Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2023 – 03:31 AM EDT

PDB ID	:	2B9V
Title	:	Acetobacter turbidans alpha-amino acid ester hydrolase
Authors	:	Barends, T.R.M.
Deposited on	:	2005-10-13
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

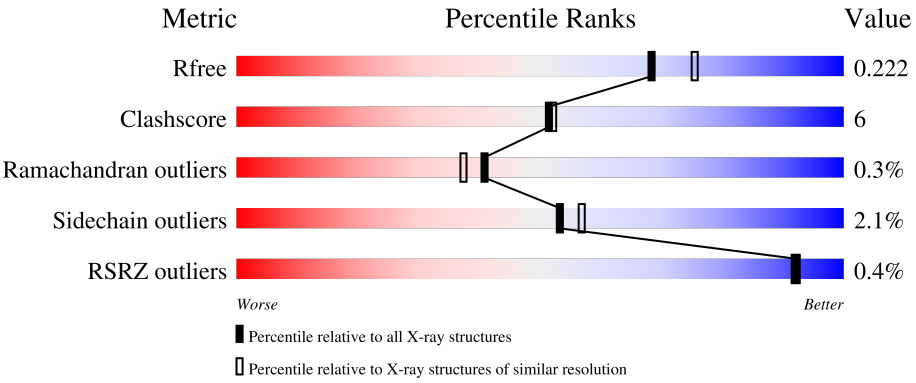
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	652	86% 6% 7%
1	B	652	83% 10% 7%
1	C	652	84% 8% 7%
1	D	652	84% 9% • 7%
1	E	652	84% 9% 7%

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Mol	Chain	Length	Quality of chain
1	F	652	85% 8% • 7%
1	G	652	83% 10% 7%
1	H	652	86% 7% 7%
1	I	652	85% 8% • 7%
1	J	652	83% 9% • 7%
1	K	652	% 84% 9% • 7%
1	L	652	% 83% 10% 7%
1	M	652	84% 8% • 7%
1	N	652	84% 8% • 7%
1	O	652	81% 12% 7%
1	P	652	86% 7% • 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 80710 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 Alpha-amino acid ester hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	608	Total	C	N	O	S	0	0	0
			4816	3071	833	893	19			
1	B	608	Total	C	N	O	S	0	0	0
			4816	3071	833	893	19			
1	C	608	Total	C	N	O	S	0	0	0
			4816	3071	833	893	19			
1	D	608	Total	C	N	O	S	0	0	0
			4816	3071	833	893	19			
1	E	608	Total	C	N	O	S	0	0	0
			4816	3071	833	893	19			
1	F	608	Total	C	N	O	S	0	0	0
			4816	3071	833	893	19			
1	G	608	Total	C	N	O	S	0	0	0
			4816	3071	833	893	19			
1	H	608	Total	C	N	O	S	0	0	0
			4816	3071	833	893	19			
1	I	608	Total	C	N	O	S	0	0	0
			4816	3071	833	893	19			
1	J	608	Total	C	N	O	S	0	0	0
			4816	3071	833	893	19			
1	K	608	Total	C	N	O	S	0	0	0
			4816	3071	833	893	19			
1	L	608	Total	C	N	O	S	0	0	0
			4816	3071	833	893	19			
1	M	608	Total	C	N	O	S	0	0	0
			4816	3071	833	893	19			
1	N	608	Total	C	N	O	S	0	0	0
			4816	3071	833	893	19			
1	O	608	Total	C	N	O	S	0	0	0
			4816	3071	833	893	19			
1	P	608	Total	C	N	O	S	0	0	0
			4816	3071	833	893	19			

There are 400 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	668	LYS	-	expression tag	UNP Q8VRK8
A	669	LEU	-	expression tag	UNP Q8VRK8
A	670	GLY	-	expression tag	UNP Q8VRK8
A	671	PRO	-	expression tag	UNP Q8VRK8
A	672	GLU	-	expression tag	UNP Q8VRK8
A	673	GLN	-	expression tag	UNP Q8VRK8
A	674	LYS	-	expression tag	UNP Q8VRK8
A	675	LEU	-	expression tag	UNP Q8VRK8
A	676	ILE	-	expression tag	UNP Q8VRK8
A	677	SER	-	expression tag	UNP Q8VRK8
A	678	GLU	-	expression tag	UNP Q8VRK8
A	679	GLU	-	expression tag	UNP Q8VRK8
A	680	ASP	-	expression tag	UNP Q8VRK8
A	681	LEU	-	expression tag	UNP Q8VRK8
A	682	ASN	-	expression tag	UNP Q8VRK8
A	683	SER	-	expression tag	UNP Q8VRK8
A	684	ALA	-	expression tag	UNP Q8VRK8
A	685	VAL	-	expression tag	UNP Q8VRK8
A	686	ASP	-	expression tag	UNP Q8VRK8
A	687	HIS	-	expression tag	UNP Q8VRK8
A	688	HIS	-	expression tag	UNP Q8VRK8
A	689	HIS	-	expression tag	UNP Q8VRK8
A	690	HIS	-	expression tag	UNP Q8VRK8
A	691	HIS	-	expression tag	UNP Q8VRK8
A	692	HIS	-	expression tag	UNP Q8VRK8
B	668	LYS	-	expression tag	UNP Q8VRK8
B	669	LEU	-	expression tag	UNP Q8VRK8
B	670	GLY	-	expression tag	UNP Q8VRK8
B	671	PRO	-	expression tag	UNP Q8VRK8
B	672	GLU	-	expression tag	UNP Q8VRK8
B	673	GLN	-	expression tag	UNP Q8VRK8
B	674	LYS	-	expression tag	UNP Q8VRK8
B	675	LEU	-	expression tag	UNP Q8VRK8
B	676	ILE	-	expression tag	UNP Q8VRK8
B	677	SER	-	expression tag	UNP Q8VRK8
B	678	GLU	-	expression tag	UNP Q8VRK8
B	679	GLU	-	expression tag	UNP Q8VRK8
B	680	ASP	-	expression tag	UNP Q8VRK8
B	681	LEU	-	expression tag	UNP Q8VRK8
B	682	ASN	-	expression tag	UNP Q8VRK8
B	683	SER	-	expression tag	UNP Q8VRK8
B	684	ALA	-	expression tag	UNP Q8VRK8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	685	VAL	-	expression tag	UNP Q8VRK8
B	686	ASP	-	expression tag	UNP Q8VRK8
B	687	HIS	-	expression tag	UNP Q8VRK8
B	688	HIS	-	expression tag	UNP Q8VRK8
B	689	HIS	-	expression tag	UNP Q8VRK8
B	690	HIS	-	expression tag	UNP Q8VRK8
B	691	HIS	-	expression tag	UNP Q8VRK8
B	692	HIS	-	expression tag	UNP Q8VRK8
C	668	LYS	-	expression tag	UNP Q8VRK8
C	669	LEU	-	expression tag	UNP Q8VRK8
C	670	GLY	-	expression tag	UNP Q8VRK8
C	671	PRO	-	expression tag	UNP Q8VRK8
C	672	GLU	-	expression tag	UNP Q8VRK8
C	673	GLN	-	expression tag	UNP Q8VRK8
C	674	LYS	-	expression tag	UNP Q8VRK8
C	675	LEU	-	expression tag	UNP Q8VRK8
C	676	ILE	-	expression tag	UNP Q8VRK8
C	677	SER	-	expression tag	UNP Q8VRK8
C	678	GLU	-	expression tag	UNP Q8VRK8
C	679	GLU	-	expression tag	UNP Q8VRK8
C	680	ASP	-	expression tag	UNP Q8VRK8
C	681	LEU	-	expression tag	UNP Q8VRK8
C	682	ASN	-	expression tag	UNP Q8VRK8
C	683	SER	-	expression tag	UNP Q8VRK8
C	684	ALA	-	expression tag	UNP Q8VRK8
C	685	VAL	-	expression tag	UNP Q8VRK8
C	686	ASP	-	expression tag	UNP Q8VRK8
C	687	HIS	-	expression tag	UNP Q8VRK8
C	688	HIS	-	expression tag	UNP Q8VRK8
C	689	HIS	-	expression tag	UNP Q8VRK8
C	690	HIS	-	expression tag	UNP Q8VRK8
C	691	HIS	-	expression tag	UNP Q8VRK8
C	692	HIS	-	expression tag	UNP Q8VRK8
D	668	LYS	-	expression tag	UNP Q8VRK8
D	669	LEU	-	expression tag	UNP Q8VRK8
D	670	GLY	-	expression tag	UNP Q8VRK8
D	671	PRO	-	expression tag	UNP Q8VRK8
D	672	GLU	-	expression tag	UNP Q8VRK8
D	673	GLN	-	expression tag	UNP Q8VRK8
D	674	LYS	-	expression tag	UNP Q8VRK8
D	675	LEU	-	expression tag	UNP Q8VRK8
D	676	ILE	-	expression tag	UNP Q8VRK8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	677	SER	-	expression tag	UNP Q8VRK8
D	678	GLU	-	expression tag	UNP Q8VRK8
D	679	GLU	-	expression tag	UNP Q8VRK8
D	680	ASP	-	expression tag	UNP Q8VRK8
D	681	LEU	-	expression tag	UNP Q8VRK8
D	682	ASN	-	expression tag	UNP Q8VRK8
D	683	SER	-	expression tag	UNP Q8VRK8
D	684	ALA	-	expression tag	UNP Q8VRK8
D	685	VAL	-	expression tag	UNP Q8VRK8
D	686	ASP	-	expression tag	UNP Q8VRK8
D	687	HIS	-	expression tag	UNP Q8VRK8
D	688	HIS	-	expression tag	UNP Q8VRK8
D	689	HIS	-	expression tag	UNP Q8VRK8
D	690	HIS	-	expression tag	UNP Q8VRK8
D	691	HIS	-	expression tag	UNP Q8VRK8
D	692	HIS	-	expression tag	UNP Q8VRK8
E	668	LYS	-	expression tag	UNP Q8VRK8
E	669	LEU	-	expression tag	UNP Q8VRK8
E	670	GLY	-	expression tag	UNP Q8VRK8
E	671	PRO	-	expression tag	UNP Q8VRK8
E	672	GLU	-	expression tag	UNP Q8VRK8
E	673	GLN	-	expression tag	UNP Q8VRK8
E	674	LYS	-	expression tag	UNP Q8VRK8
E	675	LEU	-	expression tag	UNP Q8VRK8
E	676	ILE	-	expression tag	UNP Q8VRK8
E	677	SER	-	expression tag	UNP Q8VRK8
E	678	GLU	-	expression tag	UNP Q8VRK8
E	679	GLU	-	expression tag	UNP Q8VRK8
E	680	ASP	-	expression tag	UNP Q8VRK8
E	681	LEU	-	expression tag	UNP Q8VRK8
E	682	ASN	-	expression tag	UNP Q8VRK8
E	683	SER	-	expression tag	UNP Q8VRK8
E	684	ALA	-	expression tag	UNP Q8VRK8
E	685	VAL	-	expression tag	UNP Q8VRK8
E	686	ASP	-	expression tag	UNP Q8VRK8
E	687	HIS	-	expression tag	UNP Q8VRK8
E	688	HIS	-	expression tag	UNP Q8VRK8
E	689	HIS	-	expression tag	UNP Q8VRK8
E	690	HIS	-	expression tag	UNP Q8VRK8
E	691	HIS	-	expression tag	UNP Q8VRK8
E	692	HIS	-	expression tag	UNP Q8VRK8
F	668	LYS	-	expression tag	UNP Q8VRK8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	669	LEU	-	expression tag	UNP Q8VRK8
F	670	GLY	-	expression tag	UNP Q8VRK8
F	671	PRO	-	expression tag	UNP Q8VRK8
F	672	GLU	-	expression tag	UNP Q8VRK8
F	673	GLN	-	expression tag	UNP Q8VRK8
F	674	LYS	-	expression tag	UNP Q8VRK8
F	675	LEU	-	expression tag	UNP Q8VRK8
F	676	ILE	-	expression tag	UNP Q8VRK8
F	677	SER	-	expression tag	UNP Q8VRK8
F	678	GLU	-	expression tag	UNP Q8VRK8
F	679	GLU	-	expression tag	UNP Q8VRK8
F	680	ASP	-	expression tag	UNP Q8VRK8
F	681	LEU	-	expression tag	UNP Q8VRK8
F	682	ASN	-	expression tag	UNP Q8VRK8
F	683	SER	-	expression tag	UNP Q8VRK8
F	684	ALA	-	expression tag	UNP Q8VRK8
F	685	VAL	-	expression tag	UNP Q8VRK8
F	686	ASP	-	expression tag	UNP Q8VRK8
F	687	HIS	-	expression tag	UNP Q8VRK8
F	688	HIS	-	expression tag	UNP Q8VRK8
F	689	HIS	-	expression tag	UNP Q8VRK8
F	690	HIS	-	expression tag	UNP Q8VRK8
F	691	HIS	-	expression tag	UNP Q8VRK8
F	692	HIS	-	expression tag	UNP Q8VRK8
G	668	LYS	-	expression tag	UNP Q8VRK8
G	669	LEU	-	expression tag	UNP Q8VRK8
G	670	GLY	-	expression tag	UNP Q8VRK8
G	671	PRO	-	expression tag	UNP Q8VRK8
G	672	GLU	-	expression tag	UNP Q8VRK8
G	673	GLN	-	expression tag	UNP Q8VRK8
G	674	LYS	-	expression tag	UNP Q8VRK8
G	675	LEU	-	expression tag	UNP Q8VRK8
G	676	ILE	-	expression tag	UNP Q8VRK8
G	677	SER	-	expression tag	UNP Q8VRK8
G	678	GLU	-	expression tag	UNP Q8VRK8
G	679	GLU	-	expression tag	UNP Q8VRK8
G	680	ASP	-	expression tag	UNP Q8VRK8
G	681	LEU	-	expression tag	UNP Q8VRK8
G	682	ASN	-	expression tag	UNP Q8VRK8
G	683	SER	-	expression tag	UNP Q8VRK8
G	684	ALA	-	expression tag	UNP Q8VRK8
G	685	VAL	-	expression tag	UNP Q8VRK8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	686	ASP	-	expression tag	UNP Q8VRK8
G	687	HIS	-	expression tag	UNP Q8VRK8
G	688	HIS	-	expression tag	UNP Q8VRK8
G	689	HIS	-	expression tag	UNP Q8VRK8
G	690	HIS	-	expression tag	UNP Q8VRK8
G	691	HIS	-	expression tag	UNP Q8VRK8
G	692	HIS	-	expression tag	UNP Q8VRK8
H	668	LYS	-	expression tag	UNP Q8VRK8
H	669	LEU	-	expression tag	UNP Q8VRK8
H	670	GLY	-	expression tag	UNP Q8VRK8
H	671	PRO	-	expression tag	UNP Q8VRK8
H	672	GLU	-	expression tag	UNP Q8VRK8
H	673	GLN	-	expression tag	UNP Q8VRK8
H	674	LYS	-	expression tag	UNP Q8VRK8
H	675	LEU	-	expression tag	UNP Q8VRK8
H	676	ILE	-	expression tag	UNP Q8VRK8
H	677	SER	-	expression tag	UNP Q8VRK8
H	678	GLU	-	expression tag	UNP Q8VRK8
H	679	GLU	-	expression tag	UNP Q8VRK8
H	680	ASP	-	expression tag	UNP Q8VRK8
H	681	LEU	-	expression tag	UNP Q8VRK8
H	682	ASN	-	expression tag	UNP Q8VRK8
H	683	SER	-	expression tag	UNP Q8VRK8
H	684	ALA	-	expression tag	UNP Q8VRK8
H	685	VAL	-	expression tag	UNP Q8VRK8
H	686	ASP	-	expression tag	UNP Q8VRK8
H	687	HIS	-	expression tag	UNP Q8VRK8
H	688	HIS	-	expression tag	UNP Q8VRK8
H	689	HIS	-	expression tag	UNP Q8VRK8
H	690	HIS	-	expression tag	UNP Q8VRK8
H	691	HIS	-	expression tag	UNP Q8VRK8
H	692	HIS	-	expression tag	UNP Q8VRK8
I	668	LYS	-	expression tag	UNP Q8VRK8
I	669	LEU	-	expression tag	UNP Q8VRK8
I	670	GLY	-	expression tag	UNP Q8VRK8
I	671	PRO	-	expression tag	UNP Q8VRK8
I	672	GLU	-	expression tag	UNP Q8VRK8
I	673	GLN	-	expression tag	UNP Q8VRK8
I	674	LYS	-	expression tag	UNP Q8VRK8
I	675	LEU	-	expression tag	UNP Q8VRK8
I	676	ILE	-	expression tag	UNP Q8VRK8
I	677	SER	-	expression tag	UNP Q8VRK8

