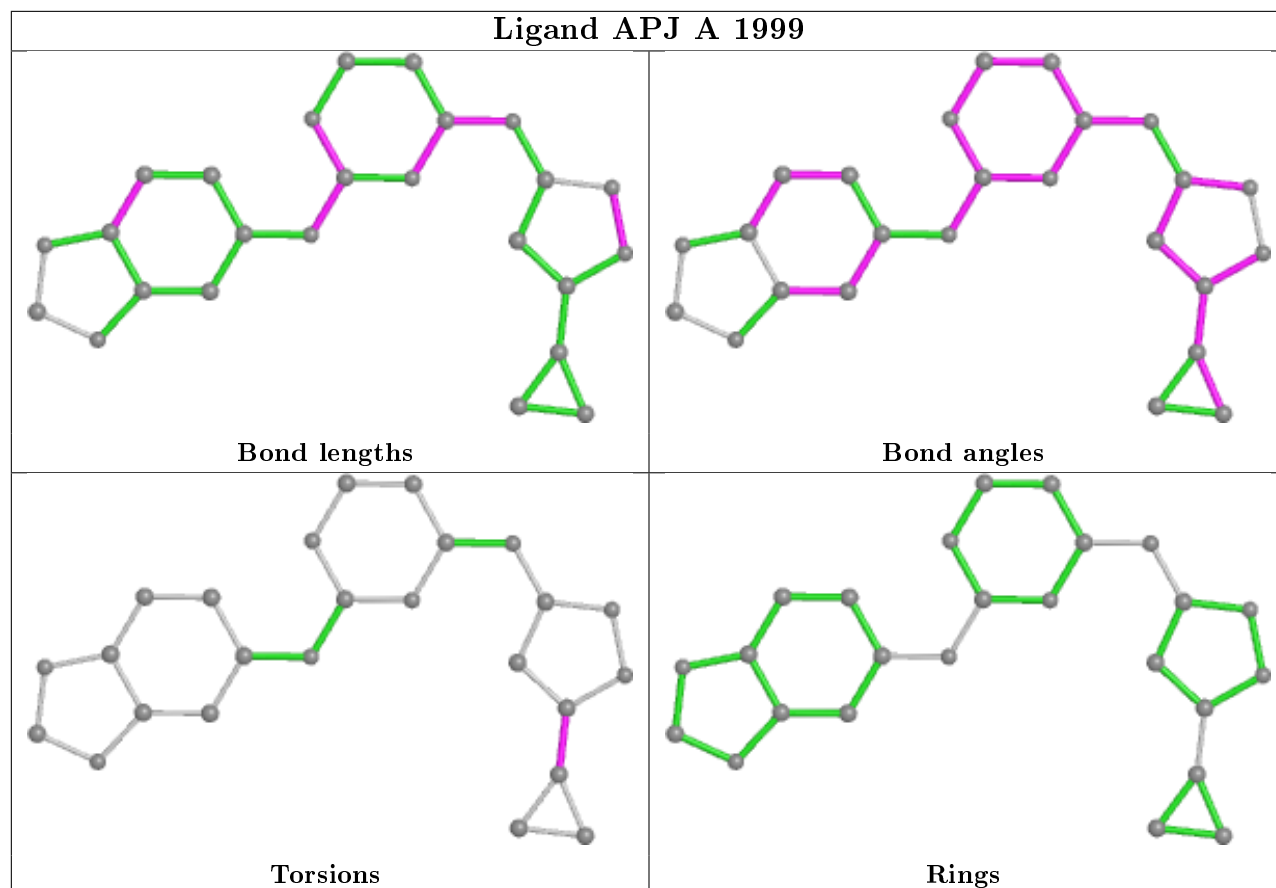


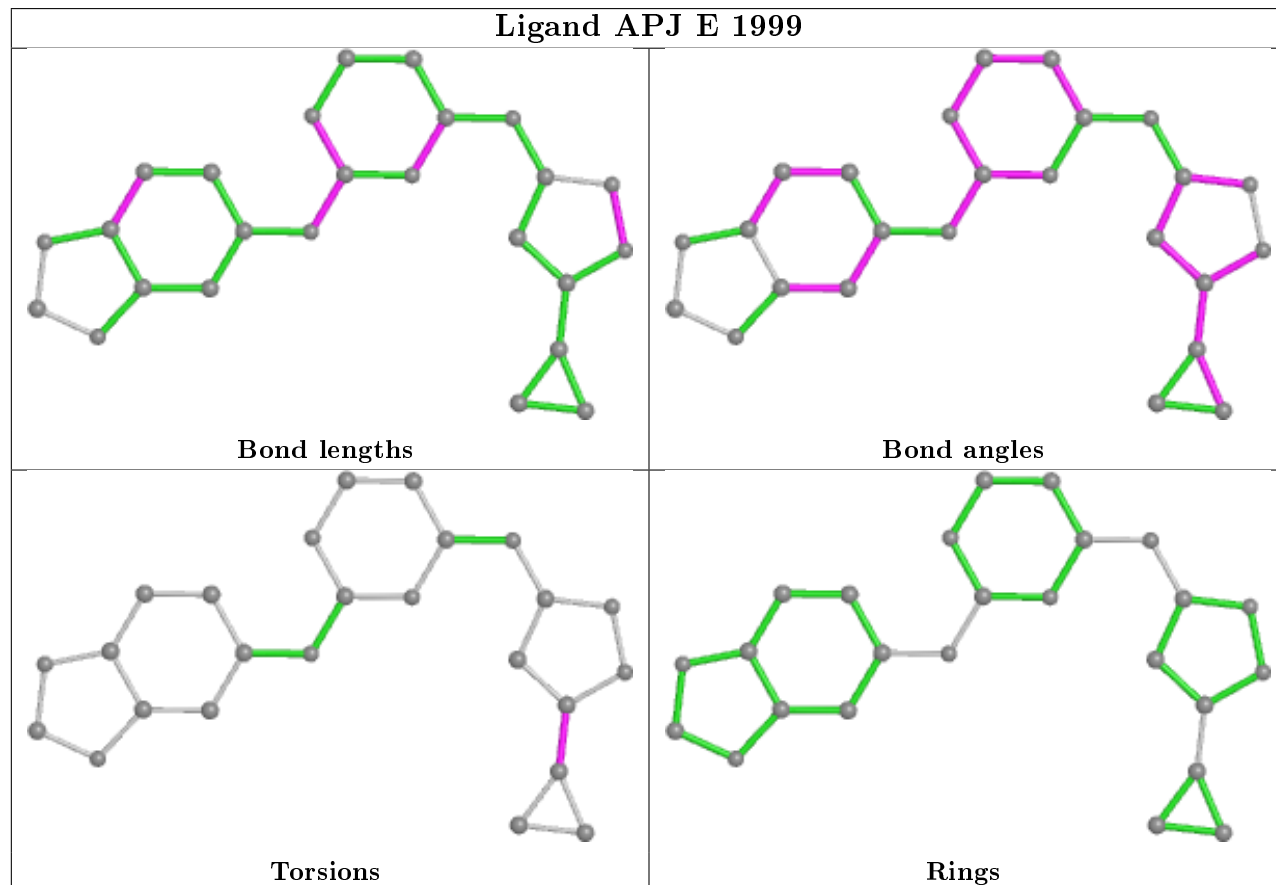
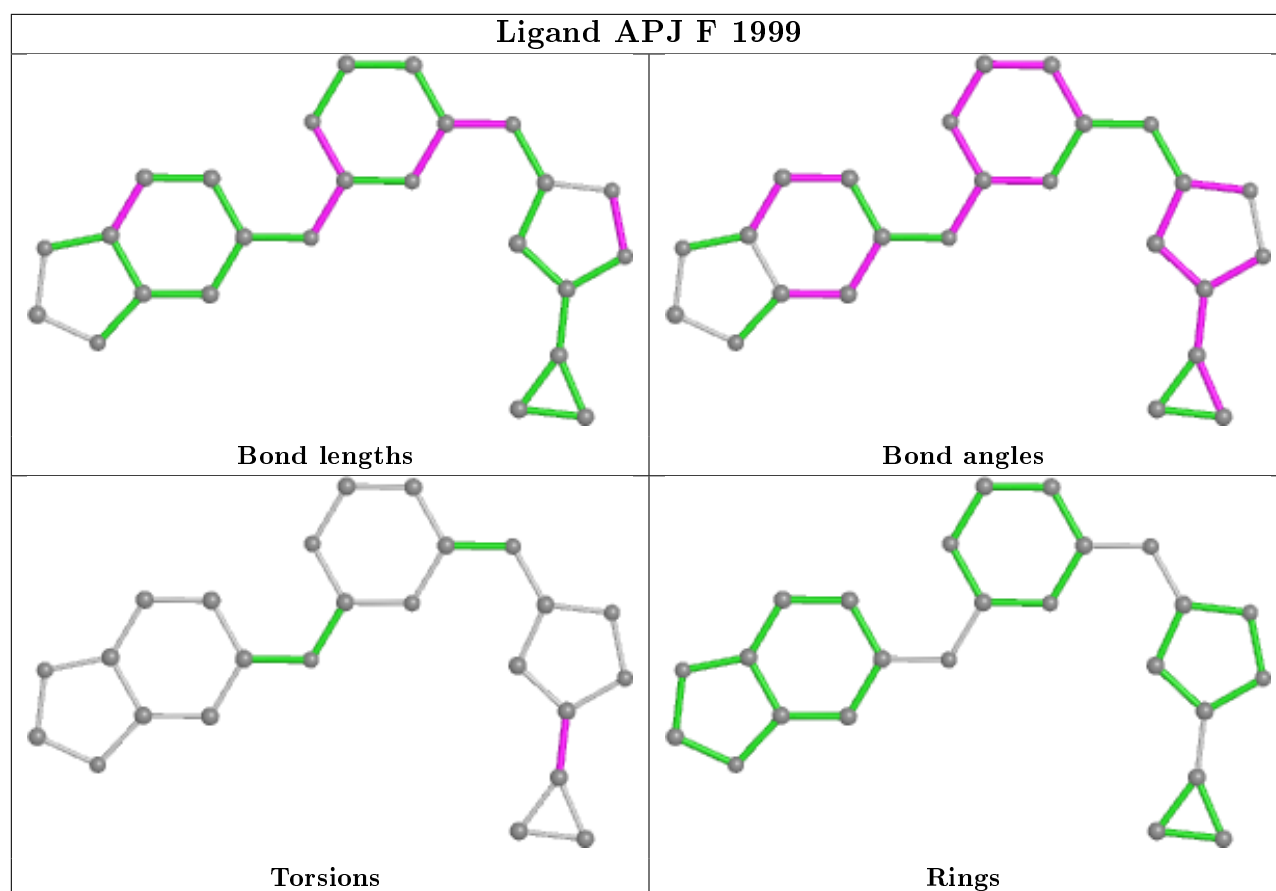


