Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:59 AM GMT

PDB ID	:	3K55
Title	:	Structure of beta hairpin deletion mutant of beta toxin from Staphylococcus aureus
Authors	:	Kruse, A.C.; Huseby, M.; Shi, K.; Digre, J.; Ohlendorf, D.H.; Earhart, C.A.
Deposited on	:	2009-10-06
Resolution	:	3.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

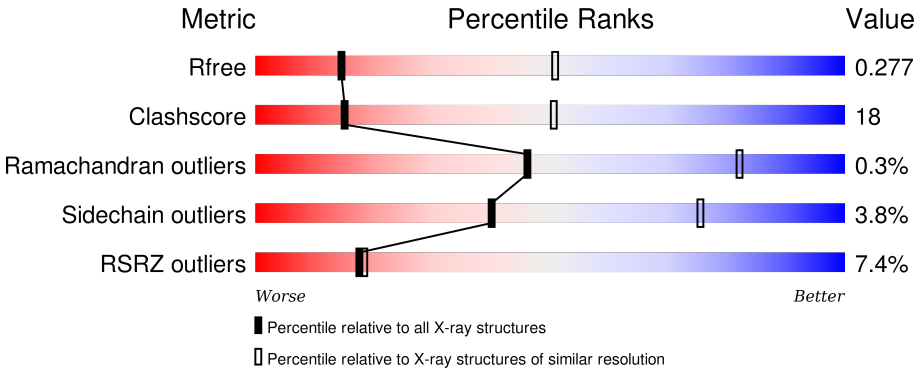
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	306	62% 26% • 8%
1	B	306	59% 30% • 8%
1	C	306	2% 59% 30% • 8%
1	D	306	3% 59% 30% • 8%
1	E	306	4% 64% 25% • 8%

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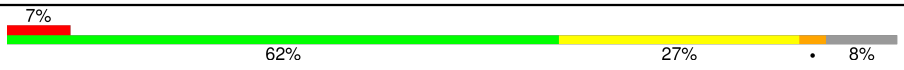
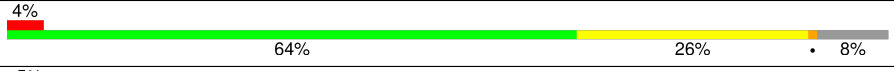
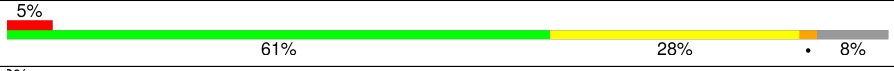
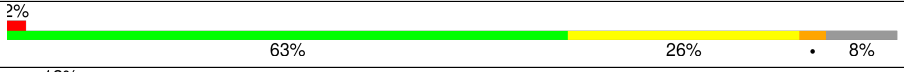
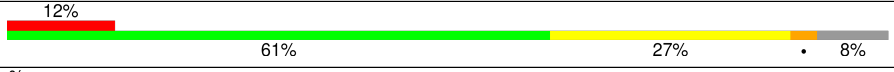
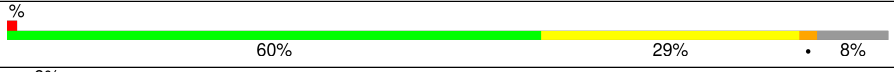
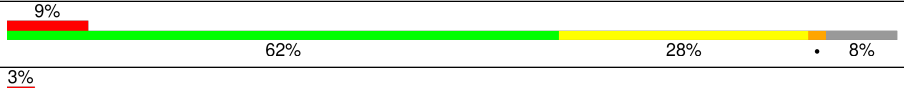
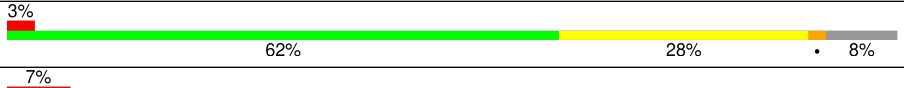
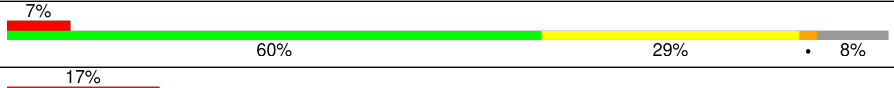
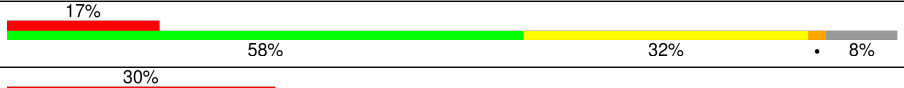
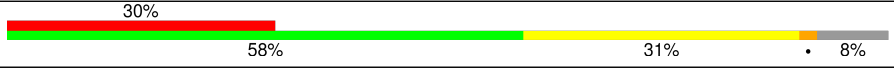
Mol	Chain	Length	Quality of chain
1	F	306	
1	G	306	
1	H	306	
1	I	306	
1	J	306	
1	K	306	
1	L	306	
1	M	306	
1	N	306	
1	O	306	
1	P	306	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 35844 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 Beta-hemolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	24	0	0
			2240	1413	383	439	5			
1	B	280	Total	C	N	O	S	20	0	0
			2240	1413	383	439	5			
1	C	280	Total	C	N	O	S	16	0	0
			2240	1413	383	439	5			
1	D	280	Total	C	N	O	S	12	0	0
			2240	1413	383	439	5			
1	E	280	Total	C	N	O	S	24	0	0
			2240	1413	383	439	5			
1	F	280	Total	C	N	O	S	20	0	0
			2240	1413	383	439	5			
1	G	280	Total	C	N	O	S	20	0	0
			2240	1413	383	439	5			
1	H	280	Total	C	N	O	S	20	0	0
			2240	1413	383	439	5			
1	I	280	Total	C	N	O	S	20	0	0
			2240	1413	383	439	5			
1	J	280	Total	C	N	O	S	16	0	0
			2240	1413	383	439	5			
1	K	280	Total	C	N	O	S	20	0	0
			2240	1413	383	439	5			
1	L	280	Total	C	N	O	S	24	0	0
			2240	1413	383	439	5			
1	M	280	Total	C	N	O	S	16	0	0
			2240	1413	383	439	5			
1	N	280	Total	C	N	O	S	12	0	0
			2240	1413	383	439	5			
1	O	280	Total	C	N	O	S	20	0	0
			2240	1413	383	439	5			
1	P	280	Total	C	N	O	S	24	0	0
			2240	1413	383	439	5			