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Chain	Residue	Modelled	Actual	Comment	Reference
I	678	GLU	-	expression tag	UNP Q8VRK8
I	679	GLU	-	expression tag	UNP Q8VRK8
I	680	ASP	-	expression tag	UNP Q8VRK8
I	681	LEU	-	expression tag	UNP Q8VRK8
I	682	ASN	-	expression tag	UNP Q8VRK8
I	683	SER	-	expression tag	UNP Q8VRK8
I	684	ALA	-	expression tag	UNP Q8VRK8
I	685	VAL	-	expression tag	UNP Q8VRK8
I	686	ASP	-	expression tag	UNP Q8VRK8
I	687	HIS	-	expression tag	UNP Q8VRK8
I	688	HIS	-	expression tag	UNP Q8VRK8
I	689	HIS	-	expression tag	UNP Q8VRK8
I	690	HIS	-	expression tag	UNP Q8VRK8
I	691	HIS	-	expression tag	UNP Q8VRK8
I	692	HIS	-	expression tag	UNP Q8VRK8
J	668	LYS	-	expression tag	UNP Q8VRK8
J	669	LEU	-	expression tag	UNP Q8VRK8
J	670	GLY	-	expression tag	UNP Q8VRK8
J	671	PRO	-	expression tag	UNP Q8VRK8
J	672	GLU	-	expression tag	UNP Q8VRK8
J	673	GLN	-	expression tag	UNP Q8VRK8
J	674	LYS	-	expression tag	UNP Q8VRK8
J	675	LEU	-	expression tag	UNP Q8VRK8
J	676	ILE	-	expression tag	UNP Q8VRK8
J	677	SER	-	expression tag	UNP Q8VRK8
J	678	GLU	-	expression tag	UNP Q8VRK8
J	679	GLU	-	expression tag	UNP Q8VRK8
J	680	ASP	-	expression tag	UNP Q8VRK8
J	681	LEU	-	expression tag	UNP Q8VRK8
J	682	ASN	-	expression tag	UNP Q8VRK8
J	683	SER	-	expression tag	UNP Q8VRK8
J	684	ALA	-	expression tag	UNP Q8VRK8
J	685	VAL	-	expression tag	UNP Q8VRK8
J	686	ASP	-	expression tag	UNP Q8VRK8
J	687	HIS	-	expression tag	UNP Q8VRK8
J	688	HIS	-	expression tag	UNP Q8VRK8
J	689	HIS	-	expression tag	UNP Q8VRK8
J	690	HIS	-	expression tag	UNP Q8VRK8
J	691	HIS	-	expression tag	UNP Q8VRK8
J	692	HIS	-	expression tag	UNP Q8VRK8
K	668	LYS	-	expression tag	UNP Q8VRK8
K	669	LEU	-	expression tag	UNP Q8VRK8

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Chain	Residue	Modelled	Actual	Comment	Reference
K	670	GLY	-	expression tag	UNP Q8VRK8
K	671	PRO	-	expression tag	UNP Q8VRK8
K	672	GLU	-	expression tag	UNP Q8VRK8
K	673	GLN	-	expression tag	UNP Q8VRK8
K	674	LYS	-	expression tag	UNP Q8VRK8
K	675	LEU	-	expression tag	UNP Q8VRK8
K	676	ILE	-	expression tag	UNP Q8VRK8
K	677	SER	-	expression tag	UNP Q8VRK8
K	678	GLU	-	expression tag	UNP Q8VRK8
K	679	GLU	-	expression tag	UNP Q8VRK8
K	680	ASP	-	expression tag	UNP Q8VRK8
K	681	LEU	-	expression tag	UNP Q8VRK8
K	682	ASN	-	expression tag	UNP Q8VRK8
K	683	SER	-	expression tag	UNP Q8VRK8
K	684	ALA	-	expression tag	UNP Q8VRK8
K	685	VAL	-	expression tag	UNP Q8VRK8
K	686	ASP	-	expression tag	UNP Q8VRK8
K	687	HIS	-	expression tag	UNP Q8VRK8
K	688	HIS	-	expression tag	UNP Q8VRK8
K	689	HIS	-	expression tag	UNP Q8VRK8
K	690	HIS	-	expression tag	UNP Q8VRK8
K	691	HIS	-	expression tag	UNP Q8VRK8
K	692	HIS	-	expression tag	UNP Q8VRK8
L	668	LYS	-	expression tag	UNP Q8VRK8
L	669	LEU	-	expression tag	UNP Q8VRK8
L	670	GLY	-	expression tag	UNP Q8VRK8
L	671	PRO	-	expression tag	UNP Q8VRK8
L	672	GLU	-	expression tag	UNP Q8VRK8
L	673	GLN	-	expression tag	UNP Q8VRK8
L	674	LYS	-	expression tag	UNP Q8VRK8
L	675	LEU	-	expression tag	UNP Q8VRK8
L	676	ILE	-	expression tag	UNP Q8VRK8
L	677	SER	-	expression tag	UNP Q8VRK8
L	678	GLU	-	expression tag	UNP Q8VRK8
L	679	GLU	-	expression tag	UNP Q8VRK8
L	680	ASP	-	expression tag	UNP Q8VRK8
L	681	LEU	-	expression tag	UNP Q8VRK8
L	682	ASN	-	expression tag	UNP Q8VRK8
L	683	SER	-	expression tag	UNP Q8VRK8
L	684	ALA	-	expression tag	UNP Q8VRK8
L	685	VAL	-	expression tag	UNP Q8VRK8
L	686	ASP	-	expression tag	UNP Q8VRK8

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Chain	Residue	Modelled	Actual	Comment	Reference
L	687	HIS	-	expression tag	UNP Q8VRK8
L	688	HIS	-	expression tag	UNP Q8VRK8
L	689	HIS	-	expression tag	UNP Q8VRK8
L	690	HIS	-	expression tag	UNP Q8VRK8
L	691	HIS	-	expression tag	UNP Q8VRK8
L	692	HIS	-	expression tag	UNP Q8VRK8
M	668	LYS	-	expression tag	UNP Q8VRK8
M	669	LEU	-	expression tag	UNP Q8VRK8
M	670	GLY	-	expression tag	UNP Q8VRK8
M	671	PRO	-	expression tag	UNP Q8VRK8
M	672	GLU	-	expression tag	UNP Q8VRK8
M	673	GLN	-	expression tag	UNP Q8VRK8
M	674	LYS	-	expression tag	UNP Q8VRK8
M	675	LEU	-	expression tag	UNP Q8VRK8
M	676	ILE	-	expression tag	UNP Q8VRK8
M	677	SER	-	expression tag	UNP Q8VRK8
M	678	GLU	-	expression tag	UNP Q8VRK8
M	679	GLU	-	expression tag	UNP Q8VRK8
M	680	ASP	-	expression tag	UNP Q8VRK8
M	681	LEU	-	expression tag	UNP Q8VRK8
M	682	ASN	-	expression tag	UNP Q8VRK8
M	683	SER	-	expression tag	UNP Q8VRK8
M	684	ALA	-	expression tag	UNP Q8VRK8
M	685	VAL	-	expression tag	UNP Q8VRK8
M	686	ASP	-	expression tag	UNP Q8VRK8
M	687	HIS	-	expression tag	UNP Q8VRK8
M	688	HIS	-	expression tag	UNP Q8VRK8
M	689	HIS	-	expression tag	UNP Q8VRK8
M	690	HIS	-	expression tag	UNP Q8VRK8
M	691	HIS	-	expression tag	UNP Q8VRK8
M	692	HIS	-	expression tag	UNP Q8VRK8
N	668	LYS	-	expression tag	UNP Q8VRK8
N	669	LEU	-	expression tag	UNP Q8VRK8
N	670	GLY	-	expression tag	UNP Q8VRK8
N	671	PRO	-	expression tag	UNP Q8VRK8
N	672	GLU	-	expression tag	UNP Q8VRK8
N	673	GLN	-	expression tag	UNP Q8VRK8
N	674	LYS	-	expression tag	UNP Q8VRK8
N	675	LEU	-	expression tag	UNP Q8VRK8
N	676	ILE	-	expression tag	UNP Q8VRK8
N	677	SER	-	expression tag	UNP Q8VRK8
N	678	GLU	-	expression tag	UNP Q8VRK8

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Chain	Residue	Modelled	Actual	Comment	Reference
N	679	GLU	-	expression tag	UNP Q8VRK8
N	680	ASP	-	expression tag	UNP Q8VRK8
N	681	LEU	-	expression tag	UNP Q8VRK8
N	682	ASN	-	expression tag	UNP Q8VRK8
N	683	SER	-	expression tag	UNP Q8VRK8
N	684	ALA	-	expression tag	UNP Q8VRK8
N	685	VAL	-	expression tag	UNP Q8VRK8
N	686	ASP	-	expression tag	UNP Q8VRK8
N	687	HIS	-	expression tag	UNP Q8VRK8
N	688	HIS	-	expression tag	UNP Q8VRK8
N	689	HIS	-	expression tag	UNP Q8VRK8
N	690	HIS	-	expression tag	UNP Q8VRK8
N	691	HIS	-	expression tag	UNP Q8VRK8
N	692	HIS	-	expression tag	UNP Q8VRK8
O	668	LYS	-	expression tag	UNP Q8VRK8
O	669	LEU	-	expression tag	UNP Q8VRK8
O	670	GLY	-	expression tag	UNP Q8VRK8
O	671	PRO	-	expression tag	UNP Q8VRK8
O	672	GLU	-	expression tag	UNP Q8VRK8
O	673	GLN	-	expression tag	UNP Q8VRK8
O	674	LYS	-	expression tag	UNP Q8VRK8
O	675	LEU	-	expression tag	UNP Q8VRK8
O	676	ILE	-	expression tag	UNP Q8VRK8
O	677	SER	-	expression tag	UNP Q8VRK8
O	678	GLU	-	expression tag	UNP Q8VRK8
O	679	GLU	-	expression tag	UNP Q8VRK8
O	680	ASP	-	expression tag	UNP Q8VRK8
O	681	LEU	-	expression tag	UNP Q8VRK8
O	682	ASN	-	expression tag	UNP Q8VRK8
O	683	SER	-	expression tag	UNP Q8VRK8
O	684	ALA	-	expression tag	UNP Q8VRK8
O	685	VAL	-	expression tag	UNP Q8VRK8
O	686	ASP	-	expression tag	UNP Q8VRK8
O	687	HIS	-	expression tag	UNP Q8VRK8
O	688	HIS	-	expression tag	UNP Q8VRK8
O	689	HIS	-	expression tag	UNP Q8VRK8
O	690	HIS	-	expression tag	UNP Q8VRK8
O	691	HIS	-	expression tag	UNP Q8VRK8
O	692	HIS	-	expression tag	UNP Q8VRK8
P	668	LYS	-	expression tag	UNP Q8VRK8
P	669	LEU	-	expression tag	UNP Q8VRK8
P	670	GLY	-	expression tag	UNP Q8VRK8

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Chain	Residue	Modelled	Actual	Comment	Reference
P	671	PRO	-	expression tag	UNP Q8VRK8
P	672	GLU	-	expression tag	UNP Q8VRK8
P	673	GLN	-	expression tag	UNP Q8VRK8
P	674	LYS	-	expression tag	UNP Q8VRK8
P	675	LEU	-	expression tag	UNP Q8VRK8
P	676	ILE	-	expression tag	UNP Q8VRK8
P	677	SER	-	expression tag	UNP Q8VRK8
P	678	GLU	-	expression tag	UNP Q8VRK8
P	679	GLU	-	expression tag	UNP Q8VRK8
P	680	ASP	-	expression tag	UNP Q8VRK8
P	681	LEU	-	expression tag	UNP Q8VRK8
P	682	ASN	-	expression tag	UNP Q8VRK8
P	683	SER	-	expression tag	UNP Q8VRK8
P	684	ALA	-	expression tag	UNP Q8VRK8
P	685	VAL	-	expression tag	UNP Q8VRK8
P	686	ASP	-	expression tag	UNP Q8VRK8
P	687	HIS	-	expression tag	UNP Q8VRK8
P	688	HIS	-	expression tag	UNP Q8VRK8
P	689	HIS	-	expression tag	UNP Q8VRK8
P	690	HIS	-	expression tag	UNP Q8VRK8
P	691	HIS	-	expression tag	UNP Q8VRK8
P	692	HIS	-	expression tag	UNP Q8VRK8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	257	Total O 257 257	0	0
2	B	226	Total O 226 226	0	0
2	C	203	Total O 203 203	0	0
2	D	234	Total O 234 234	0	0
2	E	216	Total O 216 216	0	0
2	F	185	Total O 185 185	0	0
2	G	220	Total O 220 220	0	0
2	H	265	Total O 265 265	0	0

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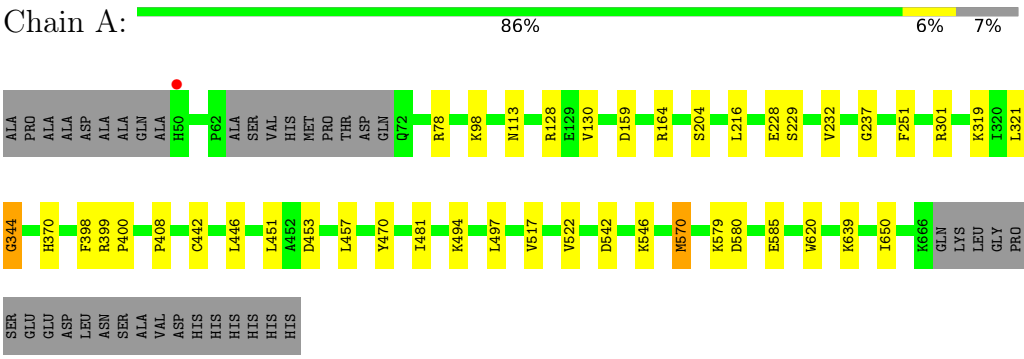
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	I	209	Total O 209 209	0	0
2	J	229	Total O 229 229	0	0
2	K	224	Total O 224 224	0	0
2	L	226	Total O 226 226	0	0
2	M	240	Total O 240 240	0	0
2	N	223	Total O 223 223	0	0
2	O	239	Total O 239 239	0	0
2	P	258	Total O 258 258	0	0

3 Residue-property plots (i)

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

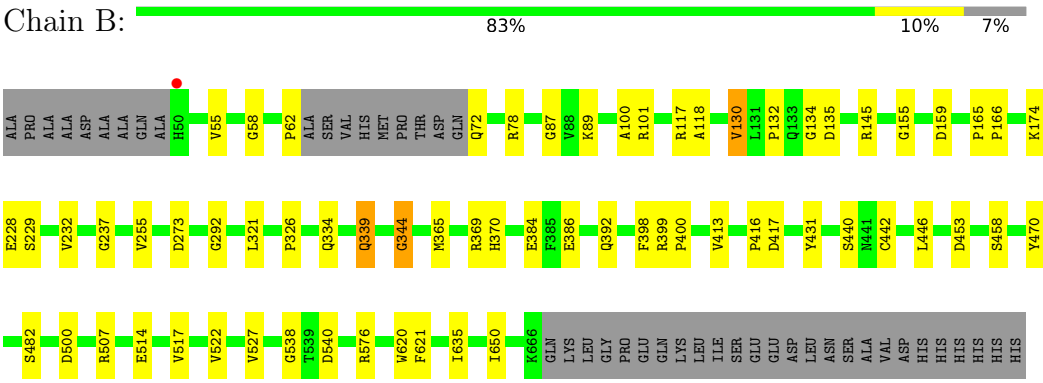
• Molecule 1: Alpha-amino acid ester hydrolase

Chain A:



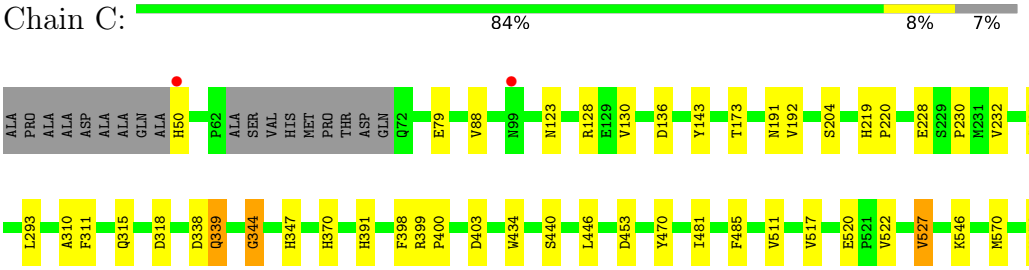
• Molecule 1: Alpha-amino acid ester hydrolase

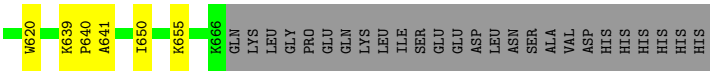
Chain B:



• Molecule 1: Alpha-amino acid ester hydrolase

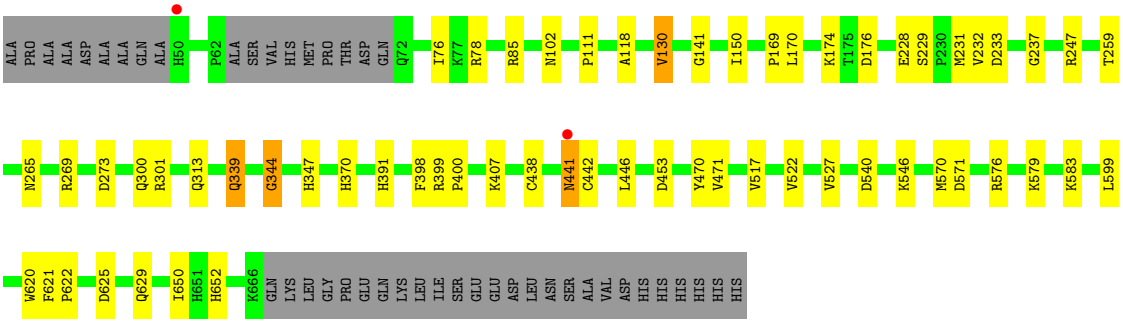
Chain C:





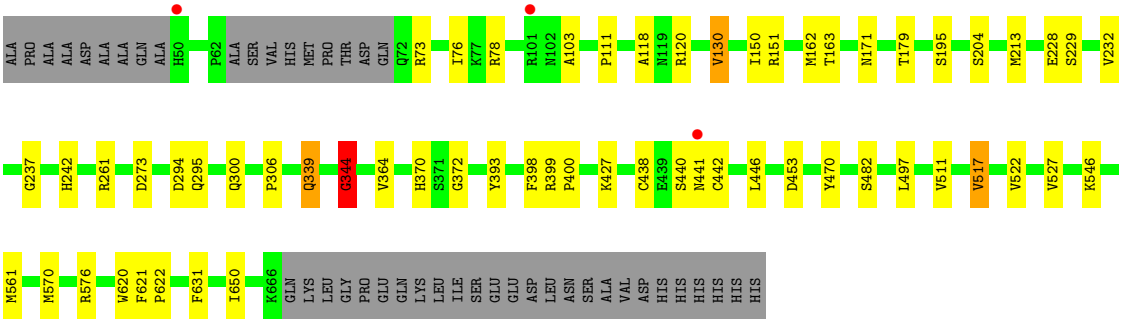
• Molecule 1: Alpha-amino acid ester hydrolase

Chain D:



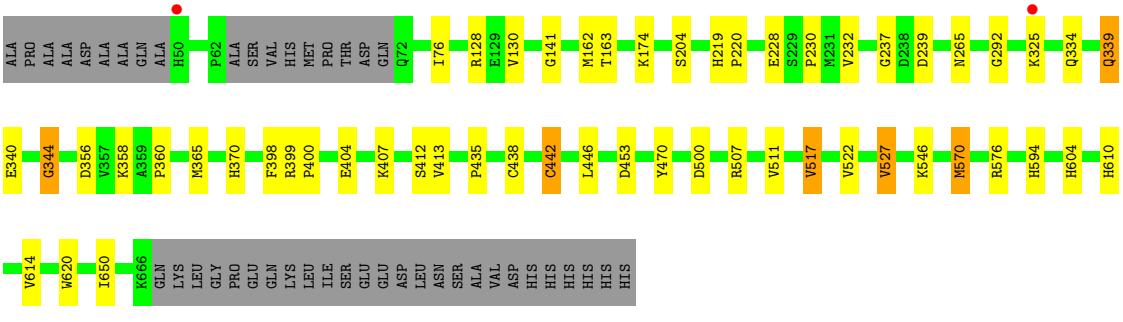
• Molecule 1: Alpha-amino acid ester hydrolase

Chain E:



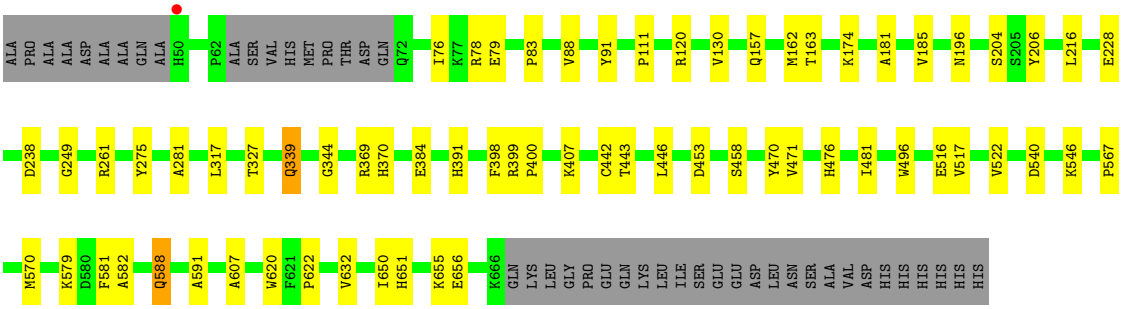
• Molecule 1: Alpha-amino acid ester hydrolase

Chain F:



• Molecule 1: Alpha-amino acid ester hydrolase

Chain G:

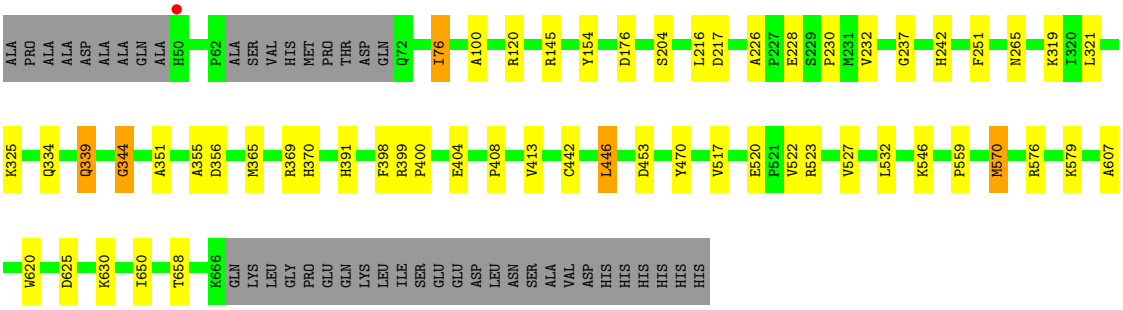


• Molecule 1: Alpha-amino acid ester hydrolase

Chain H:

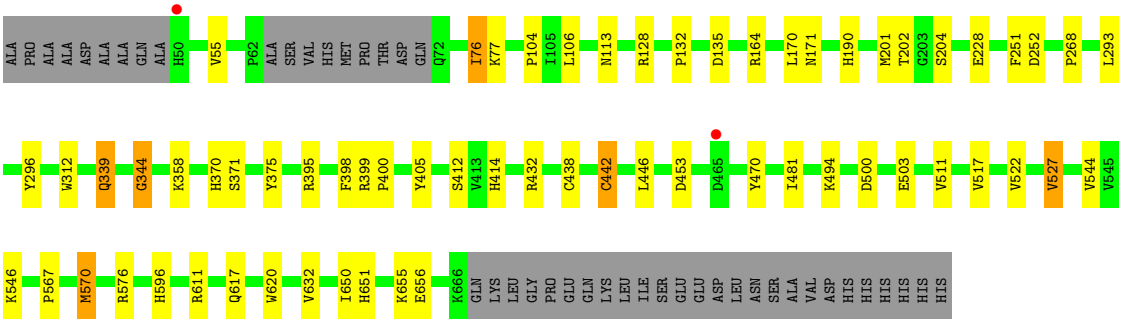
• Molecule 1: Alpha-amino acid ester hydrolase

Chain I:



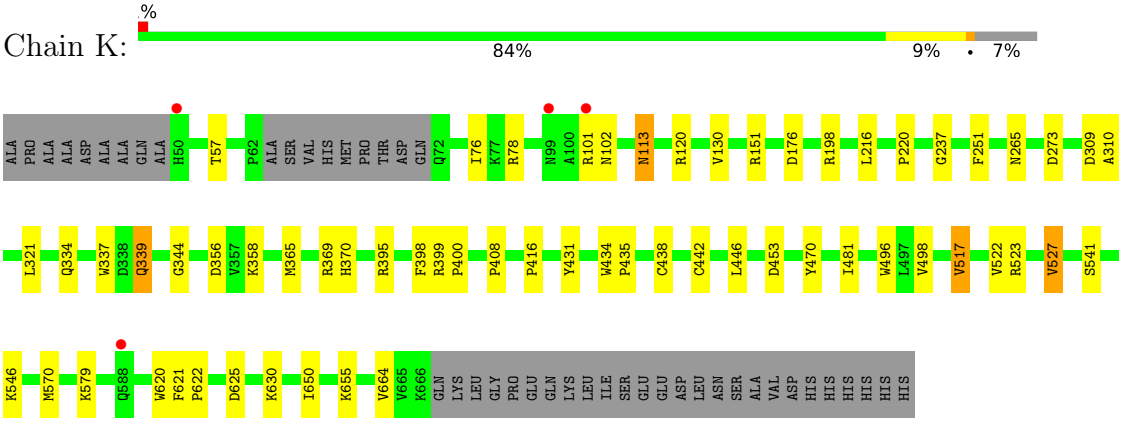
• Molecule 1: Alpha-amino acid ester hydrolase

Chain J:



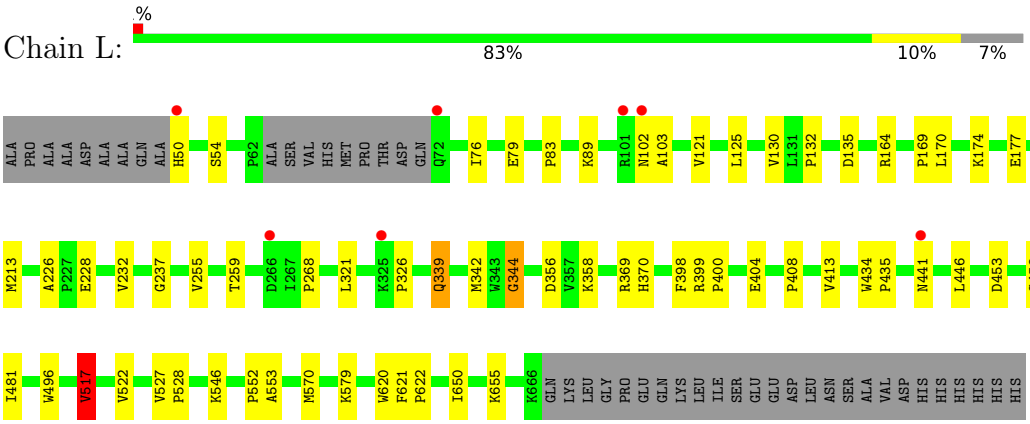
• Molecule 1: Alpha-amino acid ester hydrolase

Chain K:



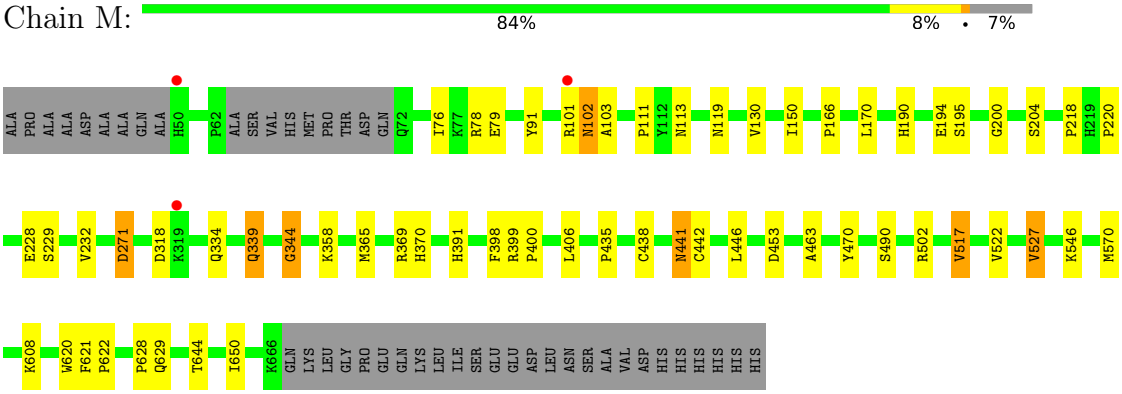
• Molecule 1: Alpha-amino acid ester hydrolase

Chain L:



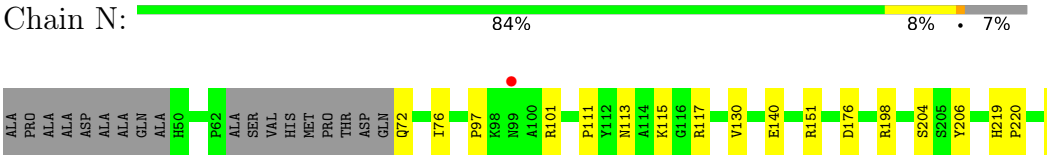
• Molecule 1: Alpha-amino acid ester hydrolase

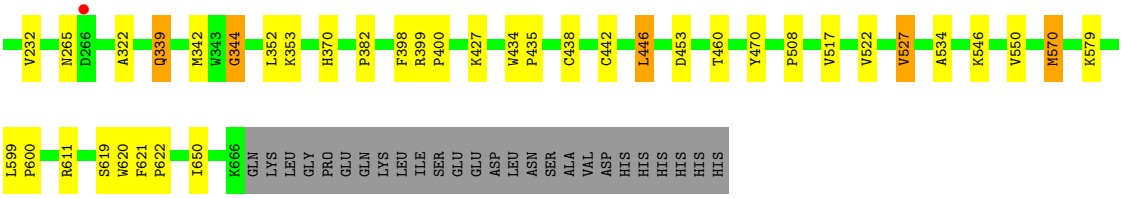
Chain M:



• Molecule 1: Alpha-amino acid ester hydrolase

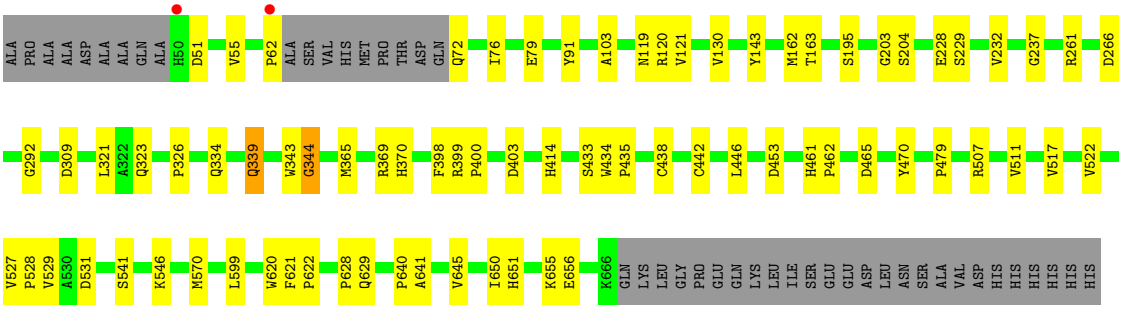
Chain N:





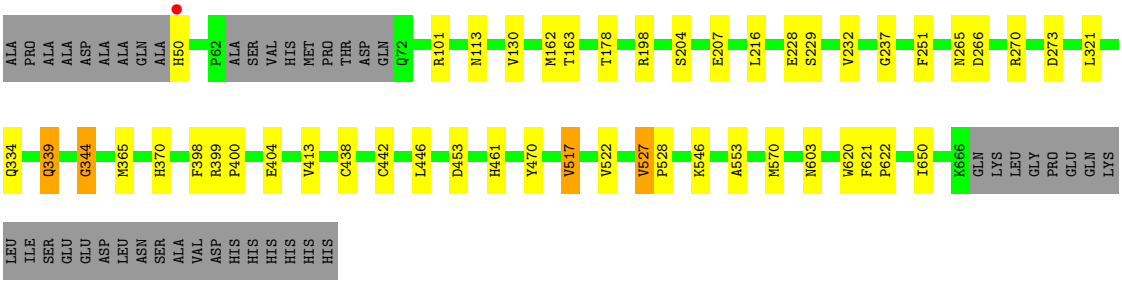
• Molecule 1: Alpha-amino acid ester hydrolase

Chain O:



• Molecule 1: Alpha-amino acid ester hydrolase

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.37Å 275.59Å 197.95Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 40.03 – 2.00	Depositor EDS
% Data completeness (in resolution range)	75.4 (40.00-2.00) 75.4 (40.03-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.91 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.235 0.190 , 0.222	Depositor DCC
R_{free} test set	25420 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å^2)	18.1	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 23.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.226 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	80710	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.71 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5111e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.40	0/4972	0.84	1/6789 (0.0%)
1	B	0.41	0/4972	0.86	8/6789 (0.1%)
1	C	0.40	0/4972	0.84	3/6789 (0.0%)
1	D	0.40	0/4972	0.85	4/6789 (0.1%)
1	E	0.39	0/4972	0.85	4/6789 (0.1%)
1	F	0.39	0/4972	0.85	5/6789 (0.1%)
1	G	0.40	0/4972	0.85	2/6789 (0.0%)
1	H	0.40	0/4972	0.86	1/6789 (0.0%)
1	I	0.40	0/4972	0.85	5/6789 (0.1%)
1	J	0.41	0/4972	0.86	5/6789 (0.1%)
1	K	0.41	0/4972	0.84	3/6789 (0.0%)
1	L	0.43	0/4972	0.81	2/6789 (0.0%)
1	M	0.43	1/4972 (0.0%)	0.83	2/6789 (0.0%)
1	N	0.42	0/4972	0.81	0/6789
1	O	0.42	0/4972	0.82	1/6789 (0.0%)
1	P	0.43	0/4972	0.81	2/6789 (0.0%)
All	All	0.41	1/79552 (0.0%)	0.84	48/108624 (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	M	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	441	ASN	C-N	-5.94	1.20	1.34