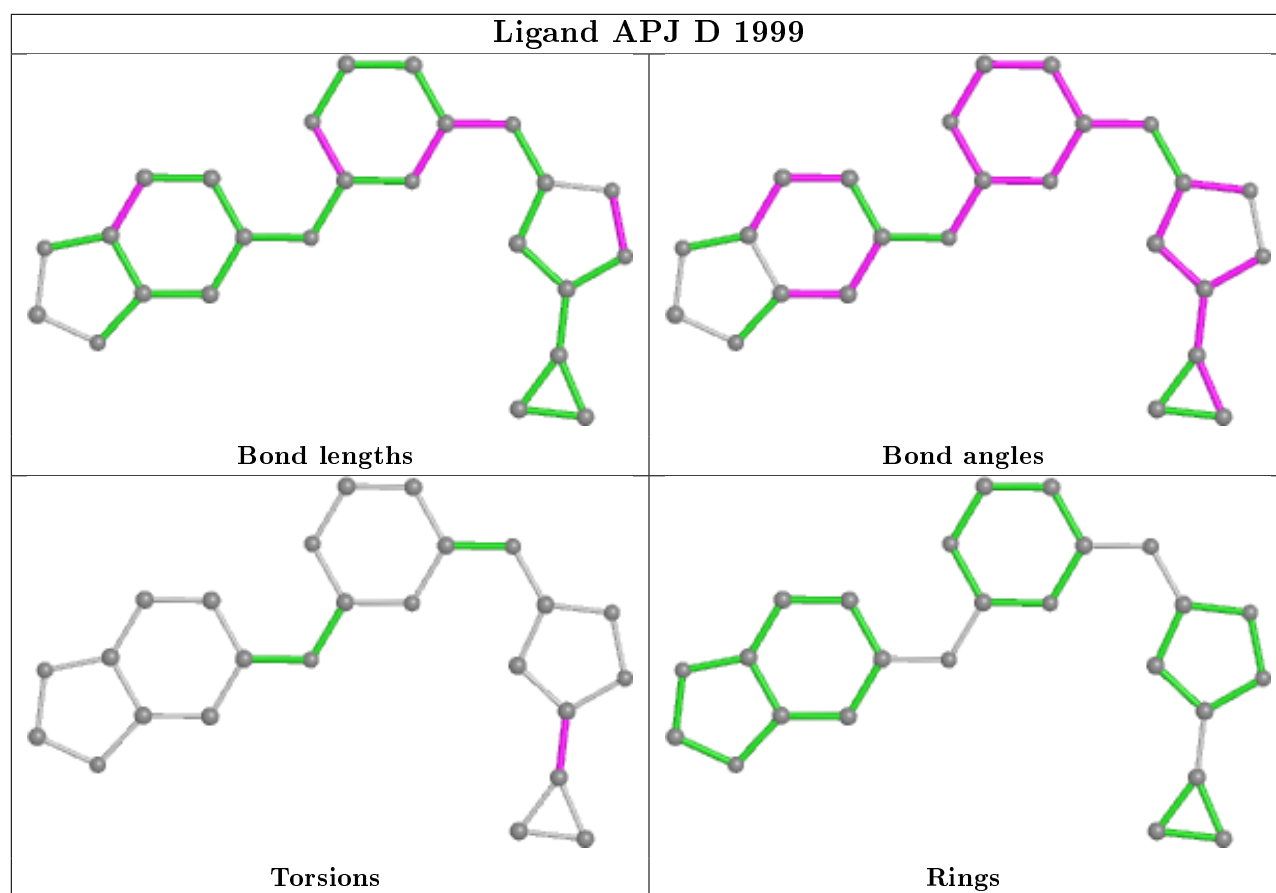












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	415/448 (92%)	-0.16	6 (1%) 75 63	53, 111, 203, 287	0
1	B	415/448 (92%)	-0.17	2 (0%) 91 86	53, 108, 202, 287	0
1	C	415/448 (92%)	-0.19	5 (1%) 79 67	41, 102, 208, 268	0
1	D	422/448 (94%)	-0.27	2 (0%) 91 86	44, 99, 190, 261	0
1	E	415/448 (92%)	-0.19	8 (1%) 66 53	70, 119, 208, 308	0
1	F	415/448 (92%)	-0.19	3 (0%) 87 81	65, 107, 200, 259	0
1	G	415/448 (92%)	0.20	22 (5%) 26 14	99, 161, 256, 323	0
1	H	415/448 (92%)	0.16	16 (3%) 39 25	109, 166, 248, 312	0
1	I	413/448 (92%)	0.19	18 (4%) 34 21	123, 185, 259, 322	0
1	J	413/448 (92%)	0.68	63 (15%) 2 1	145, 210, 301, 366	0
1	K	422/448 (94%)	0.10	10 (2%) 59 44	108, 173, 258, 302	0
1	L	415/448 (92%)	0.28	20 (4%) 30 18	122, 177, 242, 319	0
1	M	415/448 (92%)	-0.10	7 (1%) 70 57	74, 123, 209, 271	0
1	N	415/448 (92%)	-0.15	4 (0%) 82 72	70, 106, 198, 296	0
All	All	5820/6272 (92%)	0.01	186 (3%) 47 31	41, 141, 246, 366	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	864	SER	12.5
1	L	863	GLU	8.7
1	N	893	THR	7.4
1	F	864	SER	5.8
1	N	864	SER	5.8
1	F	863	GLU	5.4
1	J	772	TYR	4.9
1	I	742	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	1039	ARG	4.8
1	N	863	GLU	4.8
1	B	850	SER	4.7
1	L	835	LEU	4.4
1	G	850	SER	4.4
1	J	689	VAL	4.3
1	J	752	LEU	4.2
1	I	1003	ASP	4.1
1	J	709	CYS	4.0
1	J	740	PHE	4.0
1	J	677	GLU	4.0
1	J	742	TYR	4.0
1	J	895	ARG	3.9
1	J	701	VAL	3.9
1	I	736	THR	3.9
1	J	673	LEU	3.9
1	J	847	ASN	3.9
1	G	736	THR	3.9
1	J	704	MET	3.9
1	J	703	ARG	3.8
1	J	1040	TYR	3.8
1	J	1036	ASN	3.8
1	A	864	SER	3.8
1	J	690	PHE	3.8
1	G	740	PHE	3.7
1	G	1043	TYR	3.7
1	H	863	GLU	3.7
1	E	864	SER	3.6
1	J	1043	TYR	3.6
1	J	931	ILE	3.6
1	J	732	TYR	3.6
1	J	675	VAL	3.6
1	G	1035	ASP	3.6
1	K	1040	TYR	3.6
1	J	733	CYS	3.6
1	G	851	GLY	3.6
1	J	743	ILE	3.5
1	J	1073	MET	3.5
1	G	893	THR	3.5
1	H	671	LYS	3.4
1	G	864	SER	3.4
1	G	856	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	671	LYS	3.4
1	J	738	ASP	3.4
1	M	709	CYS	3.3
1	G	742	TYR	3.3
1	J	731	TYR	3.3
1	H	855	TRP	3.3
1	G	853	SER	3.3
1	I	1008	LEU	3.3
1	I	864	SER	3.3
1	L	842	PHE	3.2
1	J	686	GLY	3.1
1	L	760	ASN	3.1
1	A	850	SER	3.1