There are 512 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP A7LAI8
A	-18	ARG	-	EXPRESSION TAG	UNP A7LAI8
A	-17	SER	-	EXPRESSION TAG	UNP A7LAI8
A	-16	SER	-	EXPRESSION TAG	UNP A7LAI8
A	-15	HIS	-	EXPRESSION TAG	UNP A7LAI8
A	-14	HIS	-	EXPRESSION TAG	UNP A7LAI8
A	-13	HIS	-	EXPRESSION TAG	UNP A7LAI8
A	-12	HIS	-	EXPRESSION TAG	UNP A7LAI8
A	-11	HIS	-	EXPRESSION TAG	UNP A7LAI8
A	-10	HIS	-	EXPRESSION TAG	UNP A7LAI8
A	-9	SER	-	EXPRESSION TAG	UNP A7LAI8
A	-8	SER	-	EXPRESSION TAG	UNP A7LAI8
A	-7	GLY	-	EXPRESSION TAG	UNP A7LAI8
A	-6	LEU	-	EXPRESSION TAG	UNP A7LAI8
A	-5	VAL	-	EXPRESSION TAG	UNP A7LAI8
A	-4	PRO	-	EXPRESSION TAG	UNP A7LAI8
A	-3	ARG	-	EXPRESSION TAG	UNP A7LAI8
A	-2	GLY	-	EXPRESSION TAG	UNP A7LAI8
A	-1	SER	-	EXPRESSION TAG	UNP A7LAI8
A	0	HIS	-	EXPRESSION TAG	UNP A7LAI8
A	1	MET	-	EXPRESSION TAG	UNP A7LAI8
A	?	-	ASP	DELETION	UNP A7LAI8
A	?	-	VAL	DELETION	UNP A7LAI8
A	?	-	TYR	DELETION	UNP A7LAI8
A	?	-	ALA	DELETION	UNP A7LAI8
A	?	-	PHE	DELETION	UNP A7LAI8
A	?	-	PRO	DELETION	UNP A7LAI8
A	?	-	TYR	DELETION	UNP A7LAI8
A	?	-	TYR	DELETION	UNP A7LAI8
A	?	-	TYR	DELETION	UNP A7LAI8
A	?	-	VAL	DELETION	UNP A7LAI8
A	?	-	TYR	DELETION	UNP A7LAI8
B	-19	MET	-	EXPRESSION TAG	UNP A7LAI8
B	-18	ARG	-	EXPRESSION TAG	UNP A7LAI8
B	-17	SER	-	EXPRESSION TAG	UNP A7LAI8
B	-16	SER	-	EXPRESSION TAG	UNP A7LAI8
B	-15	HIS	-	EXPRESSION TAG	UNP A7LAI8
B	-14	HIS	-	EXPRESSION TAG	UNP A7LAI8
B	-13	HIS	-	EXPRESSION TAG	UNP A7LAI8
B	-12	HIS	-	EXPRESSION TAG	UNP A7LAI8
B	-11	HIS	-	EXPRESSION TAG	UNP A7LAI8
B	-10	HIS	-	EXPRESSION TAG	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	SER	-	EXPRESSION TAG	UNP A7LAI8
B	-8	SER	-	EXPRESSION TAG	UNP A7LAI8
B	-7	GLY	-	EXPRESSION TAG	UNP A7LAI8
B	-6	LEU	-	EXPRESSION TAG	UNP A7LAI8
B	-5	VAL	-	EXPRESSION TAG	UNP A7LAI8
B	-4	PRO	-	EXPRESSION TAG	UNP A7LAI8
B	-3	ARG	-	EXPRESSION TAG	UNP A7LAI8
B	-2	GLY	-	EXPRESSION TAG	UNP A7LAI8
B	-1	SER	-	EXPRESSION TAG	UNP A7LAI8
B	0	HIS	-	EXPRESSION TAG	UNP A7LAI8
B	1	MET	-	EXPRESSION TAG	UNP A7LAI8
B	?	-	ASP	DELETION	UNP A7LAI8
B	?	-	VAL	DELETION	UNP A7LAI8
B	?	-	TYR	DELETION	UNP A7LAI8
B	?	-	ALA	DELETION	UNP A7LAI8
B	?	-	PHE	DELETION	UNP A7LAI8
B	?	-	PRO	DELETION	UNP A7LAI8
B	?	-	TYR	DELETION	UNP A7LAI8
B	?	-	TYR	DELETION	UNP A7LAI8
B	?	-	TYR	DELETION	UNP A7LAI8
B	?	-	VAL	DELETION	UNP A7LAI8
B	?	-	TYR	DELETION	UNP A7LAI8
C	-19	MET	-	EXPRESSION TAG	UNP A7LAI8
C	-18	ARG	-	EXPRESSION TAG	UNP A7LAI8
C	-17	SER	-	EXPRESSION TAG	UNP A7LAI8
C	-16	SER	-	EXPRESSION TAG	UNP A7LAI8
C	-15	HIS	-	EXPRESSION TAG	UNP A7LAI8
C	-14	HIS	-	EXPRESSION TAG	UNP A7LAI8
C	-13	HIS	-	EXPRESSION TAG	UNP A7LAI8
C	-12	HIS	-	EXPRESSION TAG	UNP A7LAI8
C	-11	HIS	-	EXPRESSION TAG	UNP A7LAI8
C	-10	HIS	-	EXPRESSION TAG	UNP A7LAI8
C	-9	SER	-	EXPRESSION TAG	UNP A7LAI8
C	-8	SER	-	EXPRESSION TAG	UNP A7LAI8
C	-7	GLY	-	EXPRESSION TAG	UNP A7LAI8
C	-6	LEU	-	EXPRESSION TAG	UNP A7LAI8
C	-5	VAL	-	EXPRESSION TAG	UNP A7LAI8
C	-4	PRO	-	EXPRESSION TAG	UNP A7LAI8
C	-3	ARG	-	EXPRESSION TAG	UNP A7LAI8
C	-2	GLY	-	EXPRESSION TAG	UNP A7LAI8
C	-1	SER	-	EXPRESSION TAG	UNP A7LAI8
C	0	HIS	-	EXPRESSION TAG	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	EXPRESSION TAG	UNP A7LAI8
C	?	-	ASP	DELETION	UNP A7LAI8
C	?	-	VAL	DELETION	UNP A7LAI8
C	?	-	TYR	DELETION	UNP A7LAI8
C	?	-	ALA	DELETION	UNP A7LAI8
C	?	-	PHE	DELETION	UNP A7LAI8
C	?	-	PRO	DELETION	UNP A7LAI8
C	?	-	TYR	DELETION	UNP A7LAI8
C	?	-	TYR	DELETION	UNP A7LAI8
C	?	-	TYR	DELETION	UNP A7LAI8
C	?	-	VAL	DELETION	UNP A7LAI8
C	?	-	TYR	DELETION	UNP A7LAI8
D	-19	MET	-	EXPRESSION TAG	UNP A7LAI8
D	-18	ARG	-	EXPRESSION TAG	UNP A7LAI8
D	-17	SER	-	EXPRESSION TAG	UNP A7LAI8
D	-16	SER	-	EXPRESSION TAG	UNP A7LAI8
D	-15	HIS	-	EXPRESSION TAG	UNP A7LAI8
D	-14	HIS	-	EXPRESSION TAG	UNP A7LAI8
D	-13	HIS	-	EXPRESSION TAG	UNP A7LAI8
D	-12	HIS	-	EXPRESSION TAG	UNP A7LAI8
D	-11	HIS	-	EXPRESSION TAG	UNP A7LAI8
D	-10	HIS	-	EXPRESSION TAG	UNP A7LAI8
D	-9	SER	-	EXPRESSION TAG	UNP A7LAI8
D	-8	SER	-	EXPRESSION TAG	UNP A7LAI8
D	-7	GLY	-	EXPRESSION TAG	UNP A7LAI8
D	-6	LEU	-	EXPRESSION TAG	UNP A7LAI8
D	-5	VAL	-	EXPRESSION TAG	UNP A7LAI8
D	-4	PRO	-	EXPRESSION TAG	UNP A7LAI8
D	-3	ARG	-	EXPRESSION TAG	UNP A7LAI8
D	-2	GLY	-	EXPRESSION TAG	UNP A7LAI8
D	-1	SER	-	EXPRESSION TAG	UNP A7LAI8
D	0	HIS	-	EXPRESSION TAG	UNP A7LAI8
D	1	MET	-	EXPRESSION TAG	UNP A7LAI8
D	?	-	ASP	DELETION	UNP A7LAI8
D	?	-	VAL	DELETION	UNP A7LAI8
D	?	-	TYR	DELETION	UNP A7LAI8
D	?	-	ALA	DELETION	UNP A7LAI8
D	?	-	PHE	DELETION	UNP A7LAI8
D	?	-	PRO	DELETION	UNP A7LAI8
D	?	-	TYR	DELETION	UNP A7LAI8
D	?	-	TYR	DELETION	UNP A7LAI8
D	?	-	TYR	DELETION	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	VAL	DELETION	UNP A7LAI8
D	?	-	TYR	DELETION	UNP A7LAI8
E	-19	MET	-	EXPRESSION TAG	UNP A7LAI8
E	-18	ARG	-	EXPRESSION TAG	UNP A7LAI8
E	-17	SER	-	EXPRESSION TAG	UNP A7LAI8
E	-16	SER	-	EXPRESSION TAG	UNP A7LAI8
E	-15	HIS	-	EXPRESSION TAG	UNP A7LAI8
E	-14	HIS	-	EXPRESSION TAG	UNP A7LAI8
E	-13	HIS	-	EXPRESSION TAG	UNP A7LAI8
E	-12	HIS	-	EXPRESSION TAG	UNP A7LAI8
E	-11	HIS	-	EXPRESSION TAG	UNP A7LAI8
E	-10	HIS	-	EXPRESSION TAG	UNP A7LAI8
E	-9	SER	-	EXPRESSION TAG	UNP A7LAI8
E	-8	SER	-	EXPRESSION TAG	UNP A7LAI8
E	-7	GLY	-	EXPRESSION TAG	UNP A7LAI8
E	-6	LEU	-	EXPRESSION TAG	UNP A7LAI8
E	-5	VAL	-	EXPRESSION TAG	UNP A7LAI8
E	-4	PRO	-	EXPRESSION TAG	UNP A7LAI8
E	-3	ARG	-	EXPRESSION TAG	UNP A7LAI8
E	-2	GLY	-	EXPRESSION TAG	UNP A7LAI8
E	-1	SER	-	EXPRESSION TAG	UNP A7LAI8
E	0	HIS	-	EXPRESSION TAG	UNP A7LAI8
E	1	MET	-	EXPRESSION TAG	UNP A7LAI8
E	?	-	ASP	DELETION	UNP A7LAI8
E	?	-	VAL	DELETION	UNP A7LAI8
E	?	-	TYR	DELETION	UNP A7LAI8
E	?	-	ALA	DELETION	UNP A7LAI8
E	?	-	PHE	DELETION	UNP A7LAI8
E	?	-	PRO	DELETION	UNP A7LAI8
E	?	-	TYR	DELETION	UNP A7LAI8
E	?	-	TYR	DELETION	UNP A7LAI8
E	?	-	TYR	DELETION	UNP A7LAI8
E	?	-	VAL	DELETION	UNP A7LAI8
E	?	-	TYR	DELETION	UNP A7LAI8
F	-19	MET	-	EXPRESSION TAG	UNP A7LAI8
F	-18	ARG	-	EXPRESSION TAG	UNP A7LAI8
F	-17	SER	-	EXPRESSION TAG	UNP A7LAI8
F	-16	SER	-	EXPRESSION TAG	UNP A7LAI8
F	-15	HIS	-	EXPRESSION TAG	UNP A7LAI8
F	-14	HIS	-	EXPRESSION TAG	UNP A7LAI8
F	-13	HIS	-	EXPRESSION TAG	UNP A7LAI8
F	-12	HIS	-	EXPRESSION TAG	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-11	HIS	-	EXPRESSION TAG	UNP A7LAI8
F	-10	HIS	-	EXPRESSION TAG	UNP A7LAI8
F	-9	SER	-	EXPRESSION TAG	UNP A7LAI8
F	-8	SER	-	EXPRESSION TAG	UNP A7LAI8
F	-7	GLY	-	EXPRESSION TAG	UNP A7LAI8
F	-6	LEU	-	EXPRESSION TAG	UNP A7LAI8
F	-5	VAL	-	EXPRESSION TAG	UNP A7LAI8
F	-4	PRO	-	EXPRESSION TAG	UNP A7LAI8
F	-3	ARG	-	EXPRESSION TAG	UNP A7LAI8
F	-2	GLY	-	EXPRESSION TAG	UNP A7LAI8
F	-1	SER	-	EXPRESSION TAG	UNP A7LAI8
F	0	HIS	-	EXPRESSION TAG	UNP A7LAI8
F	1	MET	-	EXPRESSION TAG	UNP A7LAI8
F	?	-	ASP	DELETION	UNP A7LAI8
F	?	-	VAL	DELETION	UNP A7LAI8
F	?	-	TYR	DELETION	UNP A7LAI8
F	?	-	ALA	DELETION	UNP A7LAI8
F	?	-	PHE	DELETION	UNP A7LAI8
F	?	-	PRO	DELETION	UNP A7LAI8
F	?	-	TYR	DELETION	UNP A7LAI8
F	?	-	TYR	DELETION	UNP A7LAI8
F	?	-	TYR	DELETION	UNP A7LAI8
F	?	-	VAL	DELETION	UNP A7LAI8
F	?	-	TYR	DELETION	UNP A7LAI8
G	-19	MET	-	EXPRESSION TAG	UNP A7LAI8
G	-18	ARG	-	EXPRESSION TAG	UNP A7LAI8
G	-17	SER	-	EXPRESSION TAG	UNP A7LAI8
G	-16	SER	-	EXPRESSION TAG	UNP A7LAI8
G	-15	HIS	-	EXPRESSION TAG	UNP A7LAI8
G	-14	HIS	-	EXPRESSION TAG	UNP A7LAI8
G	-13	HIS	-	EXPRESSION TAG	UNP A7LAI8
G	-12	HIS	-	EXPRESSION TAG	UNP A7LAI8
G	-11	HIS	-	EXPRESSION TAG	UNP A7LAI8
G	-10	HIS	-	EXPRESSION TAG	UNP A7LAI8
G	-9	SER	-	EXPRESSION TAG	UNP A7LAI8
G	-8	SER	-	EXPRESSION TAG	UNP A7LAI8
G	-7	GLY	-	EXPRESSION TAG	UNP A7LAI8
G	-6	LEU	-	EXPRESSION TAG	UNP A7LAI8
G	-5	VAL	-	EXPRESSION TAG	UNP A7LAI8
G	-4	PRO	-	EXPRESSION TAG	UNP A7LAI8
G	-3	ARG	-	EXPRESSION TAG	UNP A7LAI8
G	-2	GLY	-	EXPRESSION TAG	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-1	SER	-	EXPRESSION TAG	UNP A7LAI8
G	0	HIS	-	EXPRESSION TAG	UNP A7LAI8
G	1	MET	-	EXPRESSION TAG	UNP A7LAI8
G	?	-	ASP	DELETION	UNP A7LAI8
G	?	-	VAL	DELETION	UNP A7LAI8
G	?	-	TYR	DELETION	UNP A7LAI8
G	?	-	ALA	DELETION	UNP A7LAI8
G	?	-	PHE	DELETION	UNP A7LAI8
G	?	-	PRO	DELETION	UNP A7LAI8
G	?	-	TYR	DELETION	UNP A7LAI8
G	?	-	TYR	DELETION	UNP A7LAI8
G	?	-	TYR	DELETION	UNP A7LAI8
G	?	-	VAL	DELETION	UNP A7LAI8
G	?	-	TYR	DELETION	UNP A7LAI8
H	-19	MET	-	EXPRESSION TAG	UNP A7LAI8
H	-18	ARG	-	EXPRESSION TAG	UNP A7LAI8
H	-17	SER	-	EXPRESSION TAG	UNP A7LAI8
H	-16	SER	-	EXPRESSION TAG	UNP A7LAI8
H	-15	HIS	-	EXPRESSION TAG	UNP A7LAI8
H	-14	HIS	-	EXPRESSION TAG	UNP A7LAI8
H	-13	HIS	-	EXPRESSION TAG	UNP A7LAI8
H	-12	HIS	-	EXPRESSION TAG	UNP A7LAI8
H	-11	HIS	-	EXPRESSION TAG	UNP A7LAI8
H	-10	HIS	-	EXPRESSION TAG	UNP A7LAI8
H	-9	SER	-	EXPRESSION TAG	UNP A7LAI8
H	-8	SER	-	EXPRESSION TAG	UNP A7LAI8
H	-7	GLY	-	EXPRESSION TAG	UNP A7LAI8
H	-6	LEU	-	EXPRESSION TAG	UNP A7LAI8
H	-5	VAL	-	EXPRESSION TAG	UNP A7LAI8
H	-4	PRO	-	EXPRESSION TAG	UNP A7LAI8
H	-3	ARG	-	EXPRESSION TAG	UNP A7LAI8
H	-2	GLY	-	EXPRESSION TAG	UNP A7LAI8
H	-1	SER	-	EXPRESSION TAG	UNP A7LAI8
H	0	HIS	-	EXPRESSION TAG	UNP A7LAI8
H	1	MET	-	EXPRESSION TAG	UNP A7LAI8
H	?	-	ASP	DELETION	UNP A7LAI8
H	?	-	VAL	DELETION	UNP A7LAI8
H	?	-	TYR	DELETION	UNP A7LAI8
H	?	-	ALA	DELETION	UNP A7LAI8
H	?	-	PHE	DELETION	UNP A7LAI8
H	?	-	PRO	DELETION	UNP A7LAI8
H	?	-	TYR	DELETION	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	TYR	DELETION	UNP A7LAI8
H	?	-	TYR	DELETION	UNP A7LAI8
H	?	-	VAL	DELETION	UNP A7LAI8
H	?	-	TYR	DELETION	UNP A7LAI8