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	500	ASP	CB-CG-OD2	7.04	124.64	118.30
1	B	500	ASP	CB-CG-OD2	6.25	123.92	118.30
1	B	540	ASP	CB-CG-OD1	6.19	123.87	118.30
1	B	273	ASP	CB-CG-OD2	6.18	123.87	118.30
1	E	273	ASP	CB-CG-OD2	6.14	123.83	118.30
1	B	117	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	576	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	J	611	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	K	120	ARG	NE-CZ-NH2	5.91	123.26	120.30
1	J	576	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	F	128	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	I	576	ARG	NE-CZ-NH1	-5.85	117.37	120.30
1	C	128	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	C	273	ASP	CB-CG-OD2	5.79	123.51	118.30
1	D	273	ASP	CB-CG-OD2	5.74	123.47	118.30
1	D	576	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	D	247	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	M	271	ASP	CB-CG-OD1	5.55	123.30	118.30
1	C	338	ASP	CB-CG-OD2	5.54	123.28	118.30
1	G	120	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	I	145	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	G	540	ASP	CB-CG-OD1	5.49	123.24	118.30
1	J	500	ASP	CB-CG-OD2	5.44	123.20	118.30
1	K	625	ASP	CB-CG-OD2	5.40	123.16	118.30
1	M	502	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	I	145	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	F	325	LYS	CD-CE-NZ	5.32	123.94	111.70
1	B	576	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	J	128	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	J	344	GLY	N-CA-C	5.28	126.30	113.10
1	A	128	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	K	273	ASP	CB-CG-OD2	5.22	123.00	118.30
1	I	625	ASP	CB-CG-OD1	-5.20	113.62	118.30
1	I	120	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	L	517	VAL	CB-CA-C	5.17	121.22	111.40
1	F	576	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	F	500	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	H	344	GLY	N-CA-C	5.12	125.89	113.10
1	B	145	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	O	531	ASP	N-CA-C	-5.09	97.27	111.00
1	E	344	GLY	N-CA-C	5.08	125.80	113.10
1	P	273	ASP	CB-CG-OD2	5.08	122.87	118.30
1	P	603	ASN	N-CA-C	-5.07	97.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	469	SER	CB-CA-C	-5.06	100.49	110.10
1	D	625	ASP	CB-CG-OD2	5.03	122.82	118.30
1	E	120	ARG	NE-CZ-NH1	-5.03	117.79	120.30
1	E	576	ARG	NE-CZ-NH2	5.01	122.80	120.30
1	B	417	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	441	ASN	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4816	0	4586	39	0
1	B	4816	0	4586	66	0
1	C	4816	0	4586	60	0
1	D	4816	0	4586	55	1
1	E	4816	0	4586	67	0
1	F	4816	0	4586	41	0
1	G	4816	0	4586	58	0
1	H	4816	0	4586	40	0
1	I	4816	0	4586	47	0
1	J	4816	0	4586	69	0
1	K	4816	0	4586	44	0
1	L	4816	0	4586	59	0
1	M	4816	0	4585	77	1
1	N	4816	0	4586	55	0
1	O	4816	0	4586	64	2
1	P	4816	0	4586	35	0
2	A	257	0	0	24	0
2	B	226	0	0	40	0
2	C	203	0	0	40	0
2	D	234	0	0	37	0
2	E	216	0	0	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	185	0	0	20	0
2	G	220	0	0	36	0
2	H	265	0	0	25	0
2	I	209	0	0	34	0
2	J	229	0	0	46	0
2	K	224	0	0	20	0
2	L	226	0	0	21	0
2	M	240	0	0	21	0
2	N	223	0	0	29	0
2	O	239	0	0	36	0
2	P	258	0	0	11	0
All	All	80710	0	73375	829	2

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 6.