1	J	734	SER	3.1
1	L	893	THR	3.1
1	J	843	ARG	3.0
1	J	938	LEU	3.0
1	H	864	SER	3.0
1	J	1037	LEU	3.0
1	C	763	ASP	3.0
1	F	893	THR	3.0
1	J	853	SER	3.0
1	C	851	GLY	2.9
1	H	1040	TYR	2.9
1	E	863	GLU	2.9
1	J	760	ASN	2.9
1	L	1012	PHE	2.9
1	J	705	LEU	2.9
1	J	682	TYR	2.9
1	L	729	ILE	2.8
1	E	847	ASN	2.8
1	C	864	SER	2.8
1	A	742	TYR	2.8
1	J	859	GLU	2.8
1	J	1041	ARG	2.8
1	L	794	ILE	2.8
1	B	742	TYR	2.8
1	L	902	ASP	2.8
1	G	741	LEU	2.8
1	J	674	VAL	2.8
1	J	849	PRO	2.7
1	J	729	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	856	ARG	2.7
1	L	764	GLU	2.6
1	J	1067	GLU	2.6
1	L	765	ASN	2.6
1	J	1113	LEU	2.6
1	J	894	LYS	2.6
1	E	850	SER	2.6
1	J	964	ASP	2.6
1	K	1013	ASP	2.6
1	G	670	LEU	2.6
1	H	1033	PHE	2.5
1	M	1040	TYR	2.5
1	D	738	ASP	2.5
1	H	1058	LYS	2.5
1	J	767	LYS	2.5
1	G	963	HIS	2.5
1	K	1033	PHE	2.5
1	G	843	ARG	2.5
1	G	1040	TYR	2.5
1	L	763	ASP	2.5
1	J	702	LYS	2.5
1	L	761	VAL	2.4
1	J	1033	PHE	2.4
1	G	733	CYS	2.4
1	H	742	TYR	2.4
1	I	961	ILE	2.4
1	J	711	ILE	2.4
1	K	1012	PHE	2.4
1	J	715	GLU	2.4
1	E	893	THR	2.4
1	I	1012	PHE	2.3
1	J	771	GLU	2.3
1	L	702	LYS	2.3
1	J	685	SER	2.3
1	K	794	ILE	2.3
1	L	858	PRO	2.3
1	H	847	ASN	2.3
1	K	742	TYR	2.3
1	G	817	THR	2.3
1	G	1036	ASN	2.3
1	G	737	THR	2.3
1	K	1047	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	843	ARG	2.3
1	L	793	ILE	2.3
1	J	1072	LEU	2.3
1	H	702	LYS	2.3
1	L	682	TYR	2.3
1	I	836	ASP	2.2
1	K	895	ARG	2.2
1	M	895	ARG	2.2
1	I	732	TYR	2.2
1	J	1039	ARG	2.2
1	H	794	ILE	2.2
1	E	849	PRO	2.2
1	D	1012	PHE	2.2
1	H	809	SER	2.2
1	A	853	SER	2.2
1	L	852	THR	2.2
1	I	809	SER	2.2
1	K	1091	LEU	2.2
1	E	672	ASN	2.2
1	C	709	CYS	2.2
1	I	700	ALA	2.1
1	G	842	PHE	2.1
1	L	860	LEU	2.1
1	J	707	ASP	2.1
1	G	895	ARG	2.1
1	J	893	THR	2.1
1	J	1058	LYS	2.1
1	J	1038	GLU	2.1
1	I	835	LEU	2.1
1	K	864	SER	2.1
1	H	737	THR	2.1
1	H	682	TYR	2.1
1	H	673	LEU	2.1
1	I	852	THR	2.1
1	H	706	ILE	2.1
1	J	836	ASP	2.1
1	N	1040	TYR	2.1
1	I	743	ILE	2.1
1	J	854	GLY	2.1
1	J	848	ASN	2.1
1	M	671	LYS	2.1
1	M	1030	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	742	TYR	2.0
1	J	741	LEU	2.0
1	A	863	GLU	2.0
1	I	1019	VAL	2.0
1	M	893	THR	2.0
1	I	921	PHE	2.0
1	I	855	TRP	2.0
1	A	670	LEU	2.0
1	J	803	ILE	2.0
1	J	747	LEU	2.0