I	-19	MET	-	EXPRESSION TAG	UNP A7LAI8
I	-18	ARG	-	EXPRESSION TAG	UNP A7LAI8
I	-17	SER	-	EXPRESSION TAG	UNP A7LAI8
I	-16	SER	-	EXPRESSION TAG	UNP A7LAI8
I	-15	HIS	-	EXPRESSION TAG	UNP A7LAI8
I	-14	HIS	-	EXPRESSION TAG	UNP A7LAI8
I	-13	HIS	-	EXPRESSION TAG	UNP A7LAI8
I	-12	HIS	-	EXPRESSION TAG	UNP A7LAI8
I	-11	HIS	-	EXPRESSION TAG	UNP A7LAI8
I	-10	HIS	-	EXPRESSION TAG	UNP A7LAI8
I	-9	SER	-	EXPRESSION TAG	UNP A7LAI8
I	-8	SER	-	EXPRESSION TAG	UNP A7LAI8
I	-7	GLY	-	EXPRESSION TAG	UNP A7LAI8
I	-6	LEU	-	EXPRESSION TAG	UNP A7LAI8
I	-5	VAL	-	EXPRESSION TAG	UNP A7LAI8
I	-4	PRO	-	EXPRESSION TAG	UNP A7LAI8
I	-3	ARG	-	EXPRESSION TAG	UNP A7LAI8
I	-2	GLY	-	EXPRESSION TAG	UNP A7LAI8
I	-1	SER	-	EXPRESSION TAG	UNP A7LAI8
I	0	HIS	-	EXPRESSION TAG	UNP A7LAI8
I	1	MET	-	EXPRESSION TAG	UNP A7LAI8
I	?	-	ASP	DELETION	UNP A7LAI8
I	?	-	VAL	DELETION	UNP A7LAI8
I	?	-	TYR	DELETION	UNP A7LAI8
I	?	-	ALA	DELETION	UNP A7LAI8
I	?	-	PHE	DELETION	UNP A7LAI8
I	?	-	PRO	DELETION	UNP A7LAI8
I	?	-	TYR	DELETION	UNP A7LAI8
I	?	-	TYR	DELETION	UNP A7LAI8
I	?	-	TYR	DELETION	UNP A7LAI8
I	?	-	VAL	DELETION	UNP A7LAI8
I	?	-	TYR	DELETION	UNP A7LAI8
J	-19	MET	-	EXPRESSION TAG	UNP A7LAI8
J	-18	ARG	-	EXPRESSION TAG	UNP A7LAI8
J	-17	SER	-	EXPRESSION TAG	UNP A7LAI8
J	-16	SER	-	EXPRESSION TAG	UNP A7LAI8
J	-15	HIS	-	EXPRESSION TAG	UNP A7LAI8
J	-14	HIS	-	EXPRESSION TAG	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-13	HIS	-	EXPRESSION TAG	UNP A7LAI8
J	-12	HIS	-	EXPRESSION TAG	UNP A7LAI8
J	-11	HIS	-	EXPRESSION TAG	UNP A7LAI8
J	-10	HIS	-	EXPRESSION TAG	UNP A7LAI8
J	-9	SER	-	EXPRESSION TAG	UNP A7LAI8
J	-8	SER	-	EXPRESSION TAG	UNP A7LAI8
J	-7	GLY	-	EXPRESSION TAG	UNP A7LAI8
J	-6	LEU	-	EXPRESSION TAG	UNP A7LAI8
J	-5	VAL	-	EXPRESSION TAG	UNP A7LAI8
J	-4	PRO	-	EXPRESSION TAG	UNP A7LAI8
J	-3	ARG	-	EXPRESSION TAG	UNP A7LAI8
J	-2	GLY	-	EXPRESSION TAG	UNP A7LAI8
J	-1	SER	-	EXPRESSION TAG	UNP A7LAI8
J	0	HIS	-	EXPRESSION TAG	UNP A7LAI8
J	1	MET	-	EXPRESSION TAG	UNP A7LAI8
J	?	-	ASP	DELETION	UNP A7LAI8
J	?	-	VAL	DELETION	UNP A7LAI8
J	?	-	TYR	DELETION	UNP A7LAI8
J	?	-	ALA	DELETION	UNP A7LAI8
J	?	-	PHE	DELETION	UNP A7LAI8
J	?	-	PRO	DELETION	UNP A7LAI8
J	?	-	TYR	DELETION	UNP A7LAI8
J	?	-	TYR	DELETION	UNP A7LAI8
J	?	-	TYR	DELETION	UNP A7LAI8
J	?	-	VAL	DELETION	UNP A7LAI8
J	?	-	TYR	DELETION	UNP A7LAI8
K	-19	MET	-	EXPRESSION TAG	UNP A7LAI8
K	-18	ARG	-	EXPRESSION TAG	UNP A7LAI8
K	-17	SER	-	EXPRESSION TAG	UNP A7LAI8
K	-16	SER	-	EXPRESSION TAG	UNP A7LAI8
K	-15	HIS	-	EXPRESSION TAG	UNP A7LAI8
K	-14	HIS	-	EXPRESSION TAG	UNP A7LAI8
K	-13	HIS	-	EXPRESSION TAG	UNP A7LAI8
K	-12	HIS	-	EXPRESSION TAG	UNP A7LAI8
K	-11	HIS	-	EXPRESSION TAG	UNP A7LAI8
K	-10	HIS	-	EXPRESSION TAG	UNP A7LAI8
K	-9	SER	-	EXPRESSION TAG	UNP A7LAI8
K	-8	SER	-	EXPRESSION TAG	UNP A7LAI8
K	-7	GLY	-	EXPRESSION TAG	UNP A7LAI8
K	-6	LEU	-	EXPRESSION TAG	UNP A7LAI8
K	-5	VAL	-	EXPRESSION TAG	UNP A7LAI8
K	-4	PRO	-	EXPRESSION TAG	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-3	ARG	-	EXPRESSION TAG	UNP A7LAI8
K	-2	GLY	-	EXPRESSION TAG	UNP A7LAI8
K	-1	SER	-	EXPRESSION TAG	UNP A7LAI8
K	0	HIS	-	EXPRESSION TAG	UNP A7LAI8
K	1	MET	-	EXPRESSION TAG	UNP A7LAI8
K	?	-	ASP	DELETION	UNP A7LAI8
K	?	-	VAL	DELETION	UNP A7LAI8
K	?	-	TYR	DELETION	UNP A7LAI8
K	?	-	ALA	DELETION	UNP A7LAI8
K	?	-	PHE	DELETION	UNP A7LAI8
K	?	-	PRO	DELETION	UNP A7LAI8
K	?	-	TYR	DELETION	UNP A7LAI8
K	?	-	TYR	DELETION	UNP A7LAI8
K	?	-	TYR	DELETION	UNP A7LAI8
K	?	-	VAL	DELETION	UNP A7LAI8
K	?	-	TYR	DELETION	UNP A7LAI8
L	-19	MET	-	EXPRESSION TAG	UNP A7LAI8
L	-18	ARG	-	EXPRESSION TAG	UNP A7LAI8
L	-17	SER	-	EXPRESSION TAG	UNP A7LAI8
L	-16	SER	-	EXPRESSION TAG	UNP A7LAI8
L	-15	HIS	-	EXPRESSION TAG	UNP A7LAI8
L	-14	HIS	-	EXPRESSION TAG	UNP A7LAI8
L	-13	HIS	-	EXPRESSION TAG	UNP A7LAI8
L	-12	HIS	-	EXPRESSION TAG	UNP A7LAI8
L	-11	HIS	-	EXPRESSION TAG	UNP A7LAI8
L	-10	HIS	-	EXPRESSION TAG	UNP A7LAI8
L	-9	SER	-	EXPRESSION TAG	UNP A7LAI8
L	-8	SER	-	EXPRESSION TAG	UNP A7LAI8
L	-7	GLY	-	EXPRESSION TAG	UNP A7LAI8
L	-6	LEU	-	EXPRESSION TAG	UNP A7LAI8
L	-5	VAL	-	EXPRESSION TAG	UNP A7LAI8
L	-4	PRO	-	EXPRESSION TAG	UNP A7LAI8
L	-3	ARG	-	EXPRESSION TAG	UNP A7LAI8
L	-2	GLY	-	EXPRESSION TAG	UNP A7LAI8
L	-1	SER	-	EXPRESSION TAG	UNP A7LAI8
L	0	HIS	-	EXPRESSION TAG	UNP A7LAI8
L	1	MET	-	EXPRESSION TAG	UNP A7LAI8
L	?	-	ASP	DELETION	UNP A7LAI8
L	?	-	VAL	DELETION	UNP A7LAI8
L	?	-	TYR	DELETION	UNP A7LAI8
L	?	-	ALA	DELETION	UNP A7LAI8
L	?	-	PHE	DELETION	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
L	?	-	PRO	DELETION	UNP A7LAI8
L	?	-	TYR	DELETION	UNP A7LAI8
L	?	-	TYR	DELETION	UNP A7LAI8
L	?	-	TYR	DELETION	UNP A7LAI8
L	?	-	VAL	DELETION	UNP A7LAI8
L	?	-	TYR	DELETION	UNP A7LAI8
M	-19	MET	-	EXPRESSION TAG	UNP A7LAI8
M	-18	ARG	-	EXPRESSION TAG	UNP A7LAI8
M	-17	SER	-	EXPRESSION TAG	UNP A7LAI8
M	-16	SER	-	EXPRESSION TAG	UNP A7LAI8
M	-15	HIS	-	EXPRESSION TAG	UNP A7LAI8
M	-14	HIS	-	EXPRESSION TAG	UNP A7LAI8
M	-13	HIS	-	EXPRESSION TAG	UNP A7LAI8
M	-12	HIS	-	EXPRESSION TAG	UNP A7LAI8
M	-11	HIS	-	EXPRESSION TAG	UNP A7LAI8
M	-10	HIS	-	EXPRESSION TAG	UNP A7LAI8
M	-9	SER	-	EXPRESSION TAG	UNP A7LAI8
M	-8	SER	-	EXPRESSION TAG	UNP A7LAI8
M	-7	GLY	-	EXPRESSION TAG	UNP A7LAI8
M	-6	LEU	-	EXPRESSION TAG	UNP A7LAI8
M	-5	VAL	-	EXPRESSION TAG	UNP A7LAI8
M	-4	PRO	-	EXPRESSION TAG	UNP A7LAI8
M	-3	ARG	-	EXPRESSION TAG	UNP A7LAI8
M	-2	GLY	-	EXPRESSION TAG	UNP A7LAI8
M	-1	SER	-	EXPRESSION TAG	UNP A7LAI8
M	0	HIS	-	EXPRESSION TAG	UNP A7LAI8
M	1	MET	-	EXPRESSION TAG	UNP A7LAI8
M	?	-	ASP	DELETION	UNP A7LAI8
M	?	-	VAL	DELETION	UNP A7LAI8
M	?	-	TYR	DELETION	UNP A7LAI8
M	?	-	ALA	DELETION	UNP A7LAI8
M	?	-	PHE	DELETION	UNP A7LAI8
M	?	-	PRO	DELETION	UNP A7LAI8
M	?	-	TYR	DELETION	UNP A7LAI8
M	?	-	TYR	DELETION	UNP A7LAI8
M	?	-	TYR	DELETION	UNP A7LAI8
M	?	-	VAL	DELETION	UNP A7LAI8
M	?	-	TYR	DELETION	UNP A7LAI8
N	-19	MET	-	EXPRESSION TAG	UNP A7LAI8
N	-18	ARG	-	EXPRESSION TAG	UNP A7LAI8
N	-17	SER	-	EXPRESSION TAG	UNP A7LAI8
N	-16	SER	-	EXPRESSION TAG	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
N	-15	HIS	-	EXPRESSION TAG	UNP A7LAI8
N	-14	HIS	-	EXPRESSION TAG	UNP A7LAI8
N	-13	HIS	-	EXPRESSION TAG	UNP A7LAI8
N	-12	HIS	-	EXPRESSION TAG	UNP A7LAI8
N	-11	HIS	-	EXPRESSION TAG	UNP A7LAI8
N	-10	HIS	-	EXPRESSION TAG	UNP A7LAI8
N	-9	SER	-	EXPRESSION TAG	UNP A7LAI8
N	-8	SER	-	EXPRESSION TAG	UNP A7LAI8
N	-7	GLY	-	EXPRESSION TAG	UNP A7LAI8
N	-6	LEU	-	EXPRESSION TAG	UNP A7LAI8
N	-5	VAL	-	EXPRESSION TAG	UNP A7LAI8
N	-4	PRO	-	EXPRESSION TAG	UNP A7LAI8
N	-3	ARG	-	EXPRESSION TAG	UNP A7LAI8
N	-2	GLY	-	EXPRESSION TAG	UNP A7LAI8
N	-1	SER	-	EXPRESSION TAG	UNP A7LAI8
N	0	HIS	-	EXPRESSION TAG	UNP A7LAI8
N	1	MET	-	EXPRESSION TAG	UNP A7LAI8
N	?	-	ASP	DELETION	UNP A7LAI8
N	?	-	VAL	DELETION	UNP A7LAI8
N	?	-	TYR	DELETION	UNP A7LAI8
N	?	-	ALA	DELETION	UNP A7LAI8
N	?	-	PHE	DELETION	UNP A7LAI8
N	?	-	PRO	DELETION	UNP A7LAI8
N	?	-	TYR	DELETION	UNP A7LAI8
N	?	-	TYR	DELETION	UNP A7LAI8
N	?	-	TYR	DELETION	UNP A7LAI8
N	?	-	VAL	DELETION	UNP A7LAI8
N	?	-	TYR	DELETION	UNP A7LAI8
O	-19	MET	-	EXPRESSION TAG	UNP A7LAI8
O	-18	ARG	-	EXPRESSION TAG	UNP A7LAI8
O	-17	SER	-	EXPRESSION TAG	UNP A7LAI8
O	-16	SER	-	EXPRESSION TAG	UNP A7LAI8
O	-15	HIS	-	EXPRESSION TAG	UNP A7LAI8
O	-14	HIS	-	EXPRESSION TAG	UNP A7LAI8
O	-13	HIS	-	EXPRESSION TAG	UNP A7LAI8
O	-12	HIS	-	EXPRESSION TAG	UNP A7LAI8
O	-11	HIS	-	EXPRESSION TAG	UNP A7LAI8
O	-10	HIS	-	EXPRESSION TAG	UNP A7LAI8
O	-9	SER	-	EXPRESSION TAG	UNP A7LAI8
O	-8	SER	-	EXPRESSION TAG	UNP A7LAI8
O	-7	GLY	-	EXPRESSION TAG	UNP A7LAI8
O	-6	LEU	-	EXPRESSION TAG	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-5	VAL	-	EXPRESSION TAG	UNP A7LAI8
O	-4	PRO	-	EXPRESSION TAG	UNP A7LAI8
O	-3	ARG	-	EXPRESSION TAG	UNP A7LAI8
O	-2	GLY	-	EXPRESSION TAG	UNP A7LAI8
O	-1	SER	-	EXPRESSION TAG	UNP A7LAI8
O	0	HIS	-	EXPRESSION TAG	UNP A7LAI8
O	1	MET	-	EXPRESSION TAG	UNP A7LAI8
O	?	-	ASP	DELETION	UNP A7LAI8
O	?	-	VAL	DELETION	UNP A7LAI8
O	?	-	TYR	DELETION	UNP A7LAI8
O	?	-	ALA	DELETION	UNP A7LAI8
O	?	-	PHE	DELETION	UNP A7LAI8
O	?	-	PRO	DELETION	UNP A7LAI8
O	?	-	TYR	DELETION	UNP A7LAI8
O	?	-	TYR	DELETION	UNP A7LAI8
O	?	-	TYR	DELETION	UNP A7LAI8
O	?	-	VAL	DELETION	UNP A7LAI8
O	?	-	TYR	DELETION	UNP A7LAI8
P	-19	MET	-	EXPRESSION TAG	UNP A7LAI8
P	-18	ARG	-	EXPRESSION TAG	UNP A7LAI8
P	-17	SER	-	EXPRESSION TAG	UNP A7LAI8
P	-16	SER	-	EXPRESSION TAG	UNP A7LAI8
P	-15	HIS	-	EXPRESSION TAG	UNP A7LAI8
P	-14	HIS	-	EXPRESSION TAG	UNP A7LAI8
P	-13	HIS	-	EXPRESSION TAG	UNP A7LAI8
P	-12	HIS	-	EXPRESSION TAG	UNP A7LAI8
P	-11	HIS	-	EXPRESSION TAG	UNP A7LAI8
P	-10	HIS	-	EXPRESSION TAG	UNP A7LAI8
P	-9	SER	-	EXPRESSION TAG	UNP A7LAI8
P	-8	SER	-	EXPRESSION TAG	UNP A7LAI8
P	-7	GLY	-	EXPRESSION TAG	UNP A7LAI8
P	-6	LEU	-	EXPRESSION TAG	UNP A7LAI8
P	-5	VAL	-	EXPRESSION TAG	UNP A7LAI8
P	-4	PRO	-	EXPRESSION TAG	UNP A7LAI8
P	-3	ARG	-	EXPRESSION TAG	UNP A7LAI8
P	-2	GLY	-	EXPRESSION TAG	UNP A7LAI8
P	-1	SER	-	EXPRESSION TAG	UNP A7LAI8
P	0	HIS	-	EXPRESSION TAG	UNP A7LAI8
P	1	MET	-	EXPRESSION TAG	UNP A7LAI8
P	?	-	ASP	DELETION	UNP A7LAI8
P	?	-	VAL	DELETION	UNP A7LAI8
P	?	-	TYR	DELETION	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
P	?	-	ALA	DELETION	UNP A7LAI8
P	?	-	PHE	DELETION	UNP A7LAI8
P	?	-	PRO	DELETION	UNP A7LAI8
P	?	-	TYR	DELETION	UNP A7LAI8
P	?	-	TYR	DELETION	UNP A7LAI8
P	?	-	TYR	DELETION	UNP A7LAI8
P	?	-	VAL	DELETION	UNP A7LAI8
P	?	-	TYR	DELETION	UNP A7LAI8