All (829) 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:E:295:GLN:HA	1:M:101:ARG:CD	1.42	1.50
1:E:295:GLN:CA	1:M:101:ARG:HD3	1.48	1.40
1:G:632:VAL:HG22	2:G:893:HOH:O	1.34	1.27
1:L:83:PRO:HB3	2:L:828:HOH:O	1.36	1.24
1:K:356:ASP:O	1:K:358:LYS:NZ	1.75	1.19
1:H:50:HIS:HB3	2:H:910:HOH:O	1.36	1.19
1:C:655:LYS:HE3	2:C:841:HOH:O	1.42	1.18
1:J:412:SER:HB3	2:J:838:HOH:O	1.45	1.15
1:G:651:HIS:HB2	2:G:827:HOH:O	1.43	1.15
1:E:295:GLN:HE21	1:M:102:ASN:ND2	1.45	1.13
1:M:608:LYS:HE3	2:M:872:HOH:O	1.48	1.11
1:C:136:ASP:HB2	2:C:876:HOH:O	1.52	1.08
1:F:265:ASN:HB2	2:F:755:HOH:O	1.52	1.07
1:J:358:LYS:HE2	2:J:850:HOH:O	1.55	1.05
1:E:295:GLN:HA	1:M:101:ARG:HD2	1.34	1.03
1:O:72:GLN:HA	2:O:825:HOH:O	1.58	1.03
1:B:58:GLY:HA3	2:B:900:HOH:O	1.56	1.03
1:I:265:ASN:HB2	2:I:811:HOH:O	1.58	1.03
1:B:132:PRO:HB2	2:B:825:HOH:O	1.59	1.01
1:I:351:ALA:HB3	2:I:884:HOH:O	1.57	1.01
1:J:76:ILE:HD13	2:J:889:HOH:O	1.63	0.99
1:C:310:ALA:HB3	2:C:880:HOH:O	1.63	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:579:LYS:HD2	2:I:836:HOH:O	1.61	0.99
1:I:408:PRO:HG3	2:I:887:HOH:O	1.63	0.98
1:B:440:SER:HB3	2:B:746:HOH:O	1.64	0.98
1:A:98:LYS:HE2	2:A:876:HOH:O	1.63	0.97
1:G:327:THR:HB	2:G:908:HOH:O	1.63	0.97
1:N:265:ASN:HB2	2:N:815:HOH:O	1.64	0.95
1:A:579:LYS:HE3	2:A:821:HOH:O	1.65	0.95
1:O:655:LYS:HE3	2:O:930:HOH:O	1.66	0.95
1:I:355:ALA:HB1	2:I:865:HOH:O	1.66	0.94
1:C:592:THR:HG21	2:C:830:HOH:O	1.68	0.94
1:E:295:GLN:HA	1:M:101:ARG:HD3	0.95	0.94
1:N:438:CYS:HG	1:N:442:CYS:HG	1.14	0.93
1:C:434:TRP:CD1	2:C:878:HOH:O	2.22	0.93
1:H:408:PRO:HG3	2:H:911:HOH:O	1.67	0.92
1:G:391:HIS:HD2	2:G:865:HOH:O	1.52	0.92
1:N:115:LYS:HE2	2:N:858:HOH:O	1.69	0.92
1:N:534:ALA:HB2	2:N:848:HOH:O	1.68	0.92
1:G:275:TYR:HB2	2:G:881:HOH:O	1.68	0.91
1:H:441:ASN:HB3	2:H:827:HOH:O	1.68	0.91
1:L:79:GLU:HG3	2:L:799:HOH:O	1.71	0.91
1:B:386:GLU:HG3	2:B:914:HOH:O	1.71	0.90
1:E:561:MET:HE2	2:E:905:HOH:O	1.70	0.90
1:O:645:VAL:HG23	2:O:917:HOH:O	1.72	0.90
1:C:391:HIS:HD2	2:D:871:HOH:O	1.54	0.89
1:D:300:GLN:HB2	2:D:820:HOH:O	1.72	0.88
1:M:218:PRO:HG3	2:M:868:HOH:O	1.73	0.88
1:E:517:VAL:HG13	2:E:754:HOH:O	1.72	0.88
1:N:101:ARG:HG3	2:N:817:HOH:O	1.72	0.88
1:L:226:ALA:HB1	2:L:873:HOH:O	1.72	0.87
1:M:470:TYR:HE2	1:M:650:ILE:HD11	1.39	0.87
1:H:440:SER:HB2	2:H:873:HOH:O	1.75	0.87
1:O:438:CYS:HG	1:O:442:CYS:HG	0.89	0.86
1:D:438:CYS:HG	1:D:442:CYS:HG	0.86	0.86
1:G:470:TYR:HE2	1:G:650:ILE:HD11	1.40	0.86
1:I:408:PRO:CG	2:I:887:HOH:O	2.21	0.85
1:L:89:LYS:HG2	2:L:828:HOH:O	1.76	0.85
1:B:166:PRO:HD3	2:B:862:HOH:O	1.75	0.85
1:E:295:GLN:NE2	1:M:102:ASN:ND2	2.25	0.85
1:G:458:SER:HB3	2:G:821:HOH:O	1.76	0.85
1:O:470:TYR:HE2	1:O:650:ILE:HD11	1.39	0.85
1:J:190:HIS:HE1	2:J:854:HOH:O	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:TYR:HE2	1:A:650:ILE:HD11	1.42	0.84
1:F:360:PRO:HD2	2:F:868:HOH:O	1.78	0.84
1:E:295:GLN:N	1:M:101:ARG:HD3	1.93	0.84
1:B:400:PRO:HA	2:B:884:HOH:O	1.77	0.83
1:P:50:HIS:CE1	2:P:889:HOH:O	2.31	0.83
1:N:352:LEU:HA	2:N:890:HOH:O	1.78	0.83
1:E:295:GLN:CA	1:M:101:ARG:CD	2.25	0.83
1:B:470:TYR:HE2	1:B:650:ILE:HD11	1.44	0.83
1:H:470:TYR:HE2	1:H:650:ILE:HD11	1.43	0.83
1:O:292:GLY:HA2	2:O:839:HOH:O	1.79	0.83
1:J:202:THR:HG22	2:J:895:HOH:O	1.79	0.82
1:G:83:PRO:HG3	1:M:358:LYS:HG3	1.61	0.82
1:M:438:CYS:HG	1:M:442:CYS:HG	1.23	0.82
1:B:635:ILE:HB	2:B:726:HOH:O	1.79	0.82
1:G:581:PHE:HB2	2:G:906:HOH:O	1.77	0.82
1:E:470:TYR:HE2	1:E:650:ILE:HD11	1.45	0.81
1:J:470:TYR:HE2	1:J:650:ILE:HD11	1.43	0.81
1:J:405:TYR:HB2	2:J:907:HOH:O	1.80	0.81
1:L:470:TYR:HE2	1:L:650:ILE:HD11	1.43	0.81
1:N:650:ILE:HG23	2:N:848:HOH:O	1.81	0.81
1:B:174:LYS:HD2	2:B:839:HOH:O	1.82	0.80
1:D:441:ASN:HB3	2:D:892:HOH:O	1.79	0.80
1:B:62:PRO:C	1:L:102:ASN:ND2	2.34	0.80
1:D:85:ARG:HA	2:D:918:HOH:O	1.79	0.79
1:D:579:LYS:HE2	2:D:907:HOH:O	1.81	0.79
1:H:408:PRO:CG	2:H:911:HOH:O	2.28	0.79
1:O:62:PRO:CA	2:O:882:HOH:O	2.31	0.79
1:O:433:SER:HB2	2:O:902:HOH:O	1.81	0.79
1:J:202:THR:CB	2:J:895:HOH:O	2.30	0.79
1:I:470:TYR:HE2	1:I:650:ILE:HD11	1.48	0.79
1:K:438:CYS:HG	1:K:442:CYS:HG	1.28	0.79
1:A:470:TYR:CE2	1:A:650:ILE:HD11	2.18	0.79
1:C:88:VAL:HA	2:C:888:HOH:O	1.82	0.79
1:O:62:PRO:CB	2:O:882:HOH:O	2.31	0.78
1:B:292:GLY:HA2	2:B:860:HOH:O	1.82	0.78
1:I:226:ALA:C	2:I:849:HOH:O	2.21	0.78
1:B:165:PRO:HA	2:B:862:HOH:O	1.84	0.78
1:I:408:PRO:CA	2:I:887:HOH:O	2.31	0.78
1:E:78:ARG:HD3	2:E:851:HOH:O	1.83	0.78
1:M:470:TYR:CE2	1:M:650:ILE:HD11	2.19	0.78
1:O:470:TYR:CE2	1:O:650:ILE:HD11	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:174:LYS:HG3	2:D:895:HOH:O	1.84	0.77
1:O:599:LEU:HD12	2:O:844:HOH:O	1.84	0.77
1:P:266:ASP:HA	2:P:785:HOH:O	1.85	0.76
1:G:622:PRO:HD3	2:G:881:HOH:O	1.86	0.76
1:N:470:TYR:HE2	1:N:650:ILE:HD11	1.50	0.76
1:O:203:GLY:HA2	2:O:915:HOH:O	1.85	0.76
1:F:517:VAL:HG12	2:F:877:HOH:O	1.85	0.76
1:D:300:GLN:CB	2:D:820:HOH:O	2.32	0.75
1:L:458:SER:HB2	2:L:880:HOH:O	1.87	0.75
1:E:213:MET:SD	2:E:891:HOH:O	2.44	0.75
1:M:391:HIS:HD2	2:N:907:HOH:O	1.70	0.74
1:E:295:GLN:CB	1:M:101:ARG:HD3	2.18	0.74
1:K:470:TYR:HE2	1:K:650:ILE:HD11	1.51	0.74
1:B:62:PRO:C	1:L:102:ASN:CG	2.44	0.74
1:N:223:LYS:HD2	2:N:789:HOH:O	1.85	0.74
1:L:517:VAL:HG13	2:L:836:HOH:O	1.87	0.74
1:J:432:ARG:HD3	2:J:829:HOH:O	1.85	0.74
1:L:470:TYR:CE2	1:L:650:ILE:HD11	2.22	0.74
1:C:315:GLN:HB3	2:C:768:HOH:O	1.86	0.73
1:H:470:TYR:CE2	1:H:650:ILE:HD11	2.22	0.73
1:O:339:GLN:HE22	1:O:370:HIS:H	1.34	0.73
1:D:233:ASP:HA	2:D:885:HOH:O	1.88	0.73
1:D:265:ASN:HB2	2:D:869:HOH:O	1.87	0.73
1:K:102:ASN:ND2	2:K:850:HOH:O	2.21	0.73
1:K:310:ALA:HB3	2:K:871:HOH:O	1.88	0.73
1:O:309:ASP:CG	2:O:879:HOH:O	2.26	0.73
1:P:101:ARG:NH1	2:P:884:HOH:O	2.20	0.73
1:I:470:TYR:CE2	1:I:650:ILE:HD11	2.24	0.72
1:D:583:LYS:HA	2:D:857:HOH:O	1.89	0.72
1:M:608:LYS:CE	2:M:872:HOH:O	2.20	0.72
1:A:579:LYS:CE	2:A:821:HOH:O	2.30	0.72
1:J:202:THR:N	2:J:895:HOH:O	2.22	0.72
1:P:438:CYS:HG	1:P:442:CYS:HG	0.76	0.72
1:K:470:TYR:CE2	1:K:650:ILE:HD11	2.25	0.72
1:F:470:TYR:HE2	1:F:650:ILE:HD11	1.54	0.71
1:G:470:TYR:CE2	1:G:650:ILE:HD11	2.25	0.71
1:B:470:TYR:CE2	1:B:650:ILE:HD11	2.25	0.71
1:J:202:THR:CG2	2:J:895:HOH:O	2.34	0.71
1:P:470:TYR:HE2	1:P:650:ILE:HD11	1.53	0.71
1:L:655:LYS:HD2	2:L:853:HOH:O	1.90	0.71
1:J:470:TYR:CE2	1:J:650:ILE:HD11	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:650:ILE:HD12	1:P:650:ILE:N	2.04	0.71
1:K:655:LYS:HD3	2:K:913:HOH:O	1.90	0.71
1:N:470:TYR:CE2	1:N:650:ILE:HD11	2.26	0.71
1:J:202:THR:HB	2:J:895:HOH:O	1.88	0.70
1:G:516:GLU:HG2	2:G:842:HOH:O	1.89	0.70
1:B:62:PRO:C	1:L:102:ASN:OD1	2.30	0.70
1:F:470:TYR:CE2	1:F:650:ILE:HD11	2.27	0.70
1:M:101:ARG:HG2	1:M:102:ASN:HD21	1.56	0.70
1:O:323:GLN:HB2	2:O:862:HOH:O	1.91	0.70
1:N:339:GLN:H	1:N:339:GLN:HE21	1.40	0.70
1:O:528:PRO:HB2	2:O:844:HOH:O	1.90	0.69
1:P:470:TYR:CE2	1:P:650:ILE:HD11	2.27	0.69
1:F:438:CYS:HG	1:F:442:CYS:HG	1.40	0.69
1:I:408:PRO:HA	2:I:887:HOH:O	1.89	0.69
1:B:458:SER:HB3	2:B:842:HOH:O	1.91	0.69
1:I:650:ILE:HD12	1:I:650:ILE:N	2.08	0.69
1:H:408:PRO:CB	2:H:911:HOH:O	2.41	0.69
1:L:339:GLN:HE22	1:L:370:HIS:H	1.38	0.69
1:M:194:GLU:HG2	2:M:887:HOH:O	1.92	0.69
1:E:339:GLN:HE22	1:E:370:HIS:H	1.39	0.68
1:E:295:GLN:CB	1:M:102:ASN:HD21	2.06	0.68
1:D:470:TYR:HE2	1:D:650:ILE:HD11	1.59	0.68
1:J:655:LYS:HG3	2:J:732:HOH:O	1.94	0.68
1:C:470:TYR:CE2	1:C:650:ILE:HD11	2.29	0.68
1:I:523:ARG:HG3	2:I:885:HOH:O	1.93	0.68
1:C:173:THR:HA	2:C:865:HOH:O	1.93	0.68
1:E:151:ARG:HD2	2:E:898:HOH:O	1.94	0.68
1:A:164:ARG:HD3	2:A:809:HOH:O	1.92	0.68
1:P:339:GLN:HE22	1:P:370:HIS:H	1.41	0.67
1:E:295:GLN:HB2	1:M:102:ASN:HD21	1.60	0.67
1:B:292:GLY:CA	2:B:860:HOH:O	2.38	0.67
1:C:339:GLN:HE22	1:C:370:HIS:H	1.43	0.67
1:D:174:LYS:CG	2:D:895:HOH:O	2.42	0.67
1:E:470:TYR:CE2	1:E:650:ILE:HD11	2.29	0.67
1:N:339:GLN:HE22	1:N:370:HIS:H	1.43	0.67
1:A:494:LYS:HE3	2:A:791:HOH:O	1.95	0.67
1:E:497:LEU:C	2:E:887:HOH:O	2.33	0.67
1:H:440:SER:CB	2:H:873:HOH:O	2.39	0.67
1:H:567:PRO:HB2	2:H:926:HOH:O	1.94	0.66
1:H:339:GLN:HE22	1:H:370:HIS:H	1.41	0.66
1:M:218:PRO:CG	2:M:868:HOH:O	2.34	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:641:ALA:HB2	2:C:776:HOH:O	1.96	0.66
1:D:339:GLN:HE22	1:D:370:HIS:H	1.40	0.66
1:D:579:LYS:CE	2:D:907:HOH:O	2.40	0.66
1:C:391:HIS:CD2	2:D:871:HOH:O	2.35	0.66
1:D:470:TYR:CE2	1:D:650:ILE:HD11	2.30	0.66
1:H:408:PRO:CA	2:H:911:HOH:O	2.43	0.66
1:O:62:PRO:HA	2:O:882:HOH:O	1.93	0.66
1:G:471:VAL:HB	2:G:876:HOH:O	1.95	0.65
1:M:166:PRO:HB3	2:M:876:HOH:O	1.94	0.65
1:F:239:ASP:HB2	2:F:872:HOH:O	1.96	0.65
1:G:181:ALA:HB1	2:G:864:HOH:O	1.96	0.65
1:F:339:GLN:HE22	1:F:370:HIS:H	1.44	0.65
1:O:399:ARG:HB3	1:O:400:PRO:HD3	1.78	0.65
1:C:470:TYR:HE2	1:C:650:ILE:HD11	1.62	0.65
1:L:164:ARG:HD3	2:L:806:HOH:O	1.96	0.65
1:A:98:LYS:CE	2:A:876:HOH:O	2.31	0.65
1:B:135:ASP:N	2:B:825:HOH:O	2.28	0.65
1:G:281:ALA:HB3	2:G:858:HOH:O	1.96	0.65
1:K:650:ILE:HD12	1:K:650:ILE:N	2.12	0.65
1:D:176:ASP:C	2:D:914:HOH:O	2.34	0.64
1:O:655:LYS:CE	2:O:930:HOH:O	2.33	0.64
1:L:79:GLU:CG	2:L:799:HOH:O	2.34	0.64
1:I:242:HIS:NE2	2:I:839:HOH:O	2.30	0.64
1:B:458:SER:CB	2:B:842:HOH:O	2.45	0.64
1:N:339:GLN:H	1:N:339:GLN:NE2	1.96	0.64
1:A:650:ILE:HD12	1:A:650:ILE:N	2.13	0.64
1:F:517:VAL:CG1	2:F:877:HOH:O	2.43	0.64
1:L:268:PRO:HD2	2:L:905:HOH:O	1.98	0.64
1:C:641:ALA:CB	2:C:776:HOH:O	2.44	0.64
1:H:408:PRO:HA	2:H:911:HOH:O	1.98	0.64
1:O:528:PRO:C	2:O:844:HOH:O	2.36	0.64
1:H:358:LYS:HE3	2:H:890:HOH:O	1.97	0.63
1:I:579:LYS:CE	2:I:836:HOH:O	2.46	0.63
1:N:650:ILE:N	1:N:650:ILE:HD12	2.13	0.63
1:P:265:ASN:HB2	2:P:929:HOH:O	1.98	0.63
1:B:87:GLY:HA2	2:B:898:HOH:O	1.99	0.63
1:J:171:ASN:CG	2:J:910:HOH:O	2.37	0.63
1:H:650:ILE:HD12	1:H:650:ILE:N	2.13	0.63
1:G:317:LEU:HD22	2:G:883:HOH:O	1.98	0.63
1:I:325:LYS:HD3	2:I:865:HOH:O	1.98	0.63
1:J:527:VAL:HG22	2:J:759:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:LYS:HB2	2:F:805:HOH:O	1.99	0.62
1:D:231:MET:CB	2:D:867:HOH:O	2.48	0.62
1:J:339:GLN:HE22	1:J:370:HIS:H	1.48	0.62
1:B:339:GLN:HE22	1:B:370:HIS:H	1.46	0.62
1:C:136:ASP:C	2:C:876:HOH:O	2.38	0.62
1:J:442:CYS:HB2	2:J:820:HOH:O	1.99	0.62
1:D:652:HIS:HD2	2:D:705:HOH:O	1.81	0.62
1:O:461:HIS:HD2	1:O:462:PRO:O	1.82	0.62
1:K:664:VAL:HG11	2:K:902:HOH:O	1.98	0.62
1:J:414:HIS:ND1	2:J:888:HOH:O	2.30	0.62
1:L:89:LYS:NZ	2:L:828:HOH:O	2.32	0.62
1:O:465:ASP:HB3	2:O:920:HOH:O	1.99	0.61
1:A:301:ARG:NE	2:A:714:HOH:O	2.33	0.61
1:C:640:PRO:HA	2:C:887:HOH:O	2.00	0.61
1:E:295:GLN:CB	1:M:101:ARG:HG2	2.31	0.61
1:G:327:THR:CB	2:G:908:HOH:O	2.35	0.61
1:B:413:VAL:HA	2:B:849:HOH:O	1.99	0.61
1:D:441:ASN:C	2:D:889:HOH:O	2.38	0.61
1:E:399:ARG:HB3	1:E:400:PRO:HD3	1.83	0.60
1:D:347:HIS:NE2	2:D:725:HOH:O	2.32	0.60
1:M:102:ASN:ND2	1:M:102:ASN:N	2.47	0.60
1:C:191:ASN:ND2	2:C:760:HOH:O	2.33	0.60
1:O:339:GLN:H	1:O:339:GLN:HE21	1.49	0.60
1:E:78:ARG:CD	2:E:851:HOH:O	2.45	0.60
1:B:62:PRO:HB2	1:L:102:ASN:HD21	1.65	0.60
1:C:520:GLU:HG3	2:C:838:HOH:O	2.01	0.60
1:M:608:LYS:CD	2:M:872:HOH:O	2.46	0.60
1:M:463:ALA:HB2	2:M:862:HOH:O	2.02	0.59
1:J:438:CYS:HG	1:J:442:CYS:HG	1.47	0.59
1:C:339:GLN:H	1:C:339:GLN:HE21	1.50	0.59
1:A:113:ASN:ND2	2:A:762:HOH:O	2.34	0.59
1:B:101:ARG:NE	2:B:846:HOH:O	2.35	0.59
1:E:482:SER:HB3	2:E:872:HOH:O	2.02	0.59
1:I:408:PRO:CB	2:I:887:HOH:O	2.48	0.59
1:A:339:GLN:HE22	1:A:370:HIS:H	1.50	0.59
1:I:520:GLU:HB2	2:I:709:HOH:O	2.02	0.59
1:M:119:ASN:ND2	2:M:786:HOH:O	2.34	0.59
1:M:490:SER:HB2	2:M:909:HOH:O	2.01	0.59
1:A:325:LYS:HE2	2:A:881:HOH:O	2.03	0.59
1:B:159:ASP:HB2	2:B:895:HOH:O	2.01	0.59
1:D:583:LYS:CA	2:D:857:HOH:O	2.48	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:325:LYS:HE2	2:H:939:HOH:O	2.02	0.59
1:K:523:ARG:NE	2:K:870:HOH:O	2.31	0.59
1:M:399:ARG:HB3	1:M:400:PRO:HD3	1.85	0.59
1:O:339:GLN:H	1:O:339:GLN:NE2	2.01	0.59
1:M:218:PRO:CD	2:M:868:HOH:O	2.50	0.59
1:B:78:ARG:NH2	2:B:840:HOH:O	2.36	0.59
1:M:119:ASN:HB3	2:M:786:HOH:O	2.02	0.59
1:N:151:ARG:HD3	2:N:744:HOH:O	2.02	0.59
1:N:353:LYS:NZ	1:N:434:TRP:O	2.36	0.59
1:C:592:THR:CG2	2:C:830:HOH:O	2.39	0.58
1:I:217:ASP:CG	2:I:866:HOH:O	2.41	0.58
1:P:438:CYS:HG	1:P:442:CYS:CB	2.16	0.58
1:N:223:LYS:CD	2:N:789:HOH:O	2.47	0.58
1:B:473:ASP:CG	2:B:857:HOH:O	2.42	0.58
1:E:561:MET:HG3	2:E:905:HOH:O	2.03	0.58
1:J:503:GLU:HB2	2:K:743:HOH:O	2.03	0.58
1:B:473:ASP:HB2	2:B:857:HOH:O	2.04	0.58
1:J:113:ASN:ND2	2:J:879:HOH:O	2.35	0.58
1:I:176:ASP:HB2	2:I:897:HOH:O	2.03	0.58
1:M:101:ARG:HG2	1:M:102:ASN:ND2	2.17	0.58
1:M:463:ALA:CB	2:M:862:HOH:O	2.50	0.58
1:L:655:LYS:CD	2:L:853:HOH:O	2.50	0.58
1:D:583:LYS:HD3	2:D:857:HOH:O	2.04	0.57
1:N:399:ARG:HB3	1:N:400:PRO:HD3	1.85	0.57
1:O:326:PRO:HB3	2:O:927:HOH:O	2.04	0.57
1:C:311:PHE:N	2:C:880:HOH:O	2.36	0.57
1:N:460:THR:HB	2:N:774:HOH:O	2.03	0.57
1:H:358:LYS:CE	2:H:890:HOH:O	2.50	0.57
1:J:371:SER:HA	2:J:779:HOH:O	2.04	0.57
1:B:62:PRO:C	1:L:102:ASN:HD21	2.06	0.57
1:G:655:LYS:HG3	2:G:769:HOH:O	2.03	0.57
1:J:399:ARG:HB3	1:J:400:PRO:HD3	1.86	0.57
1:F:356:ASP:O	1:F:358:LYS:NZ	2.31	0.57
1:D:650:ILE:HD12	1:D:650:ILE:N	2.20	0.57
1:E:482:SER:CB	2:E:872:HOH:O	2.51	0.57
1:H:266:ASP:HB2	2:H:915:HOH:O	2.05	0.57
1:E:294:ASP:O	1:M:101:ARG:NE	2.38	0.57
1:K:579:LYS:HD3	2:K:890:HOH:O	2.05	0.57
1:I:559:PRO:HD2	2:I:796:HOH:O	2.04	0.56
1:F:230:PRO:HD2	2:F:709:HOH:O	2.05	0.56
1:I:344:GLY:HA3	2:I:774:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:190:HIS:CE1	2:J:854:HOH:O	2.44	0.56
1:D:399:ARG:HG2	2:D:822:HOH:O	2.04	0.56
1:G:174:LYS:HG2	2:G:887:HOH:O	2.05	0.56
1:N:198:ARG:HD3	2:N:861:HOH:O	2.05	0.56
1:C:339:GLN:H	1:C:339:GLN:NE2	2.04	0.56
1:E:631:PHE:HB3	2:E:811:HOH:O	2.05	0.56
1:L:204:SER:HA	1:L:228:GLU:O	2.04	0.56
1:G:249:GLY:HA3	2:G:701:HOH:O	2.04	0.56
1:G:399:ARG:HB3	1:G:400:PRO:HD3	1.88	0.56
1:P:339:GLN:NE2	1:P:339:GLN:H	2.03	0.56
1:D:339:GLN:NE2	1:D:370:HIS:H	2.03	0.56
1:E:73:ARG:NE	2:E:774:HOH:O	2.23	0.56
1:J:405:TYR:CB	2:J:907:HOH:O	2.44	0.56
1:F:399:ARG:HB3	1:F:400:PRO:HD3	1.87	0.56
1:B:399:ARG:HB3	1:B:400:PRO:HD3	1.88	0.56
1:E:339:GLN:HE21	1:E:339:GLN:H	1.54	0.56
1:H:339:GLN:H	1:H:339:GLN:HE21	1.54	0.56
1:C:527:VAL:HG22	2:C:789:HOH:O	2.05	0.55
1:K:395:ARG:NH1	2:K:744:HOH:O	2.37	0.55
1:B:62:PRO:CA	1:L:102:ASN:OD1	2.55	0.55
1:D:118:ALA:O	1:D:130:VAL:HG22	2.06	0.55
1:J:104:PRO:HD3	2:J:899:HOH:O	2.06	0.55
1:N:322:ALA:CB	2:N:890:HOH:O	2.54	0.55
1:F:527:VAL:HG22	2:F:862:HOH:O	2.06	0.55
1:I:154:TYR:HE2	2:I:878:HOH:O	1.89	0.55
1:F:511:VAL:HG21	1:F:650:ILE:HD13	1.88	0.55
1:E:339:GLN:NE2	1:E:370:HIS:H	2.05	0.55
1:B:538:GLY:HA2	2:B:806:HOH:O	2.06	0.55
1:E:204:SER:HA	1:E:228:GLU:O	2.06	0.55
1:F:265:ASN:CB	2:F:755:HOH:O	2.29	0.55
1:P:162:MET:O	1:P:163:THR:C	2.46	0.55
1:H:520:GLU:HB3	2:H:869:HOH:O	2.06	0.54
1:I:76:ILE:HB	2:I:864:HOH:O	2.07	0.54
1:O:62:PRO:HB3	2:O:882:HOH:O	2.02	0.54
1:H:193:PRO:HB3	1:K:220:PRO:HB2	1.89	0.54
1:M:339:GLN:HE22	1:M:370:HIS:H	1.54	0.54
1:K:339:GLN:HE22	1:K:370:HIS:H	1.54	0.54
1:D:399:ARG:HB3	1:D:400:PRO:HD3	1.89	0.54
1:I:630:LYS:HD2	2:I:899:HOH:O	2.06	0.54
1:G:83:PRO:CG	1:M:358:LYS:HG3	2.34	0.54
1:J:77:LYS:HE3	2:J:855:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:CD	2:A:809:HOH:O	2.54	0.54
1:J:55:VAL:HG22	1:L:169:PRO:O	2.08	0.54
1:A:339:GLN:H	1:A:339:GLN:HE21	1.55	0.54
1:E:295:GLN:CB	1:M:101:ARG:CD	2.82	0.54
1:L:399:ARG:HB3	1:L:400:PRO:HD3	1.90	0.54
1:N:140:GLU:HB3	2:N:796:HOH:O	2.06	0.54
1:A:408:PRO:HG3	2:A:909:HOH:O	2.07	0.54
1:P:461:HIS:HE1	2:P:920:HOH:O	1.89	0.54
1:C:640:PRO:CA	2:C:887:HOH:O	2.54	0.53
1:I:100:ALA:HA	2:I:805:HOH:O	2.08	0.53
1:M:119:ASN:CB	2:M:786:HOH:O	2.56	0.53
1:P:228:GLU:O	1:P:229:SER:C	2.45	0.53
1:K:664:VAL:CG1	2:K:902:HOH:O	2.55	0.53
1:H:120:ARG:HD3	2:H:823:HOH:O	2.07	0.53
1:I:339:GLN:HE22	1:I:370:HIS:H	1.56	0.53
1:L:650:ILE:N	1:L:650:ILE:HD12	2.24	0.53
1:E:171:ASN:HB2	2:E:863:HOH:O	2.08	0.53
1:J:432:ARG:HD3	2:J:883:HOH:O	2.07	0.53
1:M:621:PHE:CG	1:M:622:PRO:HA	2.43	0.53
1:J:296:TYR:HB3	2:L:737:HOH:O	2.08	0.53
1:K:527:VAL:O	1:K:527:VAL:CG2	2.57	0.53
1:D:391:HIS:HE1	2:D:915:HOH:O	1.91	0.53
1:O:641:ALA:N	2:O:856:HOH:O	2.41	0.53
1:D:111:PRO:HB3	1:D:150:ILE:HD11	1.91	0.53
1:A:216:LEU:HD23	1:A:321:LEU:HD13	1.90	0.53
1:D:441:ASN:HA	2:D:889:HOH:O	2.09	0.53
2:H:807:HOH:O	1:K:101:ARG:HD3	2.07	0.53
1:L:369:ARG:HD3	2:L:817:HOH:O	2.09	0.53
1:G:196:ASN:CB	2:G:820:HOH:O	2.57	0.53
1:J:77:LYS:NZ	2:J:855:HOH:O	2.33	0.53
1:E:295:GLN:HB3	1:M:101:ARG:HG2	1.91	0.53
1:L:408:PRO:HA	2:L:906:HOH:O	2.08	0.53
1:M:194:GLU:CG	2:M:887:HOH:O	2.53	0.53
1:M:650:ILE:HD12	1:M:650:ILE:N	2.24	0.53
1:D:231:MET:HB3	2:D:867:HOH:O	2.09	0.52
1:J:251:PHE:HB2	2:J:890:HOH:O	2.09	0.52
1:J:511:VAL:HG21	1:J:650:ILE:HD13	1.91	0.52
1:J:596:HIS:CD2	2:J:882:HOH:O	2.62	0.52
1:E:261:ARG:CD	2:E:773:HOH:O	2.56	0.52
1:O:507:ARG:HB3	2:O:904:HOH:O	2.10	0.52
1:C:639:LYS:HD2	2:C:771:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:632:VAL:HB	2:J:741:HOH:O	2.10	0.52
1:N:223:LYS:CE	2:N:789:HOH:O	2.58	0.52
1:N:232:VAL:HB	1:N:344:GLY:HA2	1.91	0.52
1:F:412:SER:HB3	2:F:829:HOH:O	2.09	0.52
1:G:83:PRO:HG3	1:M:358:LYS:CG	2.37	0.52
1:O:121:VAL:HA	2:O:926:HOH:O	2.08	0.52
1:B:134:GLY:N	2:B:825:HOH:O	2.43	0.52
1:C:310:ALA:CA	2:C:880:HOH:O	2.58	0.52
1:C:440:SER:CA	2:C:812:HOH:O	2.57	0.52
1:F:412:SER:N	2:F:813:HOH:O	2.41	0.52
1:I:391:HIS:CE1	2:I:893:HOH:O	2.62	0.52
1:L:50:HIS:N	2:L:835:HOH:O	2.42	0.52
1:O:343:TRP:HB2	2:O:922:HOH:O	2.09	0.52
1:O:529:VAL:N	2:O:844:HOH:O	2.42	0.52
1:P:517:VAL:HG13	2:P:821:HOH:O	2.10	0.52
1:C:650:ILE:N	1:C:650:ILE:HD12	2.25	0.52
1:K:339:GLN:H	1:K:339:GLN:HE21	1.58	0.52
1:L:579:LYS:HE2	2:L:768:HOH:O	2.09	0.52
1:G:369:ARG:HG3	2:G:699:HOH:O	2.10	0.52
1:I:217:ASP:CB	2:I:866:HOH:O	2.58	0.52
1:J:77:LYS:CE	2:J:855:HOH:O	2.58	0.52
1:L:232:VAL:HB	1:L:344:GLY:HA2	1.92	0.52
1:M:271:ASP:HA	1:P:553:ALA:HB1	1.92	0.52