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

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	L	840	10/11	0.50	0.32	244,256,269,270	0
1	SEP	L	841	10/11	0.54	0.23	213,235,255,263	0
1	SEP	A	840	10/11	0.66	0.28	202,208,216,216	0
1	TPO	I	844	11/12	0.69	0.48	258,270,291,301	0
1	TPO	J	844	11/12	0.70	0.22	253,261,280,285	0
1	TPO	L	844	11/12	0.71	0.44	306,329,351,352	0
1	TPO	F	844	11/12	0.73	0.30	232,250,267,271	0
1	SEP	H	840	10/11	0.73	0.21	179,184,191,192	0
1	TPO	N	844	11/12	0.76	0.22	235,252,274,280	0
1	TPO	H	844	11/12	0.76	0.23	260,273,298,309	0
1	TPO	E	844	11/12	0.79	0.23	238,260,293,298	0
1	SEP	J	840	10/11	0.79	0.25	210,217,231,232	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	0.81	0.37	280,298,330,346	0
1	TPO	K	844	11/12	0.82	0.36	261,276,304,315	0
1	SEP	G	840	10/11	0.83	0.22	187,192,200,202	0
1	SEP	I	840	10/11	0.83	0.23	216,220,226,226	0
1	SEP	M	840	10/11	0.84	0.27	146,150,158,160	0
1	SEP	F	840	10/11	0.84	0.17	138,142,146,152	0
1	SEP	N	840	10/11	0.85	0.15	172,174,179,183	0
1	SEP	K	841	10/11	0.85	0.15	148,161,173,180	0
1	SEP	A	841	10/11	0.85	0.13	117,131,144,148	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	TPO	C	844	11/12	0.86	0.23	199,232,261,263	0
1	TPO	M	844	11/12	0.86	0.22	228,257,285,285	0
1	SEP	B	840	10/11	0.87	0.22	147,153,162,164	0
1	TPO	B	844	11/12	0.87	0.23	166,194,212,216	0
1	SEP	C	840	10/11	0.87	0.20	151,156,164,164	0
1	SEP	E	840	10/11	0.89	0.28	184,188,196,198	0
1	TPO	A	844	11/12	0.90	0.17	256,286,315,317	0
1	SEP	G	841	10/11	0.90	0.11	141,156,172,175	0
1	SEP	B	841	10/11	0.90	0.17	111,133,156,162	0
1	SEP	D	840	10/11	0.90	0.22	134,138,146,146	0
1	SEP	F	841	10/11	0.91	0.13	110,119,130,131	0
1	SEP	H	841	10/11	0.91	0.13	145,157,165,172	0
1	SEP	J	841	10/11	0.92	0.14	175,183,188,193	0
1	SEP	E	841	10/11	0.92	0.12	117,136,158,163	0
1	SEP	C	841	10/11	0.92	0.15	90,114,135,145	0
1	SEP	I	841	10/11	0.92	0.12	171,181,192,193	0
1	SEP	N	841	10/11	0.93	0.10	120,133,149,152	0
1	SEP	M	841	10/11	0.94	0.10	103,112,132,137	0
1	SEP	D	841	10/11	0.95	0.12	82,92,114,119	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

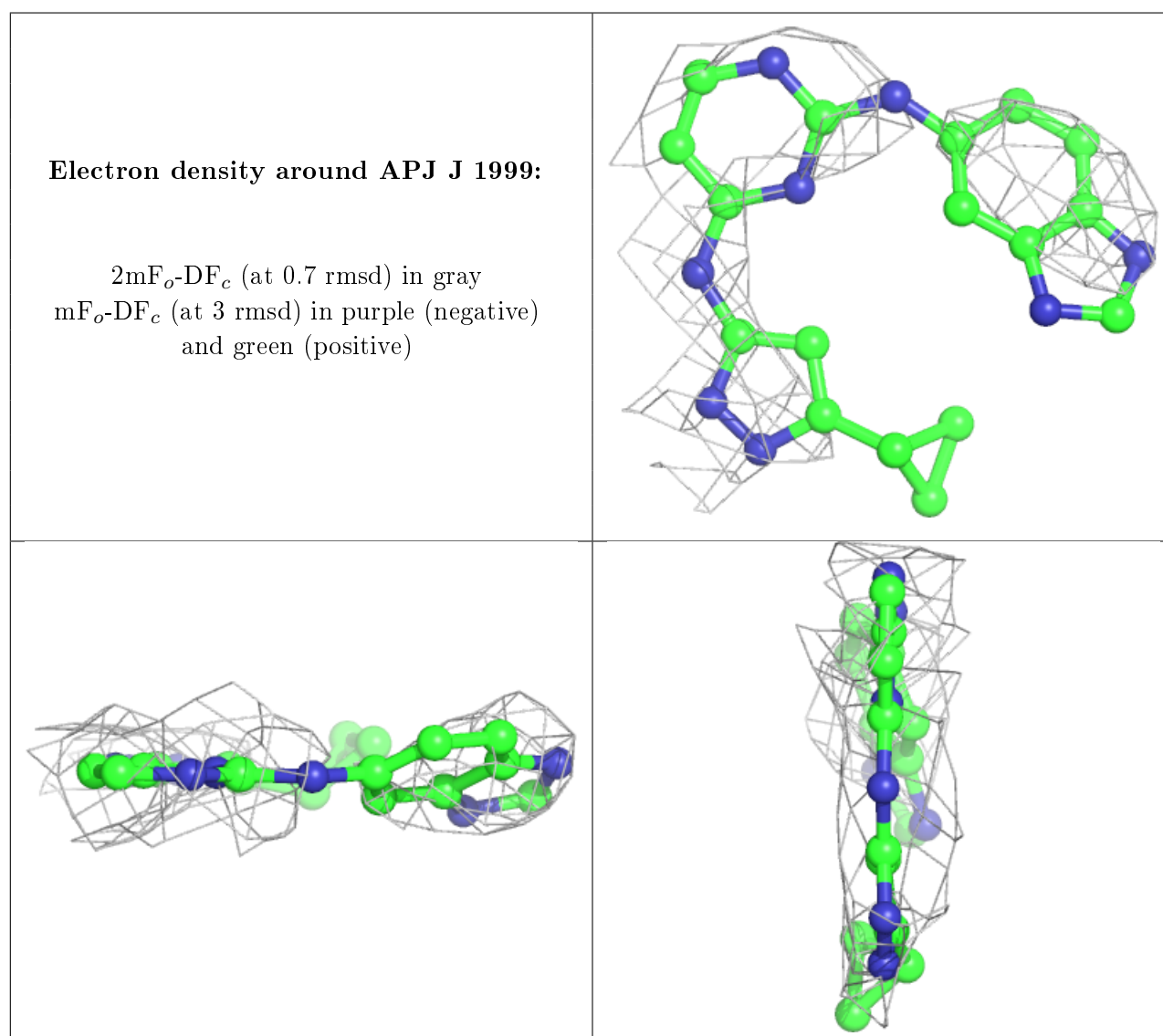
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	APJ	J	1999	25/25	0.76	0.68	197,197,197,197	0
2	APJ	H	1999	25/25	0.81	0.49	170,170,170,170	0
2	APJ	I	1999	25/25	0.83	0.29	171,171,171,171	0
2	APJ	L	1999	25/25	0.84	0.34	142,142,142,142	0
2	APJ	K	1999	25/25	0.88	0.40	135,135,135,135	0
2	APJ	M	1999	25/25	0.92	0.24	113,113,113,113	0
2	APJ	G	1999	25/25	0.92	0.31	145,145,145,145	0
2	APJ	D	1999	25/25	0.92	0.24	78,78,78,78	0
2	APJ	C	1999	25/25	0.93	0.26	66,66,66,66	0