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

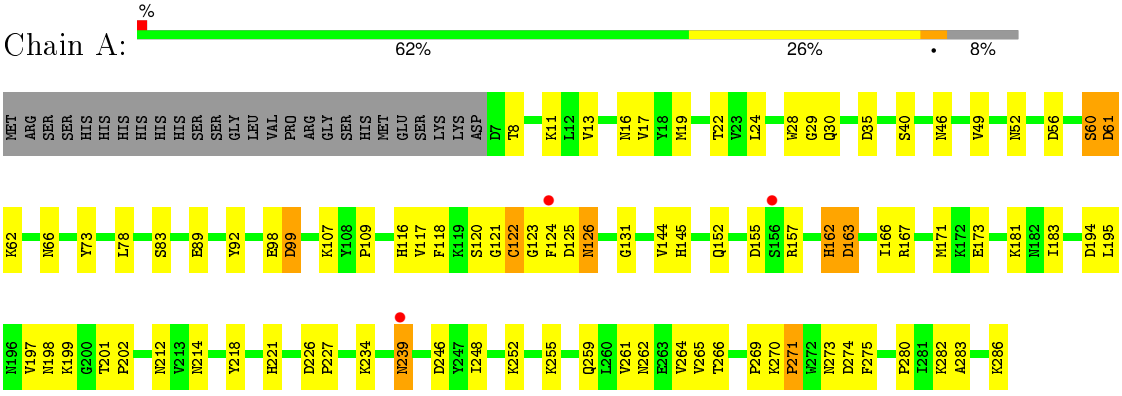
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Na 1 1	0	0