1:N:650:ILE:HA	2:N:848:HOH:O	2.10	0.52
1:A:339:GLN:H	1:A:339:GLN:NE2	2.08	0.51
1:F:141:GLY:O	1:F:407:LYS:NZ	2.36	0.51
1:P:232:VAL:HB	1:P:344:GLY:HA2	1.91	0.51
1:P:650:ILE:HD12	1:P:650:ILE:H	1.74	0.51
1:C:594:HIS:CE1	2:C:814:HOH:O	2.63	0.51
1:J:201:MET:C	2:J:895:HOH:O	2.47	0.51
1:P:399:ARG:HB3	1:P:400:PRO:HD3	1.92	0.51
1:D:583:LYS:HB3	2:D:890:HOH:O	2.10	0.51
1:E:242:HIS:CE1	2:E:844:HOH:O	2.63	0.51
1:J:395:ARG:HG3	2:J:876:HOH:O	2.10	0.51
1:O:162:MET:O	1:O:163:THR:C	2.48	0.51
1:O:621:PHE:CG	1:O:622:PRO:HA	2.45	0.51
1:F:339:GLN:H	1:F:339:GLN:NE2	2.09	0.51
1:G:204:SER:HA	1:G:228:GLU:O	2.10	0.51
1:N:265:ASN:N	2:N:815:HOH:O	2.42	0.51
2:H:807:HOH:O	1:K:101:ARG:CD	2.58	0.51
1:M:101:ARG:C	1:M:102:ASN:CG	2.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:579:LYS:HE3	2:N:860:HOH:O	2.09	0.51
1:B:58:GLY:CA	2:B:900:HOH:O	2.35	0.51
1:E:372:GLY:N	2:E:884:HOH:O	2.43	0.51
1:L:517:VAL:CG1	2:L:836:HOH:O	2.54	0.51
1:B:155:GLY:HA2	2:B:865:HOH:O	2.11	0.51
1:C:50:HIS:ND1	2:C:867:HOH:O	2.22	0.51
1:D:141:GLY:O	1:D:407:LYS:NZ	2.40	0.51
1:G:216:LEU:HD21	2:G:883:HOH:O	2.11	0.51
1:L:621:PHE:CG	1:L:622:PRO:HA	2.46	0.51
1:H:204:SER:HA	1:H:228:GLU:O	2.11	0.51
1:P:339:GLN:H	1:P:339:GLN:HE21	1.59	0.51
1:I:204:SER:HA	1:I:228:GLU:O	2.11	0.50
1:M:190:HIS:CE1	2:M:903:HOH:O	2.64	0.50
1:G:588:GLN:HG2	1:G:591:ALA:HB2	1.93	0.50
1:B:650:ILE:N	1:B:650:ILE:HD12	2.26	0.50
1:C:123:ASN:CG	2:C:840:HOH:O	2.50	0.50
1:K:176:ASP:HB2	2:K:831:HOH:O	2.11	0.50
1:K:339:GLN:H	1:K:339:GLN:NE2	2.10	0.50
1:C:230:PRO:HD2	2:C:781:HOH:O	2.12	0.50
1:F:360:PRO:CD	2:F:868:HOH:O	2.48	0.50
1:L:339:GLN:H	1:L:339:GLN:NE2	2.08	0.50
1:B:482:SER:HA	2:B:761:HOH:O	2.11	0.50
1:A:399:ARG:HB3	1:A:400:PRO:HD3	1.93	0.50
1:B:255:VAL:HG11	2:B:816:HOH:O	2.11	0.50
1:G:339:GLN:HE22	1:G:370:HIS:H	1.58	0.50
1:G:443:THR:CG2	2:G:905:HOH:O	2.59	0.50
1:G:579:LYS:HD2	2:G:848:HOH:O	2.12	0.50
1:O:438:CYS:HG	1:O:442:CYS:CB	2.25	0.50
1:O:640:PRO:C	2:O:856:HOH:O	2.49	0.50
1:F:610:HIS:HA	2:F:788:HOH:O	2.11	0.50
1:J:503:GLU:CD	2:J:745:HOH:O	2.50	0.50
1:B:89:LYS:NZ	1:L:358:LYS:HB3	2.26	0.50
1:C:88:VAL:HG22	2:C:888:HOH:O	2.12	0.50
1:C:440:SER:HA	2:C:812:HOH:O	2.11	0.50
1:C:520:GLU:CG	2:C:838:HOH:O	2.57	0.50
1:K:546:LYS:HA	1:K:570:MET:HB3	1.94	0.50
1:B:204:SER:HA	1:B:228:GLU:O	2.12	0.50
1:D:471:VAL:HB	2:D:826:HOH:O	2.12	0.50
1:F:413:VAL:HG23	2:F:740:HOH:O	2.12	0.50
1:C:79:GLU:HG3	2:C:802:HOH:O	2.10	0.49
1:O:62:PRO:CG	2:O:882:HOH:O	2.57	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:339:GLN:H	1:H:339:GLN:NE2	2.09	0.49
1:G:317:LEU:HB3	2:G:883:HOH:O	2.11	0.49
1:J:650:ILE:N	1:J:650:ILE:HD12	2.27	0.49
1:M:628:PRO:O	1:M:629:GLN:HB2	2.12	0.49
1:B:384:GLU:O	2:B:832:HOH:O	2.20	0.49
1:C:639:LYS:HE2	2:C:771:HOH:O	2.12	0.49
1:D:391:HIS:CE1	2:D:915:HOH:O	2.64	0.49
1:G:339:GLN:HE22	1:G:369:ARG:HB2	1.78	0.49
1:G:607:ALA:HB1	2:G:733:HOH:O	2.12	0.49
2:B:846:HOH:O	1:L:174:LYS:CE	2.59	0.49
1:K:399:ARG:HB3	1:K:400:PRO:HD3	1.93	0.49
1:N:427:LYS:CD	2:N:859:HOH:O	2.60	0.49
1:G:391:HIS:CD2	2:G:865:HOH:O	2.40	0.49
1:B:507:ARG:HD2	2:B:910:HOH:O	2.13	0.49
1:H:339:GLN:NE2	1:H:370:HIS:H	2.10	0.49
1:P:251:PHE:HB2	2:P:751:HOH:O	2.13	0.49
1:A:497:LEU:HB3	2:A:946:HOH:O	2.12	0.49
1:E:261:ARG:HD2	2:E:773:HOH:O	2.12	0.49
1:M:527:VAL:O	1:M:527:VAL:CG2	2.60	0.49
1:L:546:LYS:HA	1:L:570:MET:HB3	1.95	0.49
1:N:619:SER:HA	2:N:814:HOH:O	2.12	0.49
1:O:204:SER:HA	1:O:228:GLU:O	2.12	0.48
1:K:517:VAL:HG13	2:K:817:HOH:O	2.12	0.48
1:O:650:ILE:N	1:O:650:ILE:HD12	2.28	0.48
1:G:443:THR:HG22	2:G:905:HOH:O	2.14	0.48
1:J:414:HIS:HB3	2:J:888:HOH:O	2.12	0.48
1:A:639:LYS:HB3	2:A:938:HOH:O	2.12	0.48
1:O:232:VAL:HB	1:O:344:GLY:HA2	1.95	0.48
1:F:339:GLN:H	1:F:339:GLN:HE21	1.62	0.48
1:I:607:ALA:HB1	2:I:831:HOH:O	2.13	0.48
1:K:309:ASP:HB2	2:K:766:HOH:O	2.13	0.48
1:O:261:ARG:CZ	2:O:923:HOH:O	2.62	0.48
1:K:434:TRP:CG	1:K:435:PRO:HA	2.49	0.48
1:C:399:ARG:HB3	1:C:400:PRO:HD3	1.94	0.48
1:M:339:GLN:H	1:M:339:GLN:HE21	1.62	0.48
1:P:113:ASN:ND2	2:P:703:HOH:O	2.46	0.48
1:A:580:ASP:HA	2:A:925:HOH:O	2.13	0.48
1:D:269:ARG:CB	2:D:912:HOH:O	2.62	0.48
1:D:546:LYS:HA	1:D:570:MET:HB3	1.95	0.48
1:G:443:THR:HB	2:G:905:HOH:O	2.14	0.48
1:M:79:GLU:OE1	1:M:91:TYR:OH	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ALA:O	1:B:130:VAL:HG22	2.14	0.48
1:E:261:ARG:NE	2:E:773:HOH:O	2.47	0.48
1:I:546:LYS:HA	1:I:570:MET:HB3	1.96	0.48
1:L:481:ILE:HG21	1:L:496:TRP:HB2	1.96	0.48
1:I:404:GLU:OE1	1:I:413:VAL:HG22	2.13	0.47
1:B:369:ARG:HD3	2:B:815:HOH:O	2.13	0.47
1:D:313:GLN:HB3	2:D:854:HOH:O	2.13	0.47
1:E:300:GLN:NE2	1:M:101:ARG:NH1	2.62	0.47
1:F:507:ARG:HD2	2:F:702:HOH:O	2.14	0.47
1:J:494:LYS:NZ	2:J:810:HOH:O	2.47	0.47
1:C:546:LYS:HA	1:C:570:MET:HB3	1.97	0.47
1:I:369:ARG:HG3	2:I:701:HOH:O	2.14	0.47
1:C:123:ASN:ND2	2:C:840:HOH:O	2.46	0.47
1:G:88:VAL:HG13	1:G:157:GLN:HB2	1.96	0.47
1:L:404:GLU:OE1	1:L:413:VAL:HG22	2.15	0.47
1:N:621:PHE:CG	1:N:622:PRO:HA	2.49	0.47
1:C:204:SER:HA	1:C:228:GLU:O	2.14	0.47
1:G:650:ILE:N	1:G:650:ILE:HD12	2.29	0.47
1:J:567:PRO:HB2	2:J:770:HOH:O	2.14	0.47
1:M:517:VAL:HB	2:M:923:HOH:O	2.15	0.47
1:B:89:LYS:HZ1	1:L:358:LYS:CB	2.28	0.47
1:B:232:VAL:HB	1:B:344:GLY:HA2	1.97	0.47
1:B:416:PRO:HB2	1:B:431:TYR:O	2.15	0.47
2:B:846:HOH:O	1:L:174:LYS:HE2	2.14	0.47
1:E:294:ASP:C	1:M:101:ARG:HD3	2.35	0.47
1:I:579:LYS:CD	2:I:836:HOH:O	2.33	0.47
1:K:78:ARG:NH2	2:K:863:HOH:O	2.42	0.47
1:M:78:ARG:NH1	2:M:912:HOH:O	2.47	0.47
1:N:650:ILE:HD12	1:N:650:ILE:H	1.79	0.47
1:D:571:ASP:CG	2:D:888:HOH:O	2.52	0.47
1:E:171:ASN:CB	2:E:863:HOH:O	2.61	0.47
1:D:441:ASN:CA	2:D:889:HOH:O	2.63	0.47
1:G:162:MET:O	1:G:163:THR:C	2.52	0.47
1:J:481:ILE:HG22	2:J:918:HOH:O	2.14	0.47
1:K:265:ASN:HB2	2:K:888:HOH:O	2.14	0.47
1:L:103:ALA:O	1:L:195:SER:HA	2.15	0.47
1:C:440:SER:C	2:C:812:HOH:O	2.53	0.47
1:D:228:GLU:O	1:D:229:SER:C	2.53	0.47
1:F:232:VAL:HB	1:F:344:GLY:HA2	1.96	0.46
1:A:319:LYS:HE2	2:A:937:HOH:O	2.16	0.46
1:E:621:PHE:CG	1:E:622:PRO:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:164:ARG:CD	2:L:806:HOH:O	2.56	0.46
1:M:204:SER:HA	1:M:228:GLU:O	2.15	0.46
1:M:228:GLU:O	1:M:229:SER:C	2.54	0.46
1:M:546:LYS:HA	1:M:570:MET:HB3	1.97	0.46
1:A:98:LYS:NZ	2:A:876:HOH:O	2.45	0.46
1:B:55:VAL:HG22	1:D:170:LEU:HA	1.97	0.46
1:H:630:LYS:O	2:H:826:HOH:O	2.20	0.46
1:J:405:TYR:N	2:J:907:HOH:O	2.27	0.46
1:P:198:ARG:HD3	2:P:923:HOH:O	2.15	0.46
1:A:159:ASP:OD2	2:A:908:HOH:O	2.20	0.46
1:B:72:GLN:NE2	2:B:912:HOH:O	2.28	0.46
1:C:192:VAL:HG22	2:C:879:HOH:O	2.14	0.46
1:G:261:ARG:CZ	2:G:855:HOH:O	2.64	0.46
1:H:191:ASN:HB3	1:K:198:ARG:HH12	1.81	0.46
1:J:55:VAL:HG22	1:L:170:LEU:HA	1.97	0.46
1:N:342:MET:HG3	2:N:908:HOH:O	2.13	0.46
1:E:111:PRO:HB3	1:E:150:ILE:HD11	1.97	0.46
1:J:268:PRO:HB2	1:L:125:LEU:HD21	1.97	0.46
1:J:339:GLN:NE2	1:J:370:HIS:H	2.12	0.46
1:J:546:LYS:HA	1:J:570:MET:HB3	1.97	0.46
1:M:339:GLN:H	1:M:339:GLN:NE2	2.13	0.46
1:O:546:LYS:HA	1:O:570:MET:HB3	1.97	0.46
1:B:473:ASP:CB	2:B:857:HOH:O	2.62	0.46
1:C:511:VAL:HG21	1:C:650:ILE:HD13	1.97	0.46
1:E:295:GLN:HE21	1:M:102:ASN:CG	2.14	0.46
1:E:339:GLN:H	1:E:339:GLN:NE2	2.14	0.46
1:A:78:ARG:HD3	2:A:825:HOH:O	2.15	0.46
1:B:203:GLY:HA2	2:B:695:HOH:O	2.15	0.46
1:M:339:GLN:HE22	1:M:369:ARG:HB2	1.81	0.46
1:O:266:ASP:HB2	2:O:818:HOH:O	2.16	0.46
1:N:176:ASP:HB2	2:N:728:HOH:O	2.16	0.46
1:N:204:SER:HA	1:N:228:GLU:O	2.15	0.46
1:H:251:PHE:HB2	2:H:885:HOH:O	2.15	0.46
1:J:339:GLN:HE21	1:J:339:GLN:H	1.63	0.46
1:F:650:ILE:HD12	1:F:650:ILE:N	2.31	0.45
1:A:251:PHE:HB2	2:A:733:HOH:O	2.16	0.45
1:G:79:GLU:OE1	1:G:91:TYR:OH	2.26	0.45
1:N:72:GLN:HB3	1:P:270:ARG:NH2	2.31	0.45
1:P:216:LEU:HD23	1:P:321:LEU:HD13	1.97	0.45
1:P:404:GLU:OE1	1:P:413:VAL:HG22	2.16	0.45
1:J:251:PHE:CD1	1:J:293:LEU:HD13	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:339:GLN:NE2	1:L:370:HIS:H	2.10	0.45
1:P:334:GLN:O	1:P:365:MET:HA	2.16	0.45
1:A:650:ILE:HD12	1:A:650:ILE:H	1.81	0.45
1:D:621:PHE:CG	1:D:622:PRO:HA	2.51	0.45
1:F:404:GLU:OE1	1:F:413:VAL:HG22	2.17	0.45
1:F:204:SER:HA	1:F:228:GLU:O	2.17	0.45
2:F:840:HOH:O	1:G:476:HIS:CE1	2.69	0.45
1:K:621:PHE:CG	1:K:622:PRO:HA	2.52	0.45
1:M:490:SER:CB	2:M:909:HOH:O	2.63	0.45
1:O:103:ALA:O	1:O:195:SER:HA	2.16	0.45
1:G:567:PRO:HB2	2:G:777:HOH:O	2.17	0.45
1:I:232:VAL:HB	1:I:344:GLY:HA2	1.98	0.45
1:J:339:GLN:NE2	1:J:339:GLN:H	2.14	0.45
1:L:552:PRO:O	1:L:553:ALA:C	2.55	0.45
1:M:339:GLN:NE2	1:M:370:HIS:H	2.14	0.45
1:O:399:ARG:NH1	2:O:801:HOH:O	2.34	0.45
1:D:650:ILE:HD12	1:D:650:ILE:H	1.80	0.45
1:K:251:PHE:HB2	2:K:722:HOH:O	2.16	0.45
1:M:621:PHE:CD1	1:M:622:PRO:HA	2.52	0.45
1:N:508:PRO:HD2	2:O:904:HOH:O	2.17	0.45
1:P:461:HIS:CE1	2:P:920:HOH:O	2.68	0.45
1:N:228:GLU:O	1:N:229:SER:C	2.55	0.45
1:O:119:ASN:O	1:O:120:ARG:C	2.55	0.45
1:H:80:VAL:CG1	1:K:408:PRO:HB2	2.47	0.45
1:L:132:PRO:HD2	1:L:135:ASP:OD2	2.16	0.45
1:M:111:PRO:HB3	1:M:150:ILE:HD11	1.99	0.45
1:M:200:GLY:HA3	1:M:406:LEU:HD11	1.97	0.45
1:O:339:GLN:NE2	1:O:370:HIS:H	2.07	0.45
1:A:546:LYS:HA	1:A:570:MET:HB3	1.99	0.44
1:G:481:ILE:HG21	1:G:496:TRP:HB2	1.98	0.44
1:G:546:LYS:HA	1:G:570:MET:HB3	1.98	0.44
1:J:596:HIS:HD2	2:J:882:HOH:O	2.00	0.44
1:K:334:GLN:O	1:K:365:MET:HA	2.17	0.44
1:G:78:ARG:HE	1:M:220:PRO:HG3	1.82	0.44
1:P:621:PHE:CG	1:P:622:PRO:HA	2.52	0.44
1:H:178:THR:HG22	2:H:928:HOH:O	2.17	0.44
1:J:375:TYR:HB3	2:J:712:HOH:O	2.17	0.44
1:L:339:GLN:H	1:L:339:GLN:HE21	1.66	0.44
1:B:339:GLN:H	1:B:339:GLN:NE2	2.15	0.44
1:I:217:ASP:HA	2:I:866:HOH:O	2.17	0.44
1:M:334:GLN:O	1:M:365:MET:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:391:HIS:CD2	2:N:907:HOH:O	2.56	0.44
1:G:185:VAL:HG23	2:G:864:HOH:O	2.18	0.44
1:J:132:PRO:HD2	1:J:135:ASP:OD2	2.17	0.44
1:K:216:LEU:HD23	1:K:321:LEU:HD13	1.98	0.44
1:L:177:GLU:HB2	1:L:213:MET:HE2	1.98	0.44
1:F:511:VAL:HG21	1:F:650:ILE:CD1	2.46	0.44
1:G:339:GLN:H	1:G:339:GLN:NE2	2.15	0.44
1:J:414:HIS:CB	2:J:888:HOH:O	2.65	0.44
1:O:343:TRP:N	2:O:922:HOH:O	2.49	0.44
1:D:339:GLN:NE2	1:D:339:GLN:H	2.15	0.44
1:E:162:MET:O	1:E:163:THR:C	2.54	0.44
1:F:546:LYS:HA	1:F:570:MET:HB3	2.00	0.44
1:G:238:ASP:HB3	2:G:901:HOH:O	2.17	0.44
1:I:399:ARG:HB3	1:I:400:PRO:HD3	1.99	0.44
1:L:255:VAL:O	1:L:259:THR:OG1	2.33	0.44
1:L:342:MET:HB3	2:L:884:HOH:O	2.18	0.44
1:O:143:TYR:OH	1:O:403:ASP:OD2	2.25	0.44
1:J:414:HIS:CE1	2:J:913:HOH:O	2.69	0.44
1:D:301:ARG:N	2:D:820:HOH:O	2.50	0.44
1:G:407:LYS:HE2	2:G:723:HOH:O	2.17	0.44
1:K:113:ASN:ND2	2:K:740:HOH:O	2.51	0.44
1:K:151:ARG:HD3	2:K:876:HOH:O	2.17	0.44
1:M:166:PRO:CB	2:M:876:HOH:O	2.59	0.44
2:G:856:HOH:O	1:H:391:HIS:HD2	2.01	0.43
1:P:546:LYS:HA	1:P:570:MET:HB3	2.00	0.43
1:A:204:SER:HA	1:A:228:GLU:O	2.18	0.43
1:D:259:THR:HG21	2:D:851:HOH:O	2.18	0.43
1:E:482:SER:HB2	2:E:872:HOH:O	2.15	0.43
1:F:292:GLY:HA2	2:F:747:HOH:O	2.16	0.43
1:I:356:ASP:HB3	2:I:830:HOH:O	2.17	0.43
1:N:339:GLN:HE21	1:N:339:GLN:N	2.13	0.43
1:O:79:GLU:OE1	1:O:91:TYR:OH	2.24	0.43
1:O:228:GLU:O	1:O:229:SER:C	2.56	0.43
1:O:369:ARG:HG3	2:O:720:HOH:O	2.16	0.43
1:O:511:VAL:HG21	1:O:650:ILE:HD13	2.00	0.43
1:A:408:PRO:HA	2:A:909:HOH:O	2.17	0.43
1:G:384:GLU:OE2	2:G:854:HOH:O	2.21	0.43
1:I:650:ILE:N	1:I:650:ILE:CD1	2.78	0.43
1:N:527:VAL:O	1:N:527:VAL:CG2	2.66	0.43
1:O:334:GLN:O	1:O:365:MET:HA	2.18	0.43
1:B:514:GLU:OE1	2:B:730:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:321:LEU:HD11	1:O:326:PRO:HG3	2.00	0.43
1:A:228:GLU:O	1:A:229:SER:C	2.57	0.43
1:C:136:ASP:CB	2:C:876:HOH:O	2.33	0.43
1:E:295:GLN:CB	1:M:101:ARG:CG	2.97	0.43
1:K:57:THR:C	2:K:875:HOH:O	2.56	0.43
1:K:470:TYR:HA	2:K:777:HOH:O	2.18	0.43
1:B:339:GLN:NE2	1:B:370:HIS:H	2.15	0.43
1:E:179:THR:HG23	2:E:842:HOH:O	2.18	0.43
1:E:306:PRO:HG2	2:E:828:HOH:O	2.18	0.43
1:K:339:GLN:NE2	1:K:370:HIS:H	2.16	0.43
1:N:352:LEU:HG	2:N:798:HOH:O	2.18	0.43
1:N:438:CYS:HA	1:N:446:LEU:CD1	2.48	0.43
1:P:339:GLN:NE2	1:P:370:HIS:H	2.12	0.43
1:C:639:LYS:CE	2:C:771:HOH:O	2.67	0.43
1:H:216:LEU:HD23	1:H:321:LEU:HD13	2.00	0.43
1:O:641:ALA:CA	2:O:856:HOH:O	2.66	0.43
1:B:339:GLN:H	1:B:339:GLN:HE21	1.65	0.43
1:E:118:ALA:O	1:E:130:VAL:HG22	2.19	0.43
1:H:111:PRO:HB3	1:H:150:ILE:HD11	2.01	0.43
1:A:585:GLU:CD	2:A:933:HOH:O	2.57	0.43
2:A:782:HOH:O	1:B:392:GLN:HG2	2.18	0.43
1:C:232:VAL:HB	1:C:344:GLY:HA2	2.00	0.43
1:F:340:GLU:C	2:F:695:HOH:O	2.57	0.43
1:K:630:LYS:NZ	2:K:869:HOH:O	2.52	0.43
1:P:178:THR:HG22	2:P:928:HOH:O	2.19	0.43
1:B:334:GLN:O	1:B:365:MET:HA	2.19	0.43
1:C:434:TRP:HD1	2:C:878:HOH:O	1.83	0.43
1:C:650:ILE:HD12	1:C:650:ILE:H	1.83	0.43
1:E:295:GLN:HB3	1:M:102:ASN:HD21	1.81	0.43
1:N:427:LYS:HD3	2:N:859:HOH:O	2.19	0.43
1:N:434:TRP:CG	1:N:435:PRO:HA	2.54	0.43
1:A:451:LEU:HD12	1:A:457:LEU:CD2	2.49	0.42
1:B:89:LYS:NZ	1:L:358:LYS:CB	2.82	0.42
1:C:434:TRP:NE1	2:C:878:HOH:O	2.42	0.42
1:D:583:LYS:HE3	2:D:808:HOH:O	2.19	0.42
1:G:111:PRO:HG3	1:G:206:TYR:CG	2.53	0.42
1:H:468:ASP:HA	2:H:936:HOH:O	2.19	0.42
1:N:339:GLN:NE2	1:N:370:HIS:H	2.12	0.42
1:B:55:VAL:HG22	1:D:169:PRO:O	2.19	0.42
1:C:347:HIS:CE1	2:C:820:HOH:O	2.72	0.42
1:D:339:GLN:H	1:D:339:GLN:HE21	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:VAL:HB	1:E:344:GLY:HA2	2.01	0.42
1:E:517:VAL:CG1	2:E:754:HOH:O	2.49	0.42
1:F:334:GLN:O	1:F:365:MET:HA	2.19	0.42
1:H:50:HIS:O	2:H:922:HOH:O	2.21	0.42
1:J:312:TRP:CZ3	2:J:866:HOH:O	2.57	0.42
1:J:400:PRO:HA	2:J:832:HOH:O	2.19	0.42
1:N:97:PRO:HG3	2:N:696:HOH:O	2.18	0.42
1:C:143:TYR:OH	1:C:403:ASP:OD2	2.23	0.42
1:C:339:GLN:NE2	1:C:370:HIS:H	2.14	0.42
1:O:414:HIS:HB3	2:O:868:HOH:O	2.19	0.42
1:C:639:LYS:CD	2:C:771:HOH:O	2.67	0.42
1:D:231:MET:HB2	2:D:867:HOH:O	2.14	0.42
1:E:228:GLU:O	1:E:229:SER:C	2.58	0.42
1:H:399:ARG:HB3	1:H:400:PRO:HD3	2.02	0.42
1:I:216:LEU:HD23	1:I:321:LEU:HD13	2.00	0.42
1:A:481:ILE:HA	2:A:865:HOH:O	2.18	0.42
1:B:255:VAL:CG1	2:B:816:HOH:O	2.67	0.42
1:D:540:ASP:O	1:D:629:GLN:HA	2.20	0.42
1:E:171:ASN:CG	2:E:863:HOH:O	2.58	0.42
1:J:170:LEU:HD22	1:L:54:SER:O	2.19	0.42
1:K:339:GLN:HE22	1:K:369:ARG:HB2	1.84	0.42
1:H:230:PRO:HD2	2:H:762:HOH:O	2.20	0.42
1:M:232:VAL:HB	1:M:344:GLY:HA2	2.02	0.42
1:E:364:VAL:HG11	1:E:393:TYR:CD2	2.54	0.42
1:E:546:LYS:HA	1:E:570:MET:HB3	2.02	0.42
1:F:438:CYS:SG	1:F:442:CYS:SG	3.02	0.42
1:F:604:HIS:HB2	2:F:803:HOH:O	2.19	0.42
1:G:339:GLN:H	1:G:339:GLN:HE21	1.66	0.42
1:L:121:VAL:HG11	2:L:887:HOH:O	2.20	0.42
1:N:382:PRO:HA	2:N:881:HOH:O	2.19	0.42
1:A:232:VAL:HB	1:A:344:GLY:HA2	2.01	0.42
1:B:228:GLU:O	1:B:229:SER:C	2.57	0.42
1:D:232:VAL:HB	1:D:344:GLY:HA2	2.02	0.42
1:J:204:SER:HA	1:J:228:GLU:O	2.20	0.42
1:L:321:LEU:HD11	1:L:326:PRO:HG3	2.01	0.42
1:O:641:ALA:HA	2:O:856:HOH:O	2.20	0.42
1:O:651:HIS:CD2	1:O:656:GLU:HB2	2.54	0.42
1:E:103:ALA:O	1:E:195:SER:HA	2.19	0.42
1:G:582:ALA:N	2:G:906:HOH:O	2.53	0.42
1:K:416:PRO:HB2	1:K:431:TYR:O	2.20	0.42
1:N:111:PRO:HG3	1:N:206:TYR:CG	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:113:ASN:O	1:N:117:ARG:HG2	2.20	0.42
1:P:204:SER:O	1:P:207:GLU:HB2	2.20	0.42
1:B:321:LEU:HD11	1:B:326:PRO:HG3	2.02	0.42
1:E:295:GLN:HB2	1:M:101:ARG:HG2	2.02	0.42
1:I:334:GLN:O	1:I:365:MET:HA	2.20	0.42
1:O:479:PRO:HA	1:O:621:PHE:O	2.19	0.42
1:C:318:ASP:N	1:C:318:ASP:OD2	2.53	0.41
1:H:325:LYS:CE	2:H:939:HOH:O	2.62	0.41
1:H:621:PHE:CG	1:H:622:PRO:HA	2.54	0.41
1:I:251:PHE:HB2	2:I:765:HOH:O	2.19	0.41
1:J:544:VAL:HB	1:J:617:GLN:HG2	2.02	0.41
1:K:337:TRP:CE2	1:K:498:VAL:HG12	2.55	0.41
1:N:438:CYS:HA	1:N:446:LEU:HD11	2.02	0.41
1:L:434:TRP:CG	1:L:435:PRO:HA	2.55	0.41
1:O:628:PRO:O	1:O:629:GLN:HB2	2.19	0.41
1:C:579:LYS:HB3	2:C:817:HOH:O	2.20	0.41
1:E:511:VAL:HG21	1:E:650:ILE:HD13	2.02	0.41
1:J:651:HIS:CD2	1:J:656:GLU:HB2	2.55	0.41
1:M:113:ASN:ND2	2:M:747:HOH:O	2.54	0.41
1:N:599:LEU:HB3	1:N:600:PRO:HD2	2.01	0.41
1:E:438:CYS:SG	1:E:440:SER:O	2.78	0.41
1:A:542:ASP:OD2	2:A:788:HOH:O	2.22	0.41
1:F:162:MET:O	1:F:163:THR:C	2.59	0.41
1:G:339:GLN:NE2	1:G:370:HIS:H	2.19	0.41
1:J:164:ARG:HD3	2:J:844:HOH:O	2.20	0.41
1:O:434:TRP:CG	1:O:435:PRO:HA	2.56	0.41
1:D:78:ARG:HG2	2:D:774:HOH:O	2.21	0.41
1:E:650:ILE:N	1:E:650:ILE:HD12	2.36	0.41
1:I:446:LEU:HD21	2:I:819:HOH:O	2.21	0.41
1:L:356:ASP:O	1:L:358:LYS:NZ	2.50	0.41
1:F:650:ILE:HD12	1:F:650:ILE:H	1.86	0.41
1:M:170:LEU:HA	1:O:55:VAL:HG22	2.02	0.41
1:E:78:ARG:NH1	2:E:851:HOH:O	2.47	0.41
1:J:106:LEU:HD11	2:J:895:HOH:O	2.20	0.41
1:N:219:HIS:CG	1:N:220:PRO:HD2	2.56	0.41
1:O:640:PRO:HB2	2:O:856:HOH:O	2.19	0.41
1:A:339:GLN:NE2	1:A:370:HIS:H	2.16	0.41
1:B:100:ALA:HA	2:B:887:HOH:O	2.20	0.41
1:C:251:PHE:CD1	1:C:293:LEU:HD13	2.56	0.41
1:G:651:HIS:CD2	1:G:656:GLU:HB2	2.56	0.41
1:I:532:LEU:HA	1:I:658:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:481:ILE:HG21	1:K:496:TRP:HB2	2.02	0.41
1:M:103:ALA:O	1:M:195:SER:HA	2.20	0.41
1:N:113:ASN:ND2	2:N:896:HOH:O	2.54	0.41
1:P:527:VAL:O	1:P:527:VAL:CG2	2.69	0.41
1:B:101:ARG:HD3	2:B:846:HOH:O	2.21	0.41
1:J:55:VAL:CG2	1:L:169:PRO:O	2.68	0.41
1:N:550:VAL:HB	1:N:611:ARG:HB2	2.02	0.41
1:O:51:ASP:HB3	2:O:880:HOH:O	2.20	0.41
1:B:101:ARG:CD	2:B:846:HOH:O	2.68	0.40
1:C:219:HIS:CG	1:C:220:PRO:HD2	2.57	0.40
1:C:481:ILE:HD11	1:C:485:PHE:CD1	2.56	0.40
1:D:599:LEU:HA	2:D:842:HOH:O	2.21	0.40
1:J:252:ASP:HB2	2:J:767:HOH:O	2.21	0.40
1:L:527:VAL:HA	1:L:528:PRO:HD3	1.91	0.40
1:P:527:VAL:HA	1:P:528:PRO:HD3	1.96	0.40
1:F:219:HIS:CG	1:F:220:PRO:HD2	2.56	0.40
1:N:460:THR:O	2:N:774:HOH:O	2.22	0.40
1:E:427:LYS:HB3	2:E:837:HOH:O	2.21	0.40
1:F:546:LYS:O	1:F:614:VAL:HA	2.22	0.40
1:I:230:PRO:HD2	2:I:774:HOH:O	2.20	0.40
1:N:546:LYS:HA	1:N:570:MET:HB3	2.03	0.40
1:F:594:HIS:CE1	2:F:865:HOH:O	2.74	0.40
1:G:249:GLY:CA	2:G:701:HOH:O	2.66	0.40
1:H:404:GLU:OE1	1:H:413:VAL:HG22	2.20	0.40
1:J:76:ILE:HD11	2:J:754:HOH:O	2.21	0.40
1:A:650:ILE:N	1:A:650:ILE:CD1	2.84	0.40
1:B:479:PRO:HA	1:B:621:PHE:O	2.21	0.40
1:I:319:LYS:HG3	2:I:801:HOH:O	2.21	0.40