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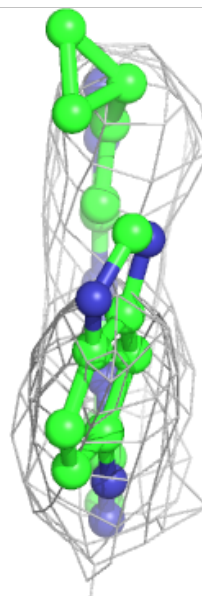
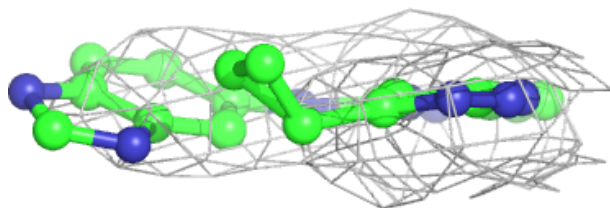
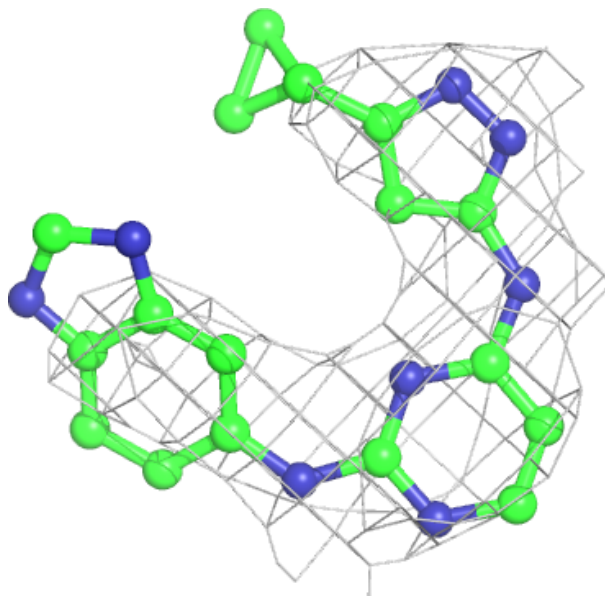
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	APJ	F	1999	25/25	0.93	0.23	93,93,93,93	0
2	APJ	A	1999	25/25	0.93	0.22	93,93,93,93	0
2	APJ	N	1999	25/25	0.94	0.21	87,87,87,87	0
2	APJ	B	1999	25/25	0.94	0.21	96,96,96,96	0
2	APJ	E	1999	25/25	0.95	0.22	101,101,101,101	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



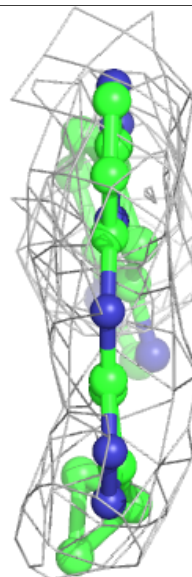
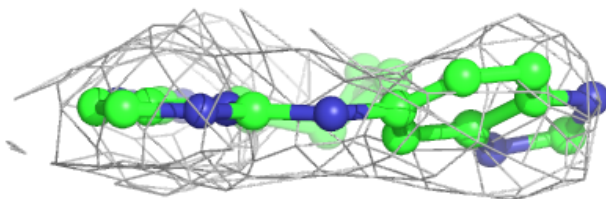
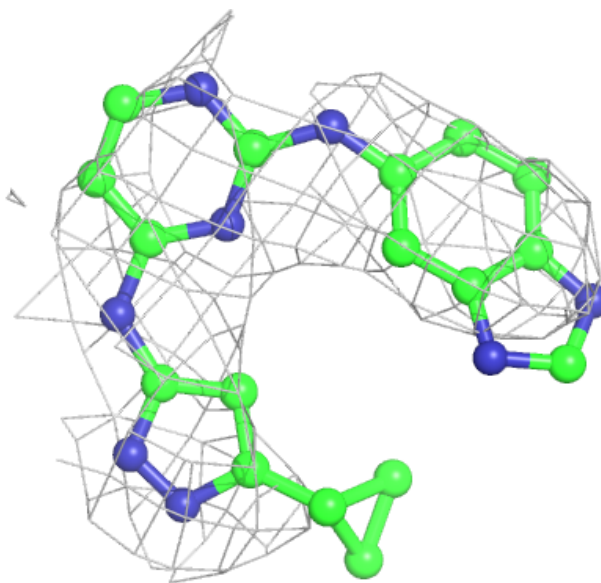
Electron density around APJ H 1999:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



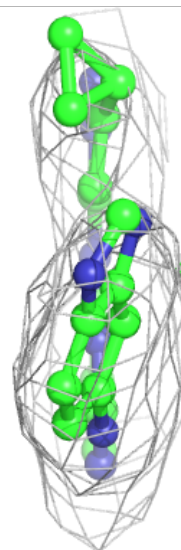
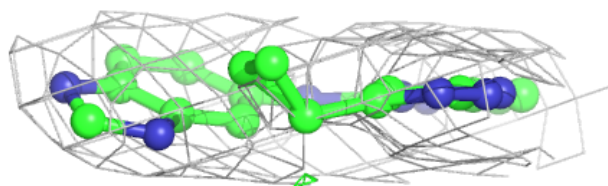
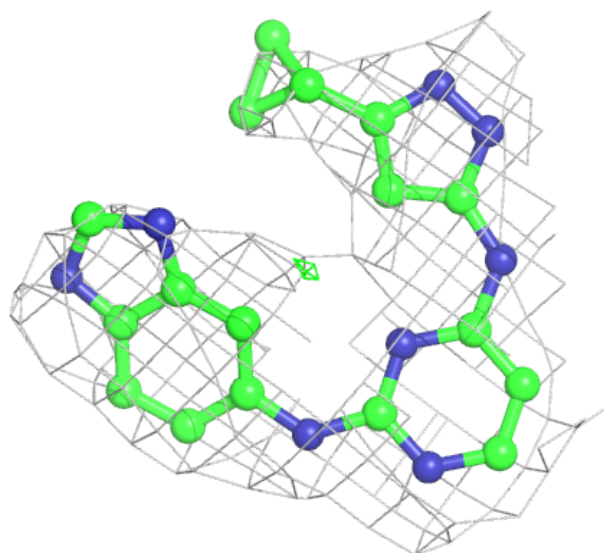
Electron density around APJ I 1999:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