3 Residue-property plots

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

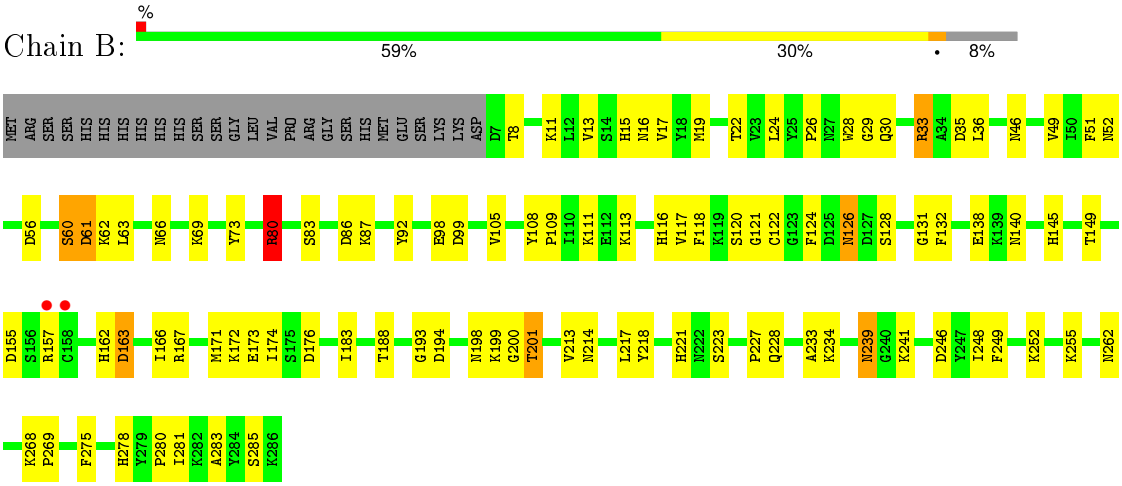
- Molecule 1: Beta-hemolysin

Chain A:



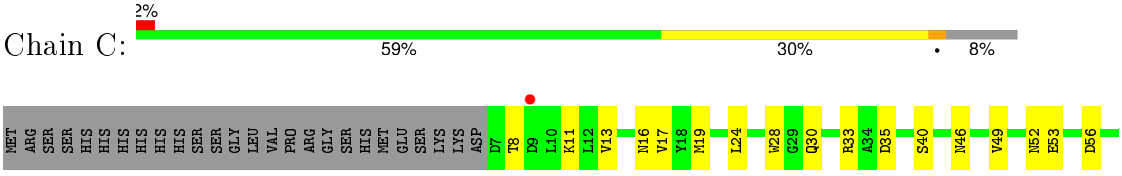
- Molecule 1: Beta-hemolysin

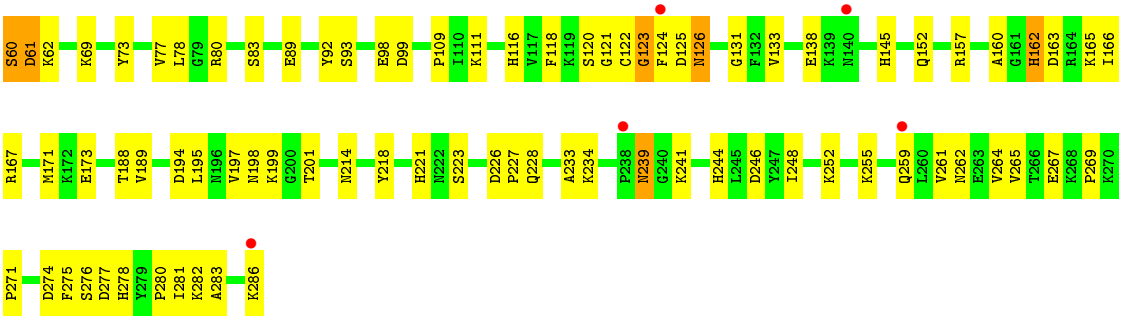
Chain B:



- Molecule 1: Beta-hemolysin

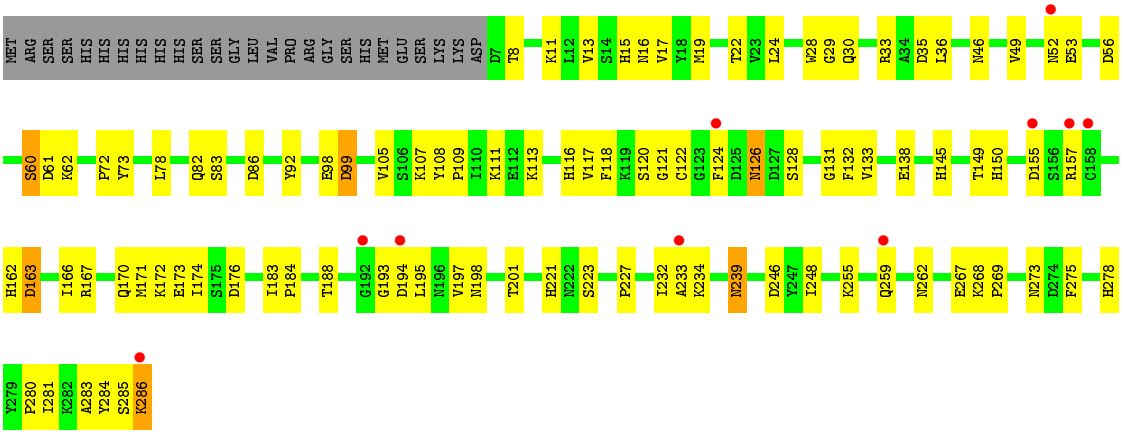
Chain C:





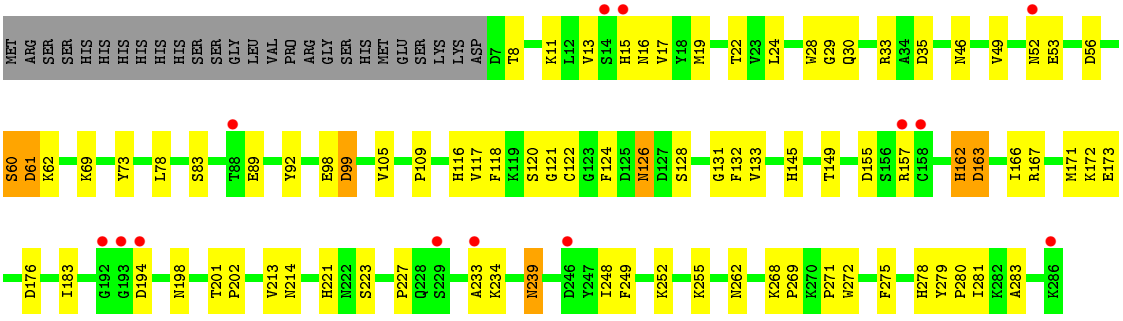
• Molecule 1: Beta-hemolysin

Chain D:



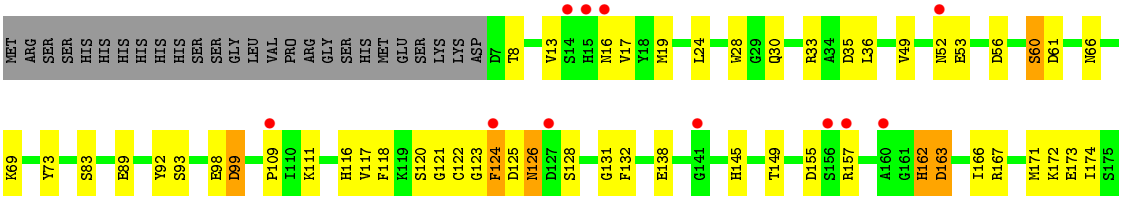
• Molecule 1: Beta-hemolysin

Chain E:



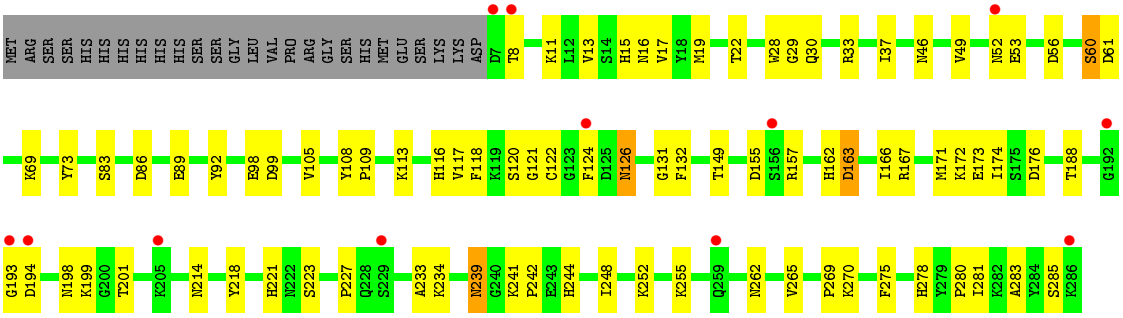
• Molecule 1: Beta-hemolysin

Chain F:



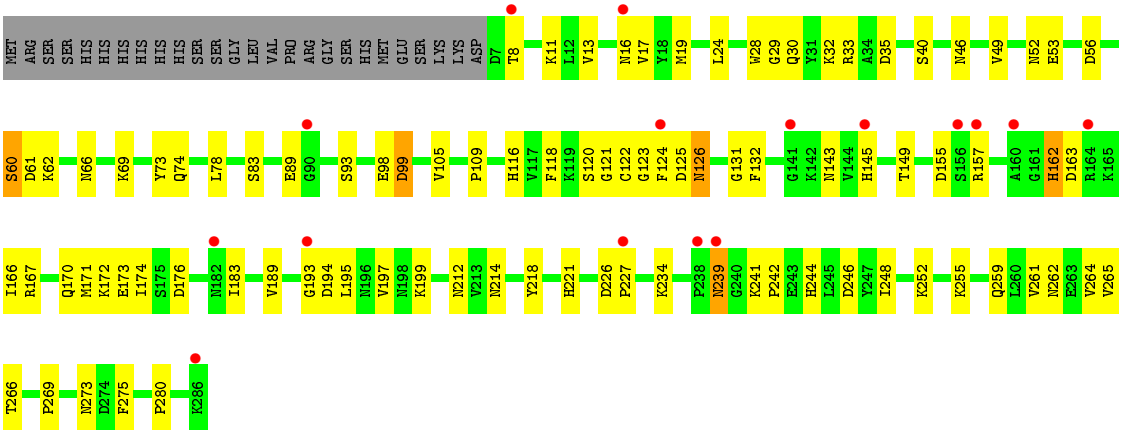
• Molecule 1: Beta-hemolysin

Chain G:



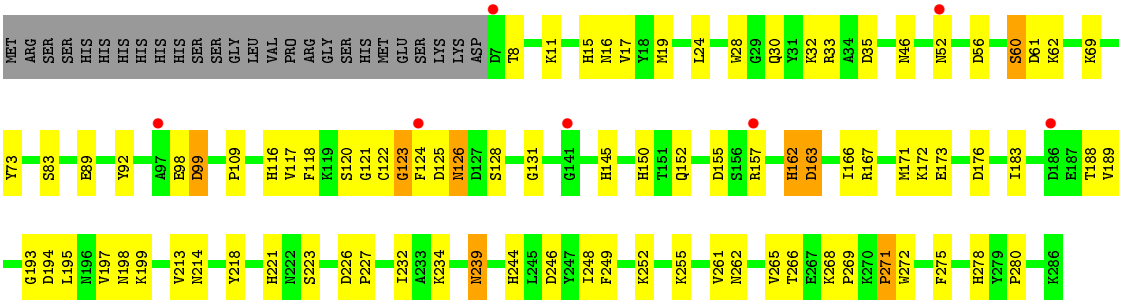
• Molecule 1: Beta-hemolysin

Chain H:



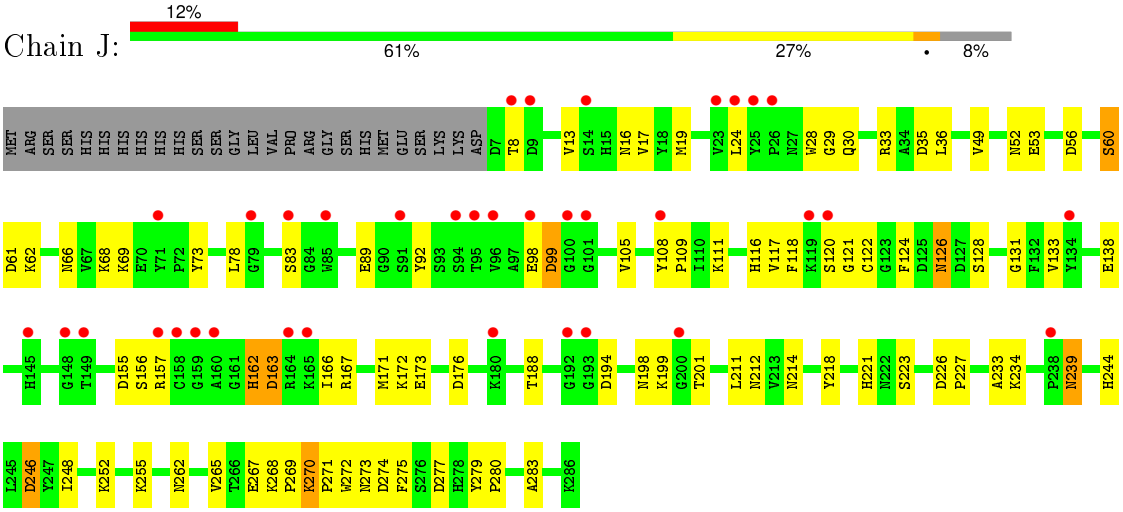
• Molecule 1: Beta-hemolysin

Chain I:



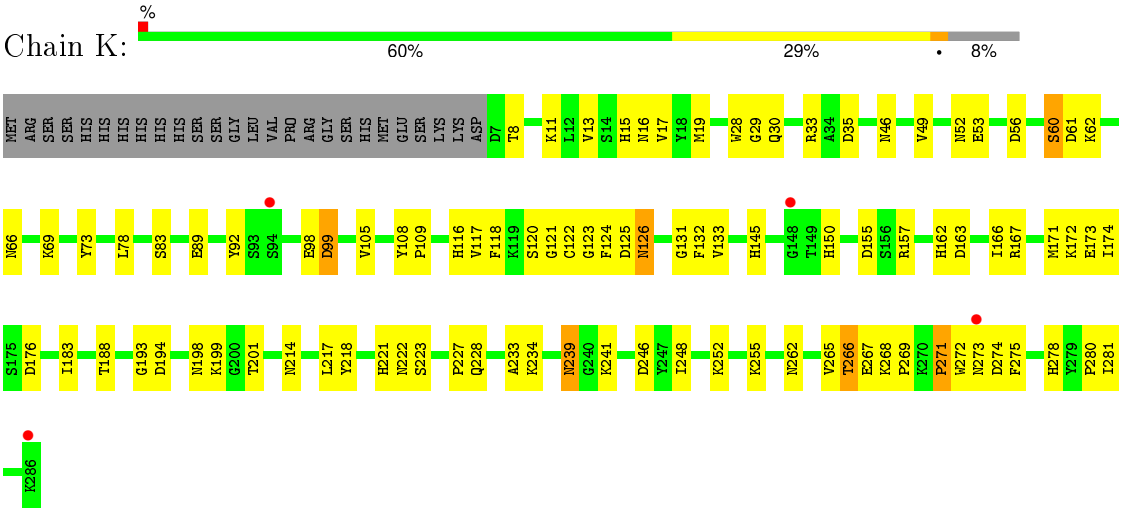
• Molecule 1: Beta-hemolysin

Chain J:



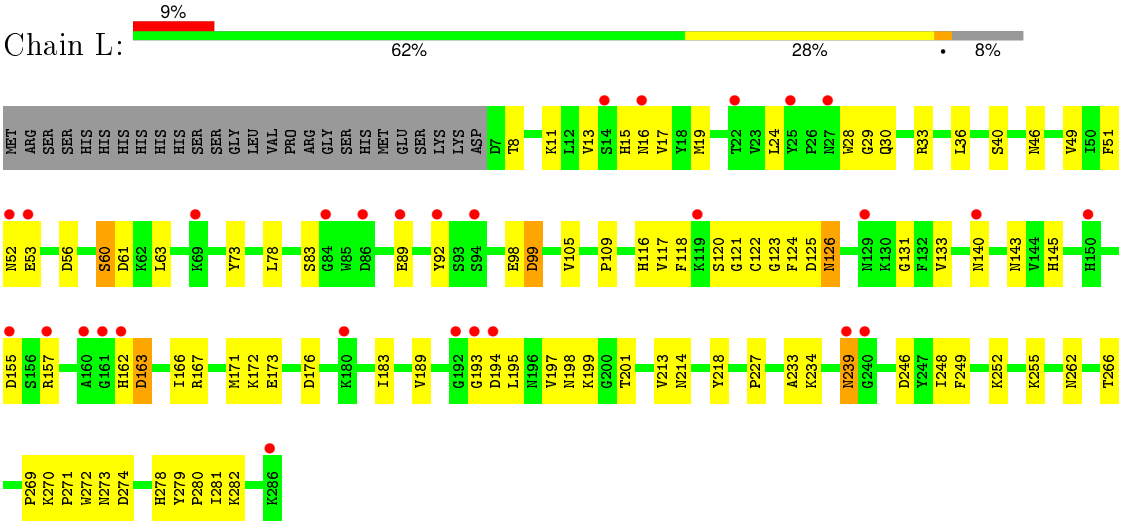
• Molecule 1: Beta-hemolysin

Chain K:



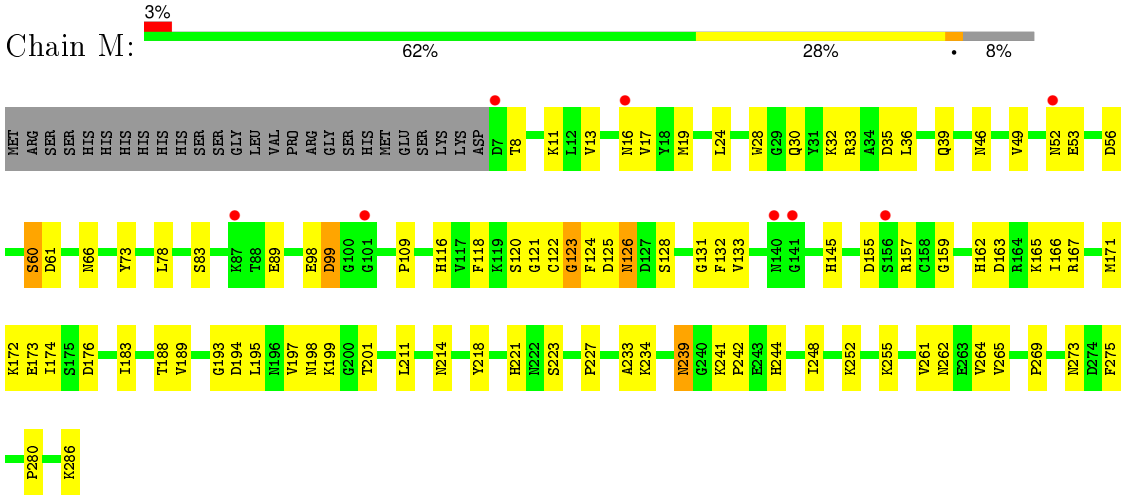
• Molecule 1: Beta-hemolysin

Chain L:



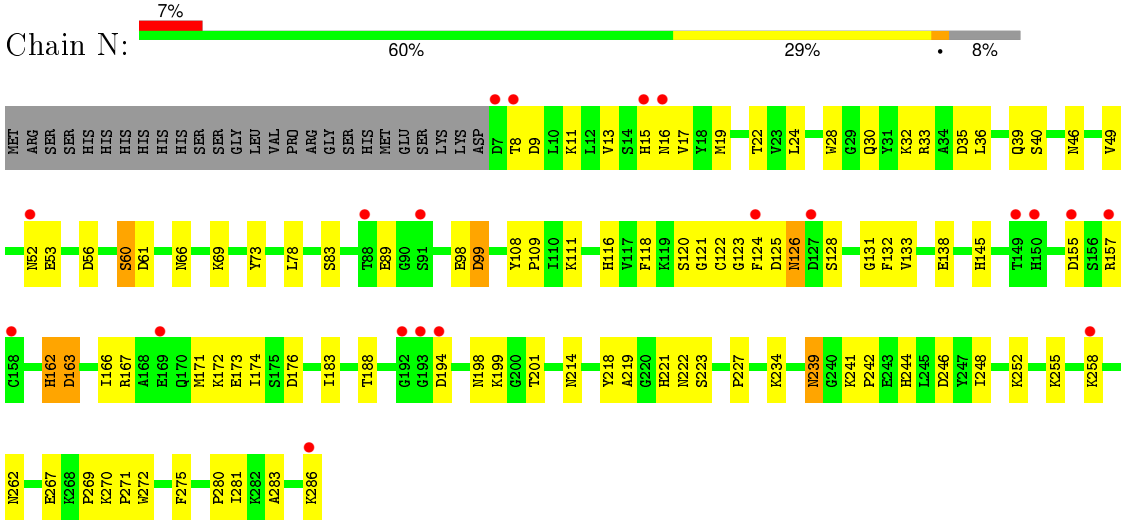
• Molecule 1: Beta-hemolysin

Chain M:



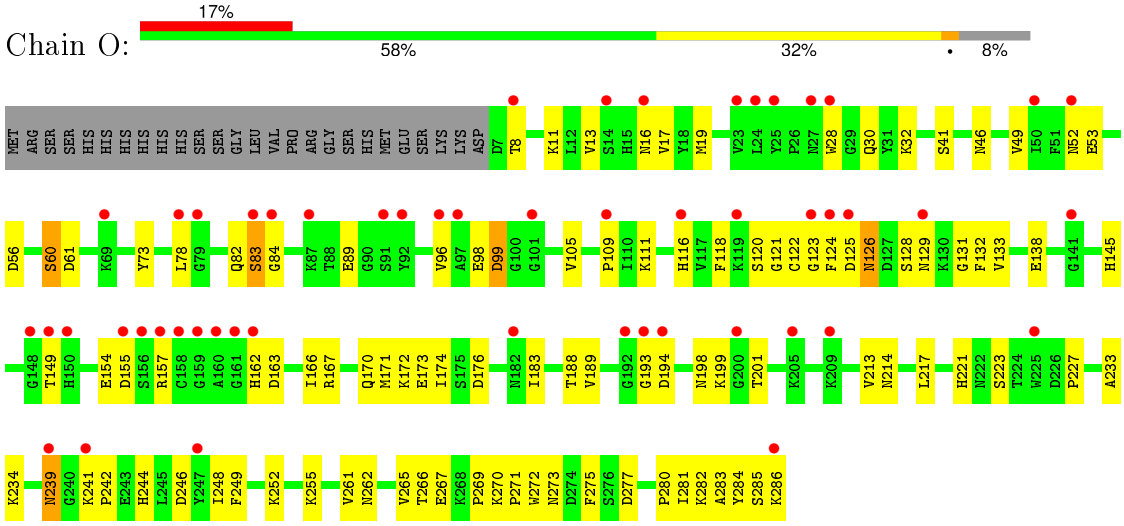
• Molecule 1: Beta-hemolysin

Chain N:



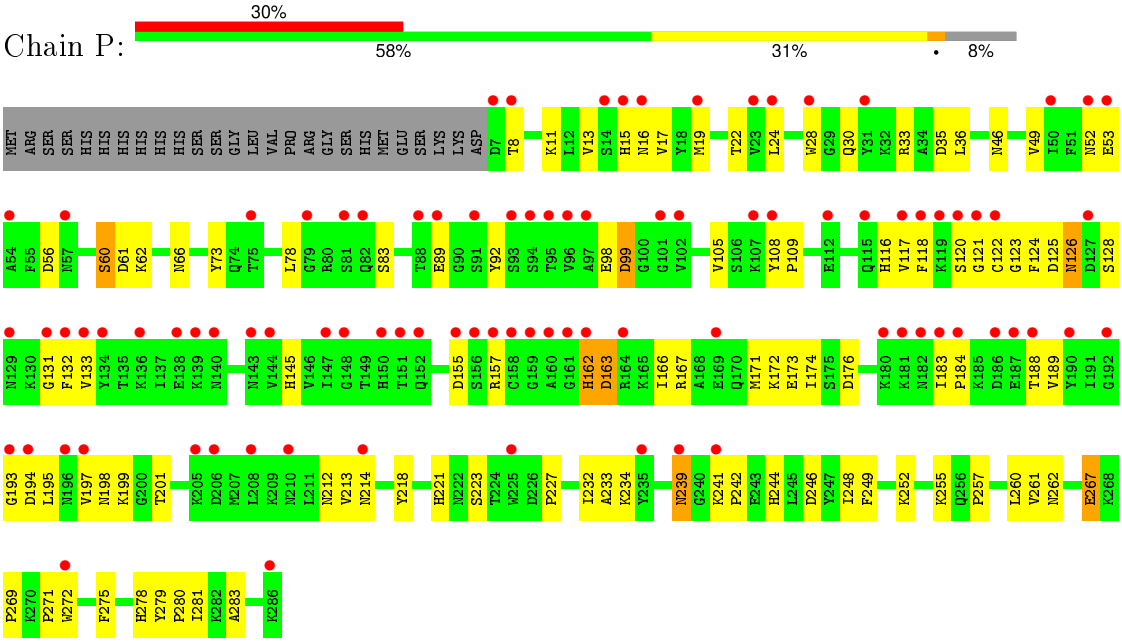
• Molecule 1: Beta-hemolysin

Chain O:



• Molecule 1: Beta-hemolysin

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	151.38Å 134.47Å 156.99Å 90.00° 116.89° 90.00°	Depositor
Resolution (Å)	31.31 – 3.35 31.31 – 3.02	Depositor EDS
% Data completeness (in resolution range)	95.5 (31.31-3.35) 75.9 (31.31-3.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.29 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.241 , 0.281 0.238 , 0.277	Depositor DCC
R_{free} test set	3827 reflections (4.96%)	DCC
Wilson B-factor (Å^2)	74.8	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 66.5	EDS
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 83795 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	35844	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.82	1/2294 (0.0%)	0.79	0/3100
1	B	0.81	0/2294	0.79	2/3100 (0.1%)
1	C	0.73	0/2294	0.73	0/3100
1	D	0.71	0/2294	0.72	0/3100
1	E	0.53	0/2294	0.61	0/3100
1	F	0.47	0/2294	0.60	0/3100
1	G	0.51	0/2294	0.61	0/3100
1	H	0.49	0/2294	0.60	0/3100
1	I	0.56	0/2294	0.64	0/3100
1	J	0.47	0/2294	0.60	0/3100
1	K	0.58	0/2294	0.87	3/3100 (0.1%)
1	L	0.50	0/2294	0.59	0/3100
1	M	0.49	0/2294	0.59	0/3100
1	N	0.45	0/2294	0.59	0/3100
1	O	0.40	0/2294	0.54	0/3100
1	P	0.34	0/2294	0.52	0/3100
All	All	0.57	1/36704 (0.0%)	0.66	5/49600 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	122	CYS	CB-SG	-6.63	1.71	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	33	ARG	NE-CZ-NH2	23.71	132.16	120.30
1	K	33	ARG	NE-CZ-NH1	-21.44	109.58	120.30
1	K	33	ARG	CD-NE-CZ	10.64	138.50	123.60
1	B	80	ARG	NE-CZ-NH2	6.59	123.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	33	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2240	0	2169	76	1
1	B	2240	0	2169	105	3
1	C	2240	0	2169	108	0
1	D	2240	0	2169	130	2
1	E	2240	0	2169	90	2
1	F	2240	0	2169	73	0
1	G	2240	0	2169	72	2
1	H	2240	0	2169	78	0
1	I	2240	0	2169	81	0
1	J	2240	0	2169	149	0
1	K	2240	0	2169	106	0
1	L	2240	0	2169	83	1
1	M	2240	0	2169	71	1
1	N	2240	0	2169	71	0
1	O	2240	0	2169	110	0
1	P	2240	0	2169	91	0
2	B	1	0	0	0	0
2	D	1	0	0	0	0
2	L	1	0	0	0	0
3	C	1	0	0	0	0
All	All	35844	0	34704	1219	6

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 18.