All (2) 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:D:102:ASN:OD1	1:O:62:PRO:C[2_645]	1.94	0.26
1:M:318:ASP:OD1	1:O:655:LYS:NZ[1_455]	2.10	0.10

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	604/652 (93%)	579 (96%)	23 (4%)	2 (0%)	41	37
1	B	604/652 (93%)	577 (96%)	25 (4%)	2 (0%)	41	37
1	C	604/652 (93%)	577 (96%)	25 (4%)	2 (0%)	41	37
1	D	604/652 (93%)	575 (95%)	27 (4%)	2 (0%)	41	37
1	E	604/652 (93%)	579 (96%)	23 (4%)	2 (0%)	41	37
1	F	604/652 (93%)	575 (95%)	27 (4%)	2 (0%)	41	37
1	G	604/652 (93%)	579 (96%)	24 (4%)	1 (0%)	47	44
1	H	604/652 (93%)	580 (96%)	22 (4%)	2 (0%)	41	37
1	I	604/652 (93%)	575 (95%)	27 (4%)	2 (0%)	41	37
1	J	604/652 (93%)	574 (95%)	29 (5%)	1 (0%)	47	44
1	K	604/652 (93%)	574 (95%)	28 (5%)	2 (0%)	41	37
1	L	604/652 (93%)	579 (96%)	23 (4%)	2 (0%)	41	37
1	M	604/652 (93%)	571 (94%)	32 (5%)	1 (0%)	47	44
1	N	604/652 (93%)	576 (95%)	27 (4%)	1 (0%)	47	44
1	O	604/652 (93%)	569 (94%)	33 (6%)	2 (0%)	41	37
1	P	604/652 (93%)	575 (95%)	27 (4%)	2 (0%)	41	37
All	All	9664/10432 (93%)	9214 (95%)	422 (4%)	28 (0%)	41	37