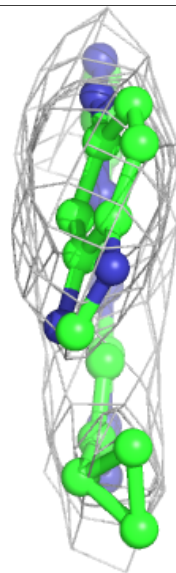
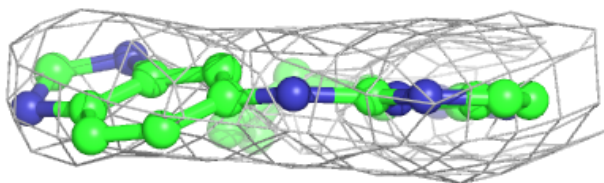
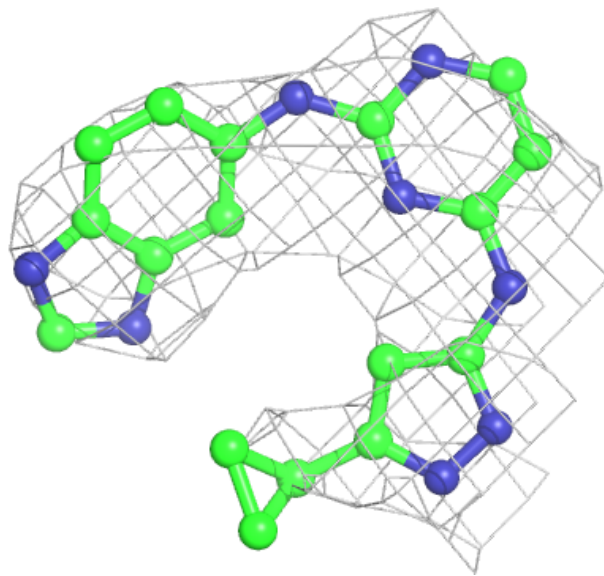
Electron density around APJ L 1999:

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and green (positive)



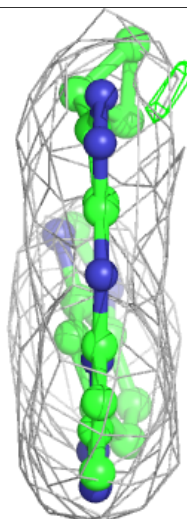
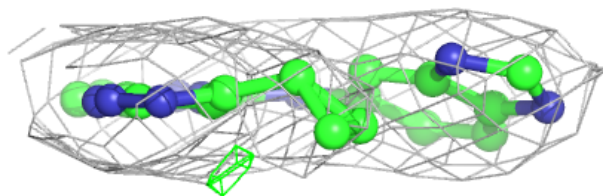
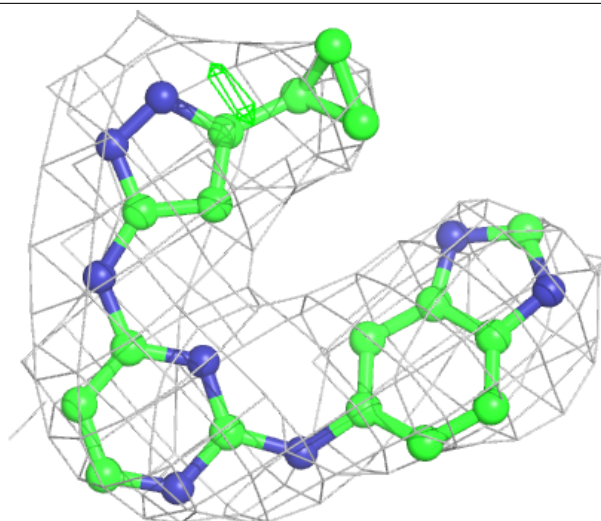
Electron density around APJ K 1999:

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and green (positive)



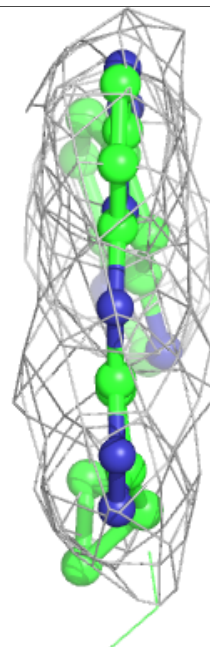
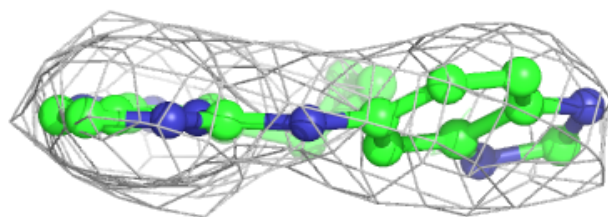
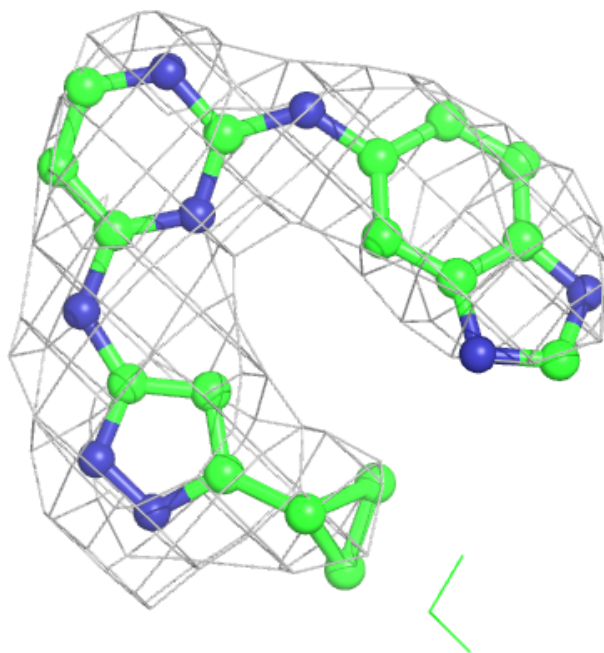
Electron density around APJ M 1999:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



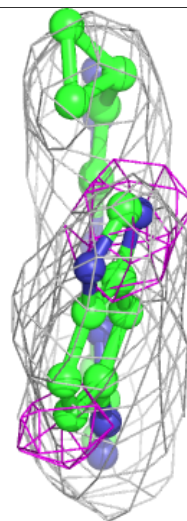
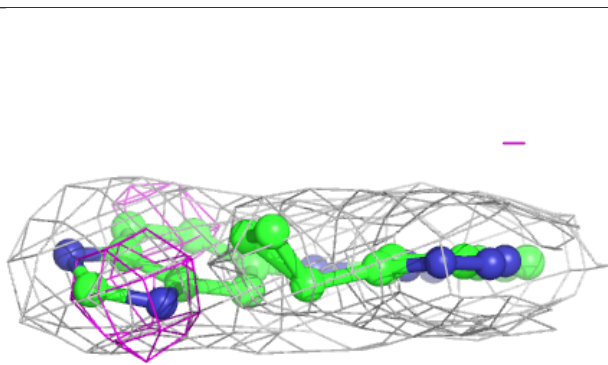
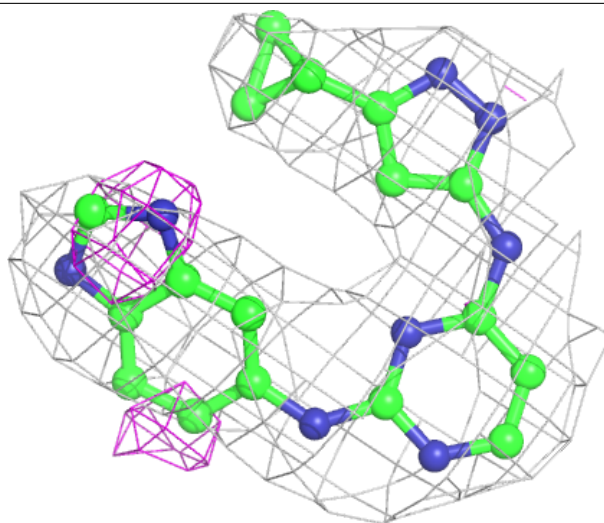
Electron density around APJ G 1999:

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and green (positive)



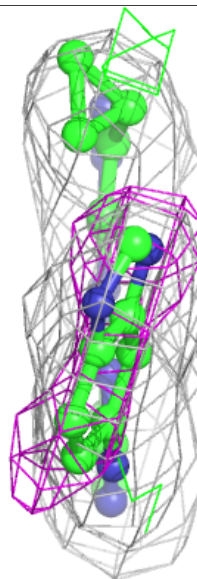
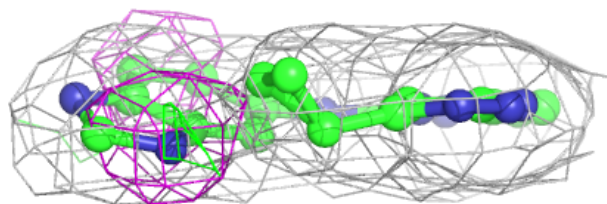
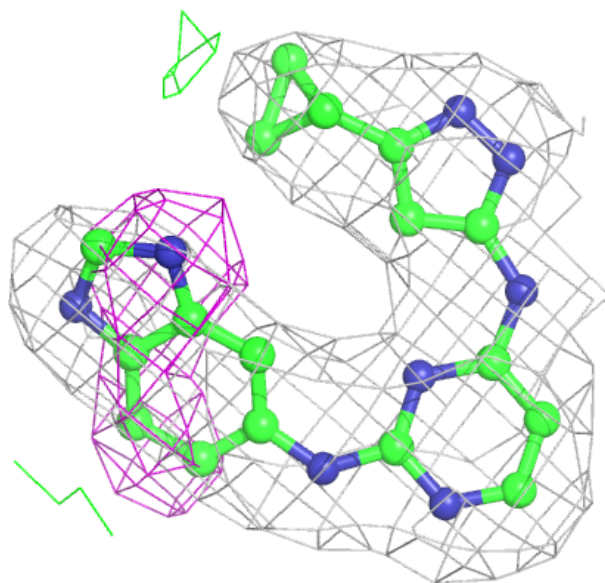
Electron density around APJ D 1999:

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and green (positive)



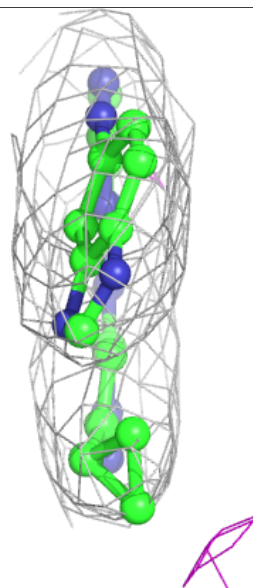
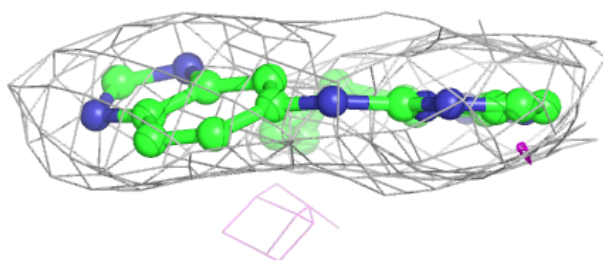
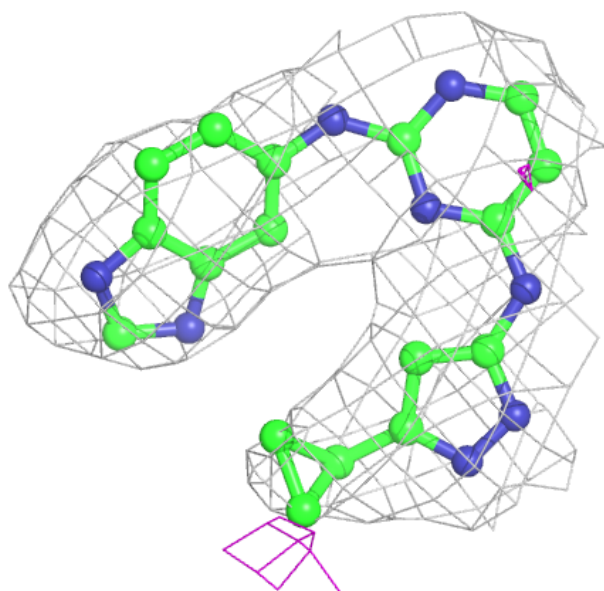
Electron density around APJ C 1999:

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and green (positive)



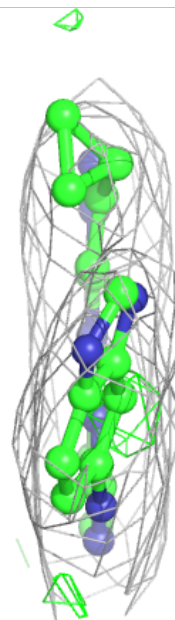
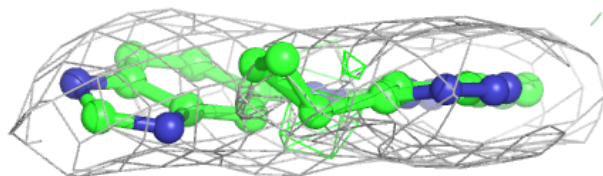
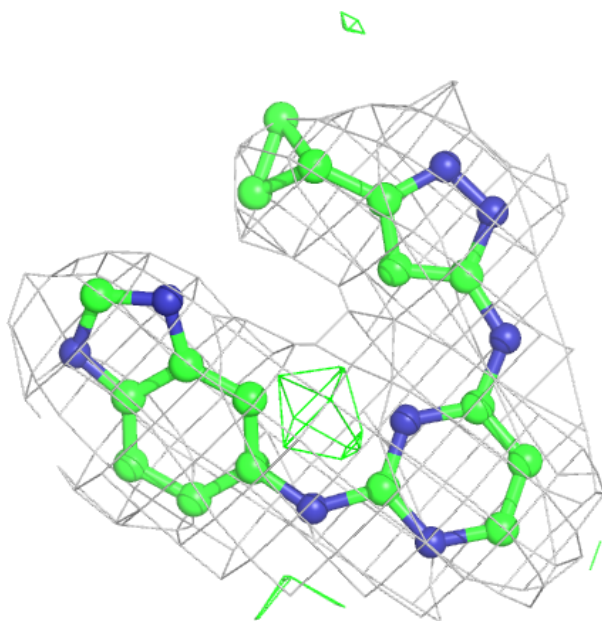
Electron density around APJ F 1999:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