All (1219) 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:K:272:TRP:CH2	1:L:28:TRP:HA	1.31	1.62
1:J:68:LYS:CE	1:O:83:SER:HA	1.54	1.38
1:K:272:TRP:CH2	1:L:28:TRP:CA	2.06	1.35
1:D:284:TYR:HD2	1:J:157:ARG:NH2	1.40	1.20
1:C:259:GLN:HB3	1:D:286:LYS:HG3	1.24	1.19
1:K:272:TRP:HH2	1:L:28:TRP:CA	1.47	1.18
1:K:272:TRP:CZ2	1:L:28:TRP:C	2.18	1.17
1:J:269:PRO:O	1:J:271:PRO:HD3	1.43	1.15
1:B:69:LYS:CD	1:C:93:SER:HB2	1.76	1.14
1:B:69:LYS:HD2	1:C:93:SER:HB2	1.17	1.13
1:B:228:GLN:HE22	1:K:241:LYS:HD3	1.18	1.08
1:D:286:LYS:HB3	1:J:124:PHE:CD1	1.87	1.08
1:J:68:LYS:HE2	1:O:83:SER:CA	1.84	1.07
1:B:241:LYS:HD3	1:K:228:GLN:NE2	1.71	1.05
1:B:241:LYS:HD3	1:K:228:GLN:HE22	1.23	1.04
1:K:272:TRP:CH2	1:L:28:TRP:C	2.31	1.02
1:D:284:TYR:CD2	1:J:157:ARG:NH2	2.28	1.02
1:E:69:LYS:HD2	1:H:93:SER:HB2	1.43	0.99
1:D:285:SER:N	1:J:157:ARG:HH22	1.60	0.99
1:J:269:PRO:O	1:J:271:PRO:CD	2.09	0.99
1:K:273:ASN:O	1:K:274:ASP:OD1	1.80	0.98
1:B:228:GLN:NE2	1:K:241:LYS:HD3	1.78	0.98
1:C:259:GLN:CB	1:D:286:LYS:HG3	1.96	0.96
1:D:284:TYR:C	1:J:157:ARG:NH2	2.19	0.95
1:C:275:PHE:O	1:D:33:ARG:HD2	1.66	0.95
1:F:93:SER:HB2	1:G:69:LYS:HD2	1.48	0.95
1:M:32:LYS:HE2	1:N:39:GLN:OE1	1.67	0.95
1:J:68:LYS:HE2	1:O:83:SER:HA	0.94	0.94
1:D:285:SER:CA	1:J:157:ARG:HH22	1.80	0.94
1:O:154:GLU:HA	1:O:163:ASP:OD2	1.67	0.93
1:C:228:GLN:HE21	1:E:202:PRO:HG3	1.30	0.93
1:K:272:TRP:CZ2	1:L:29:GLY:N	2.38	0.92
1:C:248:ILE:H	1:C:262:ASN:HD21	1.15	0.92
1:B:17:VAL:HG23	1:B:19:MET:HG3	1.53	0.90
1:J:17:VAL:HG23	1:J:19:MET:HG3	1.52	0.90
1:D:285:SER:N	1:J:157:ARG:NH2	2.18	0.89
1:A:275:PHE:O	1:B:33:ARG:HD2	1.71	0.89
1:O:275:PHE:HE2	1:P:267:GLU:O	1.55	0.89
1:D:284:TYR:C	1:J:157:ARG:HH22	1.76	0.88
1:M:248:ILE:H	1:M:262:ASN:HD21	1.22	0.87
1:A:17:VAL:HG23	1:A:19:MET:HG3	1.54	0.87
1:J:68:LYS:NZ	1:O:83:SER:HA	1.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:69:LYS:CD	1:H:93:SER:HB2	2.05	0.86
1:G:33:ARG:HD2	1:H:275:PHE:O	1.74	0.86
1:O:275:PHE:CE2	1:P:267:GLU:O	2.29	0.86
1:J:248:ILE:H	1:J:262:ASN:HD21	1.23	0.86
1:H:17:VAL:HG23	1:H:19:MET:HG3	1.56	0.86
1:C:73:TYR:CD1	1:C:109:PRO:HA	2.11	0.85
1:I:248:ILE:H	1:I:262:ASN:HD21	1.25	0.85
1:C:17:VAL:HG23	1:C:19:MET:HG3	1.58	0.85
1:A:248:ILE:H	1:A:262:ASN:HD21	1.22	0.85
1:I:17:VAL:HG23	1:I:19:MET:HG3	1.58	0.85
1:D:285:SER:N	1:J:157:ARG:HH12	1.74	0.85
1:B:16:ASN:HA	1:B:52:ASN:HB2	1.59	0.84
1:N:17:VAL:HG23	1:N:19:MET:HG3	1.59	0.84
1:K:16:ASN:HA	1:K:52:ASN:HB2	1.60	0.84
1:A:73:TYR:CD1	1:A:109:PRO:HA	2.12	0.84
1:I:269:PRO:O	1:I:271:PRO:HD3	1.78	0.84
1:C:228:GLN:NE2	1:E:202:PRO:HG3	1.92	0.83
1:L:248:ILE:H	1:L:262:ASN:HD21	1.26	0.83
1:D:73:TYR:CD1	1:D:109:PRO:HA	2.14	0.83
1:D:284:TYR:HD2	1:J:157:ARG:HH21	0.83	0.82
1:N:9:ASP:OD2	1:N:258:LYS:HE3	1.79	0.81
1:D:285:SER:N	1:J:157:ARG:NH1	2.28	0.81
1:K:227:PRO:O	1:K:234:LYS:HB2	1.80	0.81
1:E:227:PRO:O	1:E:234:LYS:HB2	1.80	0.81
1:K:17:VAL:HG23	1:K:19:MET:HG3	1.61	0.80
1:D:284:TYR:HB2	1:J:157:ARG:CZ	2.11	0.80
1:G:17:VAL:HG23	1:G:19:MET:HG3	1.62	0.80
1:P:248:ILE:H	1:P:262:ASN:HD21	1.29	0.80
1:J:68:LYS:CE	1:O:83:SER:CA	2.50	0.80
1:H:16:ASN:HA	1:H:52:ASN:HB2	1.62	0.80
1:D:285:SER:H	1:J:157:ARG:HH12	1.29	0.80
1:A:16:ASN:HA	1:A:52:ASN:HB2	1.62	0.80
1:B:73:TYR:CD1	1:B:109:PRO:HA	2.17	0.79
1:D:16:ASN:HA	1:D:52:ASN:HB2	1.63	0.79
1:M:16:ASN:HA	1:M:52:ASN:HB2	1.64	0.79
1:C:228:GLN:HE21	1:E:202:PRO:CG	1.95	0.79
1:J:16:ASN:HA	1:J:52:ASN:HB2	1.64	0.79
1:E:16:ASN:HA	1:E:52:ASN:HB2	1.62	0.79
1:D:17:VAL:HG23	1:D:19:MET:HG3	1.64	0.79
1:L:227:PRO:O	1:L:234:LYS:HB2	1.83	0.79
1:G:227:PRO:O	1:G:234:LYS:HB2	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:266:THR:HG22	1:J:279:TYR:CE1	2.19	0.78
1:C:259:GLN:HB3	1:D:286:LYS:CG	2.11	0.78
1:O:16:ASN:HA	1:O:52:ASN:HB2	1.65	0.78
1:D:248:ILE:H	1:D:262:ASN:HD21	1.31	0.78
1:H:73:TYR:CD1	1:H:109:PRO:HA	2.17	0.78
1:P:16:ASN:HA	1:P:52:ASN:HB2	1.66	0.78
1:O:248:ILE:H	1:O:262:ASN:HD21	1.30	0.78
1:D:284:TYR:CD2	1:J:157:ARG:NE	2.53	0.77
1:O:275:PHE:CE1	1:P:269:PRO:HG3	2.18	0.77
1:I:73:TYR:CD1	1:I:109:PRO:HA	2.19	0.77
1:D:239:ASN:ND2	1:D:239:ASN:H	1.81	0.77
1:D:52:ASN:ND2	1:D:194:ASP:H	1.82	0.77
1:M:73:TYR:CD1	1:M:109:PRO:HA	2.19	0.77
1:P:17:VAL:HG23	1:P:19:MET:HG3	1.66	0.77
1:L:16:ASN:HA	1:L:52:ASN:HB2	1.66	0.77
1:F:227:PRO:O	1:F:234:LYS:HB2	1.85	0.77
1:D:284:TYR:CD2	1:J:157:ARG:CZ	2.68	0.77
1:E:33:ARG:HD2	1:F:275:PHE:O	1.84	0.77
1:O:227:PRO:O	1:O:234:LYS:HB2	1.83	0.77
1:F:248:ILE:H	1:F:262:ASN:HD21	1.33	0.77
1:N:16:ASN:HA	1:N:52:ASN:HB2	1.67	0.76
1:E:248:ILE:H	1:E:262:ASN:HD21	1.31	0.76
1:K:272:TRP:HZ2	1:L:29:GLY:N	1.81	0.76
1:E:269:PRO:HD2	1:F:273:ASN:O	1.86	0.76
1:I:16:ASN:HA	1:I:52:ASN:HB2	1.68	0.76
1:A:118:PHE:CD2	1:A:131:GLY:HA2	2.21	0.76
1:F:73:TYR:CD1	1:F:109:PRO:HA	2.22	0.75
1:B:98:GLU:HG3	1:B:99:ASP:H	1.51	0.75
1:G:248:ILE:H	1:G:262:ASN:HD21	1.32	0.75
1:G:16:ASN:HA	1:G:52:ASN:HB2	1.68	0.75
1:K:239:ASN:ND2	1:K:239:ASN:H	1.84	0.75
1:I:269:PRO:HG3	1:J:275:PHE:CE1	2.22	0.75
1:P:227:PRO:O	1:P:234:LYS:HB2	1.87	0.75
1:G:73:TYR:CD1	1:G:109:PRO:HA	2.21	0.74
1:E:239:ASN:H	1:E:239:ASN:ND2	1.85	0.74
1:J:122:CYS:HB2	1:J:166:ILE:HD12	1.70	0.74
1:N:73:TYR:CD1	1:N:109:PRO:HA	2.21	0.74
1:K:52:ASN:ND2	1:K:194:ASP:H	1.85	0.74
1:J:239:ASN:H	1:J:239:ASN:ND2	1.85	0.74
1:O:73:TYR:CD1	1:O:109:PRO:HA	2.22	0.74
1:B:239:ASN:H	1:B:239:ASN:ND2	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:VAL:HG23	1:E:19:MET:HG3	1.70	0.74
1:A:118:PHE:CE2	1:A:131:GLY:HA2	2.22	0.74
1:D:227:PRO:O	1:D:234:LYS:HB2	1.87	0.74
1:H:52:ASN:ND2	1:H:194:ASP:H	1.86	0.74
1:F:17:VAL:HG23	1:F:19:MET:HG3	1.68	0.74
1:B:227:PRO:O	1:B:234:LYS:HB2	1.87	0.74
1:O:17:VAL:HG23	1:O:19:MET:HG3	1.69	0.74
1:D:286:LYS:HB3	1:J:124:PHE:CE1	2.23	0.74
1:O:52:ASN:ND2	1:O:194:ASP:H	1.86	0.74
1:C:227:PRO:O	1:C:234:LYS:HB2	1.88	0.74
1:F:16:ASN:HA	1:F:52:ASN:HB2	1.68	0.73
1:L:52:ASN:ND2	1:L:194:ASP:H	1.86	0.73
1:L:17:VAL:HG23	1:L:19:MET:HG3	1.70	0.73
1:C:280:PRO:HG3	1:D:15:HIS:CE1	2.22	0.73
1:K:73:TYR:CD1	1:K:109:PRO:HA	2.23	0.73
1:L:73:TYR:CD1	1:L:109:PRO:HA	2.23	0.73
1:J:8:THR:HG21	1:J:255:LYS:NZ	2.03	0.73
1:B:167:ARG:O	1:B:171:MET:HG3	1.88	0.73
1:M:17:VAL:HG23	1:M:19:MET:HG3	1.70	0.73
1:F:239:ASN:H	1:F:239:ASN:ND2	1.87	0.73
1:P:73:TYR:CD1	1:P:109:PRO:HA	2.23	0.73
1:A:261:VAL:O	1:B:283:ALA:HA	1.89	0.73
1:J:68:LYS:HZ1	1:O:83:SER:CA	2.01	0.73
1:H:248:ILE:H	1:H:262:ASN:HD21	1.32	0.72
1:G:52:ASN:ND2	1:G:194:ASP:H	1.88	0.72
1:G:239:ASN:ND2	1:G:239:ASN:H	1.86	0.72
1:D:285:SER:N	1:J:157:ARG:CZ	2.52	0.72
1:O:111:LYS:HD2	1:O:138:GLU:OE1	1.89	0.72
1:B:52:ASN:ND2	1:B:194:ASP:H	1.86	0.72
1:M:227:PRO:O	1:M:234:LYS:HB2	1.89	0.72
1:C:228:GLN:NE2	1:E:202:PRO:CG	2.51	0.72
1:E:52:ASN:ND2	1:E:194:ASP:H	1.88	0.72
1:B:98:GLU:HG3	1:B:99:ASP:N	2.04	0.72
1:D:118:PHE:CD2	1:D:131:GLY:HA2	2.24	0.72
1:C:16:ASN:HA	1:C:52:ASN:HB2	1.71	0.72
1:A:8:THR:HG21	1:A:255:LYS:NZ	2.05	0.71
1:B:8:THR:HG21	1:B:255:LYS:NZ	2.05	0.71
1:B:111:LYS:HE2	1:B:138:GLU:OE1	1.89	0.71
1:C:241:LYS:HE2	1:E:201:THR:HG22	1.71	0.71
1:N:248:ILE:H	1:N:262:ASN:HD21	1.36	0.71
1:C:111:LYS:HD2	1:C:138:GLU:OE1	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:73:TYR:CD1	1:J:109:PRO:HA	2.25	0.71
1:P:269:PRO:O	1:P:271:PRO:HD3	1.91	0.71
1:J:68:LYS:NZ	1:O:83:SER:CA	2.52	0.71
1:G:122:CYS:HB2	1:G:166:ILE:HD12	1.72	0.71
1:N:239:ASN:ND2	1:N:239:ASN:H	1.88	0.71
1:B:69:LYS:HD3	1:C:93:SER:HB2	1.71	0.70
1:E:73:TYR:CD1	1:E:109:PRO:HA	2.26	0.70
1:J:269:PRO:O	1:J:271:PRO:N	2.23	0.70
1:F:8:THR:HG21	1:F:255:LYS:NZ	2.06	0.70
1:I:8:THR:HG21	1:I:255:LYS:NZ	2.06	0.70
1:P:239:ASN:H	1:P:239:ASN:ND2	1.89	0.70
1:C:275:PHE:CE2	1:D:267:GLU:HG2	2.26	0.70
1:G:283:ALA:HA	1:H:261:VAL:O	1.92	0.70
1:C:8:THR:HG21	1:C:255:LYS:NZ	2.06	0.70
1:C:275:PHE:HE2	1:D:267:GLU:HG2	1.56	0.70
1:B:122:CYS:HB2	1:B:166:ILE:HD12	1.73	0.70
1:J:227:PRO:O	1:J:234:LYS:HB2	1.91	0.70
1:O:275:PHE:O	1:P:33:ARG:HD2	1.92	0.70
1:C:118:PHE:CD2	1:C:131:GLY:HA2	2.26	0.69
1:D:98:GLU:HG3	1:D:99:ASP:H	1.54	0.69
1:D:285:SER:H	1:J:157:ARG:NH1	1.89	0.69
1:N:8:THR:HG21	1:N:255:LYS:NZ	2.07	0.69
1:K:239:ASN:HD22	1:K:239:ASN:H	1.40	0.69
1:E:122:CYS:HB2	1:E:166:ILE:HD12	1.75	0.69
1:F:111:LYS:HD2	1:F:138:GLU:OE1	1.93	0.69
1:A:122:CYS:HB2	1:A:166:ILE:HD12	1.74	0.69
1:J:52:ASN:ND2	1:J:194:ASP:H	1.90	0.69
1:N:52:ASN:ND2	1:N:194:ASP:H	1.91	0.69
1:O:269:PRO:O	1:O:271:PRO:HD3	1.93	0.69
1:H:122:CYS:HB2	1:H:166:ILE:HD12	1.75	0.68
1:B:248:ILE:H	1:B:262:ASN:HD21	1.40	0.68
1:H:8:THR:HG21	1:H:255:LYS:NZ	2.08	0.68
1:E:118:PHE:CD2	1:E:131:GLY:HA2	2.28	0.68
1:I:272:TRP:CE3	1:I:272:TRP:HA	2.28	0.68
1:N:122:CYS:HB2	1:N:166:ILE:HD12	1.74	0.68
1:N:227:PRO:O	1:N:234:LYS:HB2	1.94	0.68
1:O:32:LYS:HD2	1:P:272:TRP:CZ3	2.29	0.68
1:K:122:CYS:HB2	1:K:166:ILE:HD12	1.74	0.68
1:D:239:ASN:H	1:D:239:ASN:HD22	1.39	0.68
1:D:118:PHE:CE2	1:D:131:GLY:HA2	2.28	0.68
1:O:8:THR:HG21	1:O:255:LYS:NZ	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:98:GLU:HG3	1:K:99:ASP:H	1.58	0.68
1:O:284:TYR:O	1:P:260:LEU:HD12	1.93	0.68
1:P:52:ASN:ND2	1:P:194:ASP:H	1.92	0.68
1:L:8:THR:HG21	1:L:255:LYS:NZ	2.09	0.68
1:A:239:ASN:H	1:A:239:ASN:ND2	1.92	0.68
1:M:122:CYS:HB2	1:M:166:ILE:HD12	1.74	0.68
1:M:8:THR:HG21	1:M:255:LYS:NZ	2.09	0.67
1:B:241:LYS:CD	1:K:228:GLN:NE2	2.55	0.67
1:L:121:GLY:HA3	1:L:126:ASN:HB2	1.74	0.67
1:C:121:GLY:HA3	1:C:126:ASN:HB2	1.76	0.67
1:D:8:THR:HG21	1:D:255:LYS:NZ	2.08	0.67
1:C:52:ASN:ND2	1:C:194:ASP:H	1.92	0.67
1:B:218:TYR:HB2	1:K:218:TYR:HB2	1.75	0.67
1:D:286:LYS:CG	1:J:124:PHE:CE1	2.78	0.67
1:C:28:TRP:HB2	1:C:30:GLN:OE1	1.93	0.67
1:H:239:ASN:H	1:H:239:ASN:ND2	1.93	0.67
1:O:267:GLU:O	1:P:275:PHE:HE2	1.76	0.67
1:L:122:CYS:HB2	1:L:166:ILE:HD12	1.77	0.67
1:H:227:PRO:O	1:H:234:LYS:HB2	1.95	0.67
1:M:275:PHE:O	1:N:33:ARG:HD2	1.95	0.67
1:C:118:PHE:CE2	1:C:131:GLY:HA2	2.30	0.67
1:I:121:GLY:HA3	1:I:126:ASN:HB2	1.76	0.67
1:B:69:LYS:CD	1:C:93:SER:CB	2.66	0.66
1:M:52:ASN:ND2	1:M:194:ASP:H	1.94	0.66
1:D:285:SER:CA	1:J:157:ARG:NH2	2.57	0.66
1:A:52:ASN:ND2	1:A:194:ASP:H	1.92	0.66
1:D:98:GLU:HG3	1:D:99:ASP:N	2.10	0.66
1:I:239:ASN:H	1:I:239:ASN:ND2	1.93	0.66
1:P:122:CYS:HB2	1:P:166:ILE:HD12	1.78	0.66
1:O:122:CYS:HB2	1:O:166:ILE:HD12	1.77	0.66
1:O:239:ASN:H	1:O:239:ASN:ND2	1.94	0.66
1:A:227:PRO:O	1:A:234:LYS:HB2	1.95	0.66
1:C:261:VAL:O	1:D:283:ALA:HA	1.95	0.66
1:M:239:ASN:ND2	1:M:239:ASN:H	1.93	0.66
1:I:227:PRO:O	1:I:234:LYS:HB2	1.96	0.66
1:D:122:CYS:HB2	1:D:166:ILE:HD12	1.78	0.66
1:E:239:ASN:HD22	1:E:239:ASN:H	1.43	0.65
1:B:200:GLY:O	1:K:221:HIS:CE1	2.49	0.65
1:L:239:ASN:H	1:L:239:ASN:ND2	1.93	0.65
1:E:198:ASN:O	1:E:201:THR:HG23	1.95	0.65