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	GLY
1	B	344	GLY
1	C	344	GLY
1	D	344	GLY
1	G	344	GLY
1	H	344	GLY

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Mol	Chain	Res	Type
1	I	344	GLY
1	J	344	GLY
1	K	344	GLY
1	L	344	GLY
1	M	344	GLY
1	O	344	GLY
1	P	344	GLY
1	F	344	GLY
1	N	344	GLY
1	E	344	GLY
1	O	237	GLY
1	D	237	GLY
1	E	237	GLY
1	P	237	GLY
1	A	237	GLY
1	C	237	GLY
1	F	237	GLY
1	H	237	GLY
1	I	237	GLY
1	K	237	GLY
1	L	237	GLY
1	B	237	GLY

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	509/544 (94%)	499 (98%)	10 (2%)	55	58
1	B	509/544 (94%)	499 (98%)	10 (2%)	55	58
1	C	509/544 (94%)	500 (98%)	9 (2%)	59	63
1	D	509/544 (94%)	498 (98%)	11 (2%)	52	55
1	E	509/544 (94%)	497 (98%)	12 (2%)	49	51
1	F	509/544 (94%)	496 (97%)	13 (3%)	46	48
1	G	509/544 (94%)	498 (98%)	11 (2%)	52	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	509/544 (94%)	499 (98%)	10 (2%)	55	58
1	I	509/544 (94%)	498 (98%)	11 (2%)	52	55
1	J	509/544 (94%)	498 (98%)	11 (2%)	52	55
1	K	509/544 (94%)	497 (98%)	12 (2%)	49	51
1	L	509/544 (94%)	499 (98%)	10 (2%)	55	58
1	M	509/544 (94%)	496 (97%)	13 (3%)	46	48
1	N	509/544 (94%)	498 (98%)	11 (2%)	52	55
1	O	509/544 (94%)	498 (98%)	11 (2%)	52	55
1	P	509/544 (94%)	500 (98%)	9 (2%)	59	63
All	All	8144/8704 (94%)	7970 (98%)	174 (2%)	53	57

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	VAL
1	A	339	GLN
1	A	398	PHE
1	A	442	CYS
1	A	446	LEU
1	A	453	ASP
1	A	517	VAL
1	A	522	VAL
1	A	570	MET
1	A	620	TRP
1	B	130	VAL
1	B	339	GLN
1	B	398	PHE
1	B	442	CYS
1	B	446	LEU
1	B	453	ASP
1	B	517	VAL
1	B	522	VAL
1	B	527	VAL
1	B	620	TRP
1	C	130	VAL
1	C	339	GLN
1	C	398	PHE
1	C	446	LEU
1	C	453	ASP

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Mol	Chain	Res	Type
1	C	517	VAL
1	C	522	VAL
1	C	527	VAL
1	C	620	TRP
1	D	76	ILE
1	D	130	VAL
1	D	339	GLN
1	D	398	PHE
1	D	441	ASN
1	D	446	LEU
1	D	453	ASP
1	D	517	VAL
1	D	522	VAL
1	D	527	VAL
1	D	620	TRP
1	E	76	ILE
1	E	130	VAL
1	E	339	GLN
1	E	398	PHE
1	E	441	ASN
1	E	442	CYS
1	E	446	LEU
1	E	453	ASP
1	E	517	VAL
1	E	522	VAL
1	E	527	VAL
1	E	620	TRP
1	F	76	ILE
1	F	130	VAL
1	F	339	GLN
1	F	398	PHE
1	F	435	PRO
1	F	442	CYS
1	F	446	LEU
1	F	453	ASP
1	F	517	VAL
1	F	522	VAL
1	F	527	VAL
1	F	570	MET
1	F	620	TRP
1	G	76	ILE
1	G	130	VAL

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Mol	Chain	Res	Type
1	G	339	GLN
1	G	398	PHE
1	G	442	CYS
1	G	446	LEU
1	G	453	ASP
1	G	517	VAL
1	G	522	VAL
1	G	588	GLN
1	G	620	TRP
1	H	76	ILE
1	H	130	VAL
1	H	339	GLN
1	H	398	PHE
1	H	446	LEU
1	H	453	ASP
1	H	517	VAL
1	H	522	VAL
1	H	527	VAL
1	H	620	TRP
1	I	76	ILE
1	I	339	GLN
1	I	398	PHE
1	I	442	CYS
1	I	446	LEU
1	I	453	ASP
1	I	517	VAL
1	I	522	VAL
1	I	527	VAL
1	I	570	MET
1	I	620	TRP
1	J	76	ILE
1	J	339	GLN
1	J	398	PHE
1	J	442	CYS
1	J	446	LEU
1	J	453	ASP
1	J	517	VAL
1	J	522	VAL
1	J	527	VAL
1	J	570	MET
1	J	620	TRP
1	K	76	ILE

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Mol	Chain	Res	Type
1	K	113	ASN
1	K	130	VAL
1	K	339	GLN
1	K	398	PHE
1	K	446	LEU
1	K	453	ASP
1	K	517	VAL
1	K	522	VAL
1	K	527	VAL
1	K	541	SER
1	K	620	TRP
1	L	76	ILE
1	L	130	VAL
1	L	339	GLN
1	L	398	PHE
1	L	441	ASN
1	L	446	LEU
1	L	453	ASP
1	L	517	VAL
1	L	522	VAL
1	L	620	TRP
1	M	76	ILE
1	M	102	ASN
1	M	130	VAL
1	M	339	GLN
1	M	398	PHE
1	M	435	PRO
1	M	446	LEU
1	M	453	ASP
1	M	517	VAL
1	M	522	VAL
1	M	527	VAL
1	M	620	TRP
1	M	644	THR
1	N	76	ILE
1	N	130	VAL
1	N	339	GLN
1	N	398	PHE
1	N	446	LEU
1	N	453	ASP
1	N	517	VAL
1	N	522	VAL

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Mol	Chain	Res	Type
1	N	527	VAL
1	N	570	MET
1	N	620	TRP
1	O	76	ILE
1	O	130	VAL
1	O	339	GLN
1	O	398	PHE
1	O	446	LEU
1	O	453	ASP
1	O	517	VAL
1	O	522	VAL
1	O	527	VAL
1	O	541	SER
1	O	620	TRP
1	P	130	VAL
1	P	339	GLN
1	P	398	PHE
1	P	446	LEU
1	P	453	ASP
1	P	517	VAL
1	P	522	VAL
1	P	527	VAL
1	P	620	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	133	GLN
1	A	191	ASN
1	A	339	GLN
1	A	441	ASN
1	B	113	ASN
1	B	339	GLN
1	B	441	ASN
1	B	588	GLN
1	C	113	ASN
1	C	133	GLN
1	C	191	ASN
1	C	265	ASN
1	C	339	GLN
1	C	347	HIS

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Mol	Chain	Res	Type
1	C	441	ASN
1	C	588	GLN
1	D	102	ASN
1	D	113	ASN
1	D	133	GLN
1	D	339	GLN
1	D	441	ASN
1	D	588	GLN
1	D	652	HIS
1	E	113	ASN
1	E	133	GLN
1	E	191	ASN
1	E	300	GLN
1	E	339	GLN
1	E	414	HIS
1	E	441	ASN
1	E	588	GLN
1	F	113	ASN
1	F	133	GLN
1	F	339	GLN
1	F	441	ASN
1	F	588	GLN
1	F	652	HIS
1	G	113	ASN
1	G	133	GLN
1	G	339	GLN
1	G	441	ASN
1	G	476	HIS
1	G	588	GLN
1	H	113	ASN
1	H	133	GLN
1	H	191	ASN
1	H	339	GLN
1	H	391	HIS
1	H	441	ASN
1	I	113	ASN
1	I	191	ASN
1	I	339	GLN
1	I	441	ASN
1	J	133	GLN
1	J	339	GLN
1	J	441	ASN

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Mol	Chain	Res	Type
1	J	588	GLN
1	K	113	ASN
1	K	133	GLN
1	K	191	ASN
1	K	339	GLN
1	K	441	ASN
1	K	588	GLN
1	L	113	ASN
1	L	133	GLN
1	L	295	GLN
1	L	339	GLN
1	L	441	ASN
1	L	588	GLN
1	L	652	HIS
1	M	102	ASN
1	M	113	ASN
1	M	133	GLN
1	M	191	ASN
1	M	339	GLN
1	M	588	GLN
1	N	113	ASN
1	N	133	GLN
1	N	339	GLN
1	N	391	HIS
1	N	441	ASN
1	O	113	ASN
1	O	133	GLN
1	O	295	GLN
1	O	339	GLN
1	O	391	HIS
1	O	441	ASN
1	O	461	HIS
1	O	588	GLN
1	P	50	HIS
1	P	113	ASN
1	P	133	GLN
1	P	191	ASN
1	P	339	GLN
1	P	441	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	M	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	M	441:ASN	C	442:CYS	N	1.20

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	608/652 (93%)	-0.39	1 (0%)	95	94	10, 16, 27, 54	0
1	B	608/652 (93%)	-0.40	1 (0%)	95	94	10, 17, 28, 54	0
1	C	608/652 (93%)	-0.40	2 (0%)	94	93	10, 17, 28, 54	0
1	D	608/652 (93%)	-0.42	2 (0%)	94	93	10, 17, 28, 54	0
1	E	608/652 (93%)	-0.43	3 (0%)	91	90	10, 17, 28, 54	0
1	F	608/652 (93%)	-0.48	2 (0%)	94	93	10, 17, 28, 54	0
1	G	608/652 (93%)	-0.41	1 (0%)	95	94	10, 17, 28, 54	0
1	H	608/652 (93%)	-0.43	1 (0%)	95	94	10, 16, 28, 54	0
1	I	608/652 (93%)	-0.44	1 (0%)	95	94	10, 17, 28, 54	0
1	J	608/652 (93%)	-0.36	2 (0%)	94	93	10, 17, 28, 54	0
1	K	608/652 (93%)	-0.42	4 (0%)	87	87	11, 17, 28, 54	0
1	L	608/652 (93%)	-0.39	7 (1%)	79	78	10, 17, 28, 54	0
1	M	608/652 (93%)	-0.40	3 (0%)	91	90	10, 17, 28, 54	0
1	N	608/652 (93%)	-0.41	2 (0%)	94	93	10, 16, 28, 54	0
1	O	608/652 (93%)	-0.40	2 (0%)	94	93	10, 17, 28, 54	0
1	P	608/652 (93%)	-0.39	1 (0%)	95	94	10, 16, 28, 54	0
All	All	9728/10432 (93%)	-0.41	35 (0%)	92	92	10, 17, 28, 54	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	441	ASN	5.3
1	L	50	HIS	4.9
1	J	50	HIS	4.8
1	H	50	HIS	4.7
1	E	50	HIS	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	441	ASN	3.4
1	O	50	HIS	3.3
1	A	50	HIS	3.2
1	G	50	HIS	3.1
1	P	50	HIS	3.1
1	M	50	HIS	3.0
1	C	99	ASN	2.9
1	F	50	HIS	2.8
1	B	50	HIS	2.8
1	O	62	PRO	2.8
1	J	465	ASP	2.8
1	D	441	ASN	2.6
1	D	50	HIS	2.5
1	I	50	HIS	2.5
1	L	102	ASN	2.4
1	M	319	LYS	2.3
1	N	266	ASP	2.3
1	K	50	HIS	2.2
1	L	72	GLN	2.2
1	L	325	LYS	2.2
1	K	99	ASN	2.1
1	E	101	ARG	2.1
1	K	101	ARG	2.1
1	L	101	ARG	2.1
1	K	588	GLN	2.1
1	L	266	ASP	2.0
1	M	101	ARG	2.0
1	N	99	ASN	2.0
1	F	325	LYS	2.0
1	C	50	HIS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.