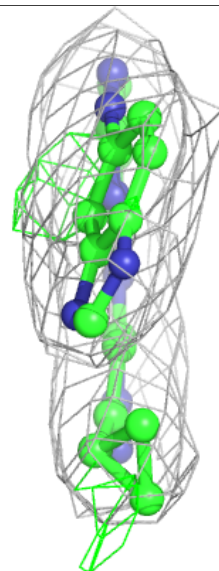
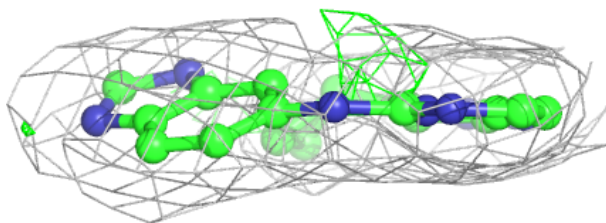
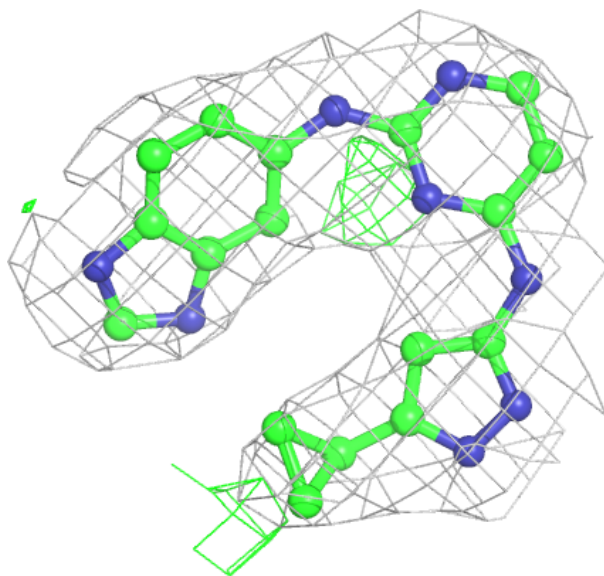
Electron density around APJ A 1999:

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and green (positive)



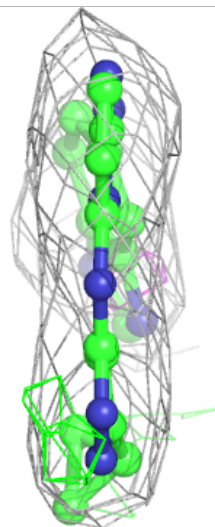
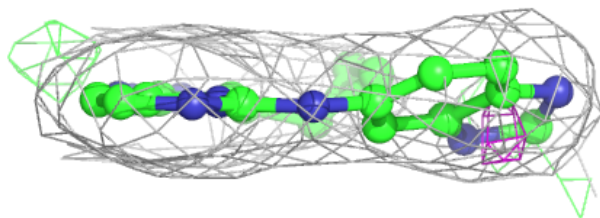
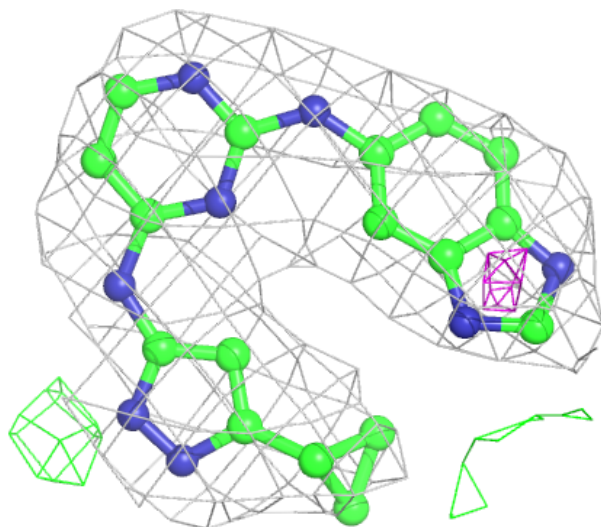
Electron density around APJ N 1999:

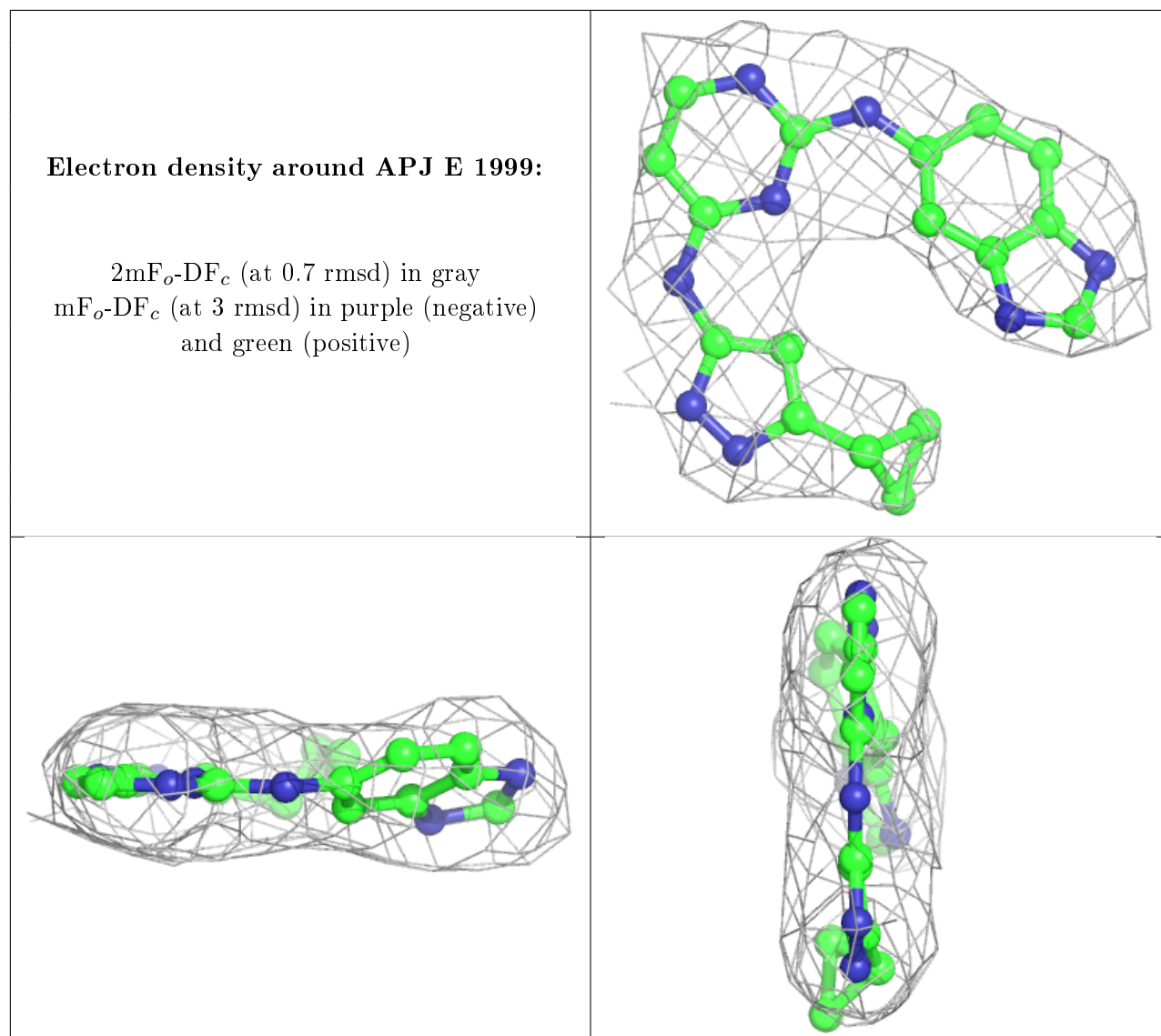
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and green (positive)



Electron density around APJ B 1999:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.