1:J:239:ASN:H	1:J:239:ASN:HD22	1.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:118:PHE:CD2	1:H:131:GLY:HA2	2.32	0.65
1:J:121:GLY:HA3	1:J:126:ASN:HB2	1.78	0.65
1:I:52:ASN:ND2	1:I:194:ASP:H	1.95	0.65
1:B:239:ASN:H	1:B:239:ASN:HD22	1.43	0.65
1:E:8:THR:HG21	1:E:255:LYS:NZ	2.12	0.65
1:C:122:CYS:HB2	1:C:166:ILE:HD12	1.78	0.65
1:J:98:GLU:HG3	1:J:99:ASP:H	1.61	0.65
1:E:275:PHE:CZ	1:F:269:PRO:HG3	2.31	0.65
1:B:36:LEU:HD22	1:B:269:PRO:HB3	1.79	0.65
1:B:118:PHE:CD2	1:B:131:GLY:HA2	2.33	0.64
1:P:8:THR:HG21	1:P:255:LYS:NZ	2.11	0.64
1:M:118:PHE:CD2	1:M:131:GLY:HA2	2.32	0.64
1:F:239:ASN:H	1:F:239:ASN:HD22	1.45	0.64
1:H:121:GLY:HA3	1:H:126:ASN:HB2	1.79	0.64
1:C:239:ASN:ND2	1:C:239:ASN:H	1.95	0.64
1:M:121:GLY:HA3	1:M:126:ASN:HB2	1.79	0.64
1:J:68:LYS:NZ	1:O:83:SER:HB3	2.12	0.64
1:P:118:PHE:CD2	1:P:131:GLY:HA2	2.31	0.64
1:L:118:PHE:CD2	1:L:131:GLY:HA2	2.31	0.64
1:I:118:PHE:CD2	1:I:131:GLY:HA2	2.32	0.64
1:G:15:HIS:CE1	1:H:280:PRO:HG3	2.33	0.64
1:G:239:ASN:H	1:G:239:ASN:HD22	1.45	0.64
1:B:140:ASN:HA	1:C:165:LYS:HZ3	1.63	0.64
1:A:121:GLY:HA3	1:A:126:ASN:HB2	1.80	0.64
1:K:248:ILE:H	1:K:262:ASN:HD21	1.43	0.64
1:L:163:ASP:OD1	1:L:163:ASP:N	2.30	0.64
1:K:272:TRP:CZ2	1:L:28:TRP:CA	2.65	0.64
1:E:118:PHE:CE2	1:E:131:GLY:HA2	2.33	0.64
1:K:8:THR:HG21	1:K:255:LYS:NZ	2.13	0.64
1:E:167:ARG:O	1:E:171:MET:HG3	1.98	0.64
1:J:111:LYS:HD2	1:J:138:GLU:OE1	1.98	0.64
1:G:8:THR:HG21	1:G:255:LYS:NZ	2.13	0.63
1:F:122:CYS:HB2	1:F:166:ILE:HD12	1.80	0.63
1:I:122:CYS:HB2	1:I:166:ILE:HD12	1.80	0.63
1:D:286:LYS:CG	1:J:124:PHE:HE1	2.11	0.63
1:C:98:GLU:HG3	1:C:99:ASP:H	1.62	0.63
1:N:111:LYS:HD2	1:N:138:GLU:OE1	1.98	0.63
1:J:124:PHE:CD2	1:J:157:ARG:HG3	2.34	0.63
1:O:269:PRO:HG3	1:P:275:PHE:CE1	2.32	0.63
1:K:118:PHE:CD2	1:K:131:GLY:HA2	2.34	0.63
1:P:239:ASN:HD22	1:P:239:ASN:H	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ASP:OD1	1:B:278:HIS:HD2	1.82	0.63
1:K:15:HIS:CE1	1:L:280:PRO:HG3	2.33	0.63
1:B:228:GLN:NE2	1:K:241:LYS:CD	2.60	0.63
1:J:68:LYS:HZ1	1:O:84:GLY:N	1.96	0.62
1:C:160:ALA:HB2	1:E:239:ASN:HB3	1.81	0.62
1:L:118:PHE:CE2	1:L:131:GLY:HA2	2.34	0.62
1:N:98:GLU:HG3	1:N:99:ASP:H	1.64	0.62
1:B:163:ASP:OD1	1:B:163:ASP:N	2.31	0.62
1:G:163:ASP:OD1	1:G:163:ASP:N	2.30	0.62
1:F:124:PHE:CD2	1:F:157:ARG:HG3	2.34	0.62
1:N:239:ASN:HD22	1:N:239:ASN:H	1.45	0.62
1:J:68:LYS:NZ	1:O:84:GLY:H	1.98	0.62
1:O:118:PHE:CD2	1:O:131:GLY:HA2	2.35	0.62
1:A:269:PRO:HG3	1:B:275:PHE:CE1	2.34	0.62
1:P:124:PHE:CD2	1:P:157:ARG:HG3	2.35	0.62
1:A:124:PHE:CD2	1:A:157:ARG:HG3	2.35	0.62
1:B:200:GLY:HA3	1:K:221:HIS:CE1	2.34	0.62
1:F:116:HIS:HE1	1:F:173:GLU:OE1	1.83	0.62
1:F:52:ASN:ND2	1:F:194:ASP:H	1.97	0.62
1:P:121:GLY:HA3	1:P:126:ASN:HB2	1.81	0.62
1:G:275:PHE:CE1	1:H:269:PRO:HG3	2.34	0.62
1:A:280:PRO:HG3	1:B:15:HIS:CE1	2.34	0.62
1:N:124:PHE:CD2	1:N:157:ARG:HG3	2.34	0.62
1:A:98:GLU:HG3	1:A:99:ASP:H	1.64	0.62
1:O:121:GLY:HA3	1:O:126:ASN:HB2	1.80	0.62
1:E:278:HIS:HD2	1:F:246:ASP:OD1	1.83	0.62
1:D:286:LYS:HG2	1:J:124:PHE:CE1	2.36	0.61
1:I:272:TRP:HE3	1:I:272:TRP:HA	1.63	0.61
1:M:118:PHE:CE2	1:M:131:GLY:HA2	2.35	0.61
1:N:118:PHE:CD2	1:N:131:GLY:HA2	2.34	0.61
1:L:98:GLU:HG3	1:L:99:ASP:H	1.64	0.61
1:I:269:PRO:HD3	1:J:275:PHE:CE2	2.35	0.61
1:J:98:GLU:HG3	1:J:99:ASP:N	2.16	0.61
1:O:214:ASN:HD21	1:O:252:LYS:HE3	1.66	0.61
1:G:124:PHE:CD2	1:G:157:ARG:HG3	2.36	0.61
1:G:28:TRP:HB2	1:G:30:GLN:OE1	2.01	0.61
1:O:266:THR:HG22	1:P:279:TYR:CE1	2.36	0.61
1:I:28:TRP:HB2	1:I:30:GLN:OE1	2.01	0.61
1:K:98:GLU:HG3	1:K:99:ASP:N	2.16	0.61
1:L:116:HIS:HE1	1:L:173:GLU:OE1	1.84	0.61
1:E:15:HIS:CE1	1:F:280:PRO:HG3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:98:GLU:HG3	1:L:99:ASP:N	2.16	0.60
1:I:124:PHE:CD2	1:I:157:ARG:HG3	2.36	0.60
1:L:227:PRO:HA	1:L:233:ALA:HB3	1.82	0.60
1:H:239:ASN:H	1:H:239:ASN:HD22	1.50	0.60
1:J:116:HIS:HE1	1:J:173:GLU:OE1	1.84	0.60
1:M:269:PRO:HG3	1:N:275:PHE:CE1	2.37	0.60
1:E:98:GLU:HG3	1:E:99:ASP:N	2.17	0.60
1:O:280:PRO:HG3	1:P:15:HIS:CE1	2.37	0.60
1:A:28:TRP:HB2	1:A:30:GLN:OE1	2.02	0.60
1:C:167:ARG:O	1:C:171:MET:HG3	2.01	0.60
1:D:163:ASP:OD1	1:D:163:ASP:N	2.33	0.60
1:C:241:LYS:NZ	1:E:198:ASN:ND2	2.50	0.60
1:K:267:GLU:HG2	1:K:268:LYS:N	2.15	0.60
1:A:98:GLU:HG3	1:A:99:ASP:N	2.16	0.60
1:G:98:GLU:HG3	1:G:99:ASP:H	1.67	0.60
1:B:200:GLY:O	1:K:221:HIS:HE1	1.84	0.60
1:G:98:GLU:HG3	1:G:99:ASP:N	2.17	0.60
1:K:281:ILE:O	1:L:13:VAL:HA	2.02	0.60
1:C:124:PHE:CD2	1:C:157:ARG:HG3	2.37	0.60
1:N:98:GLU:HG3	1:N:99:ASP:N	2.16	0.60
1:N:121:GLY:HA3	1:N:126:ASN:HB2	1.83	0.60
1:D:124:PHE:CD2	1:D:157:ARG:HG3	2.37	0.60
1:P:98:GLU:HG3	1:P:99:ASP:H	1.67	0.60
1:J:28:TRP:HB2	1:J:30:GLN:OE1	2.02	0.60
1:J:118:PHE:CD2	1:J:131:GLY:HA2	2.37	0.59
1:A:239:ASN:H	1:A:239:ASN:HD22	1.49	0.59
1:M:239:ASN:H	1:M:239:ASN:HD22	1.51	0.59
1:I:269:PRO:HD3	1:J:275:PHE:CZ	2.37	0.59
1:M:167:ARG:O	1:M:171:MET:HG3	2.03	0.59
1:D:36:LEU:HD22	1:D:269:PRO:HB3	1.84	0.59
1:C:98:GLU:HG3	1:C:99:ASP:N	2.18	0.59
1:C:228:GLN:CG	1:E:202:PRO:HG3	2.32	0.59
1:K:275:PHE:O	1:L:33:ARG:HD2	2.02	0.59
1:D:286:LYS:CB	1:J:124:PHE:CE1	2.86	0.59
1:I:266:THR:HG22	1:J:279:TYR:CD1	2.36	0.59
1:K:116:HIS:HE1	1:K:173:GLU:OE1	1.85	0.59
1:D:111:LYS:HD2	1:D:138:GLU:OE1	2.02	0.59
1:G:116:HIS:HE1	1:G:173:GLU:OE1	1.84	0.59
1:P:118:PHE:CE2	1:P:131:GLY:HA2	2.37	0.59
1:C:269:PRO:HG3	1:D:275:PHE:CE1	2.38	0.59
1:D:285:SER:CA	1:J:157:ARG:HH12	2.15	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:33:ARG:HD2	1:J:275:PHE:O	2.03	0.58
1:H:124:PHE:CD2	1:H:157:ARG:HG3	2.37	0.58
1:B:124:PHE:CD2	1:B:157:ARG:HG3	2.38	0.58
1:B:217:LEU:HB3	1:K:217:LEU:HB3	1.84	0.58
1:K:118:PHE:CE2	1:K:131:GLY:HA2	2.39	0.58
1:F:98:GLU:HG3	1:F:99:ASP:H	1.69	0.58
1:P:167:ARG:O	1:P:171:MET:HG3	2.04	0.58
1:O:118:PHE:CE2	1:O:131:GLY:HA2	2.39	0.58
1:C:116:HIS:HE1	1:C:173:GLU:OE1	1.85	0.58
1:J:272:TRP:O	1:J:273:ASN:HB2	2.03	0.58
1:K:121:GLY:HA3	1:K:126:ASN:HB2	1.85	0.58
1:I:118:PHE:CE2	1:I:131:GLY:HA2	2.38	0.58
1:O:167:ARG:O	1:O:171:MET:HG3	2.03	0.58
1:F:118:PHE:CD2	1:F:131:GLY:HA2	2.39	0.58
1:J:68:LYS:HE2	1:O:82:GLN:O	2.04	0.58
1:H:118:PHE:CE2	1:H:131:GLY:HA2	2.38	0.58
1:D:198:ASN:O	1:D:201:THR:HG23	2.04	0.58
1:I:239:ASN:H	1:I:239:ASN:HD22	1.50	0.58
1:C:33:ARG:HD2	1:D:275:PHE:O	2.03	0.58
1:P:98:GLU:HG3	1:P:99:ASP:N	2.19	0.58
1:C:277:ASP:HB3	1:D:232:ILE:HG22	1.85	0.58
1:F:121:GLY:HA3	1:F:126:ASN:HB2	1.85	0.58
1:N:116:HIS:HE1	1:N:173:GLU:OE1	1.86	0.58
1:B:116:HIS:HE1	1:B:173:GLU:OE1	1.87	0.58
1:O:124:PHE:CD2	1:O:157:ARG:HG3	2.39	0.57
1:E:98:GLU:HG3	1:E:99:ASP:H	1.68	0.57
1:M:116:HIS:HE1	1:M:173:GLU:OE1	1.87	0.57
1:J:68:LYS:HZ1	1:O:84:GLY:H	1.52	0.57
1:F:98:GLU:HG3	1:F:99:ASP:N	2.19	0.57
1:D:284:TYR:CB	1:J:157:ARG:CZ	2.82	0.57
1:M:124:PHE:CD2	1:M:157:ARG:HG3	2.39	0.57
1:I:167:ARG:O	1:I:171:MET:HG3	2.04	0.57
1:H:56:ASP:O	1:H:60:SER:HB2	2.04	0.57
1:P:116:HIS:HE1	1:P:173:GLU:OE1	1.87	0.57
1:D:28:TRP:HB2	1:D:30:GLN:OE1	2.05	0.57
1:K:124:PHE:CD2	1:K:157:ARG:HG3	2.39	0.57
1:I:266:THR:HG22	1:J:279:TYR:CZ	2.39	0.57
1:K:124:PHE:HB2	1:K:155:ASP:OD2	2.04	0.57
1:M:39:GLN:OE1	1:N:32:LYS:HE2	2.05	0.57
1:L:36:LEU:HD22	1:L:269:PRO:CB	2.34	0.57
1:N:167:ARG:O	1:N:171:MET:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:269:PRO:HD2	1:H:273:ASN:O	2.04	0.57
1:B:140:ASN:HA	1:C:165:LYS:NZ	2.19	0.56
1:L:28:TRP:HB2	1:L:30:GLN:OE1	2.05	0.56
1:G:121:GLY:HA3	1:G:126:ASN:HB2	1.85	0.56
1:I:32:LYS:HD2	1:J:270:LYS:HD2	1.87	0.56
1:O:239:ASN:H	1:O:239:ASN:HD22	1.52	0.56
1:L:239:ASN:HD22	1:L:239:ASN:H	1.50	0.56
1:C:265:VAL:O	1:D:280:PRO:HD2	2.06	0.56
1:J:167:ARG:O	1:J:171:MET:HG3	2.04	0.56
1:B:228:GLN:HE22	1:K:241:LYS:CD	2.03	0.56
1:C:8:THR:HG21	1:C:255:LYS:HZ1	1.69	0.56
1:O:98:GLU:HG3	1:O:99:ASP:H	1.70	0.56
1:O:246:ASP:OD1	1:P:278:HIS:HD2	1.88	0.56
1:E:28:TRP:HB2	1:E:30:GLN:OE1	2.05	0.56
1:G:118:PHE:CD2	1:G:131:GLY:HA2	2.40	0.56
1:N:118:PHE:CE2	1:N:131:GLY:HA2	2.40	0.56
1:I:98:GLU:HG3	1:I:99:ASP:N	2.21	0.56
1:C:248:ILE:N	1:C:262:ASN:HD21	1.95	0.56
1:L:227:PRO:HA	1:L:233:ALA:CB	2.35	0.56
1:C:239:ASN:HD22	1:C:239:ASN:H	1.52	0.56
1:L:36:LEU:HD22	1:L:269:PRO:HB3	1.86	0.56
1:O:98:GLU:HG3	1:O:99:ASP:N	2.21	0.56
1:M:159:GLY:HA3	1:M:162:HIS:CE1	2.41	0.56
1:L:124:PHE:CD2	1:L:157:ARG:HG3	2.41	0.56
1:K:272:TRP:HH2	1:L:28:TRP:HA	0.58	0.56
1:D:56:ASP:O	1:D:60:SER:HB2	2.06	0.56
1:G:280:PRO:HD2	1:H:265:VAL:O	2.06	0.56
1:E:124:PHE:CD2	1:E:157:ARG:HG3	2.41	0.56
1:O:261:VAL:O	1:P:283:ALA:HA	2.05	0.56
1:D:286:LYS:HG2	1:J:124:PHE:HE1	1.69	0.56
1:D:73:TYR:N	1:D:73:TYR:CD2	2.73	0.56
1:M:33:ARG:HD2	1:N:275:PHE:O	2.05	0.56
1:I:275:PHE:O	1:J:33:ARG:HD2	2.06	0.55
1:B:200:GLY:HA3	1:K:221:HIS:ND1	2.20	0.55
1:K:35:ASP:OD1	1:K:62:LYS:HE3	2.06	0.55
1:K:227:PRO:HA	1:K:233:ALA:CB	2.36	0.55
1:F:167:ARG:O	1:F:171:MET:HG3	2.05	0.55
1:K:227:PRO:HA	1:K:233:ALA:HB3	1.87	0.55
1:O:283:ALA:HB3	1:P:248:ILE:HD12	1.87	0.55
1:L:167:ARG:O	1:L:171:MET:HG3	2.06	0.55
1:K:167:ARG:O	1:K:171:MET:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:98:GLU:HG3	1:M:99:ASP:H	1.72	0.55
1:C:56:ASP:O	1:C:60:SER:HB2	2.06	0.55
1:I:278:HIS:HD2	1:J:246:ASP:OD1	1.88	0.55
1:D:285:SER:C	1:J:157:ARG:NH1	2.60	0.55
1:I:89:GLU:O	1:I:116:HIS:HA	2.06	0.55
1:C:259:GLN:CG	1:D:286:LYS:HG3	2.37	0.55
1:M:98:GLU:HG3	1:M:99:ASP:N	2.22	0.55
1:F:28:TRP:HB2	1:F:30:GLN:OE1	2.06	0.55
1:D:285:SER:O	1:J:157:ARG:NH1	2.39	0.55
1:K:28:TRP:HB2	1:K:30:GLN:OE1	2.06	0.55
1:M:261:VAL:O	1:N:283:ALA:HA	2.06	0.55
1:C:145:HIS:HB2	1:C:189:VAL:HG22	1.89	0.55
1:H:167:ARG:O	1:H:171:MET:HG3	2.07	0.55
1:H:28:TRP:HB2	1:H:30:GLN:OE1	2.07	0.55
1:P:36:LEU:HD22	1:P:269:PRO:HB3	1.88	0.55
1:O:283:ALA:CB	1:P:248:ILE:HD12	2.37	0.55
1:D:116:HIS:HE1	1:D:173:GLU:OE1	1.90	0.55
1:G:270:LYS:HG3	1:H:32:LYS:NZ	2.22	0.55
1:J:221:HIS:HD2	1:J:223:SER:H	1.54	0.55
1:O:272:TRP:CH2	1:P:28:TRP:HA	2.41	0.55
1:D:286:LYS:HB3	1:J:124:PHE:HD1	1.62	0.54
1:D:124:PHE:HB2	1:D:155:ASP:OD2	2.07	0.54
1:O:116:HIS:HE1	1:O:173:GLU:OE1	1.90	0.54
1:K:13:VAL:HA	1:L:281:ILE:O	2.07	0.54
1:B:241:LYS:CD	1:K:228:GLN:HE22	2.07	0.54
1:B:108:TYR:CE1	1:C:162:HIS:CE1	2.96	0.54
1:B:218:TYR:N	1:K:218:TYR:O	2.37	0.54
1:D:92:TYR:HA	1:D:117:VAL:HG21	1.89	0.54
1:I:280:PRO:HD2	1:J:265:VAL:O	2.07	0.54
1:K:221:HIS:HD2	1:K:223:SER:H	1.55	0.54
1:D:167:ARG:O	1:D:171:MET:HG3	2.08	0.54
1:H:98:GLU:HG3	1:H:99:ASP:N	2.23	0.54
1:M:28:TRP:HB2	1:M:30:GLN:OE1	2.07	0.54
1:L:56:ASP:O	1:L:60:SER:HB2	2.08	0.54
1:M:32:LYS:CE	1:N:39:GLN:OE1	2.48	0.54
1:E:283:ALA:HA	1:F:261:VAL:O	2.08	0.54
1:D:286:LYS:CD	1:J:124:PHE:HE1	2.21	0.54
1:P:28:TRP:HB2	1:P:30:GLN:OE1	2.08	0.54
1:J:68:LYS:NZ	1:O:83:SER:CB	2.71	0.54
1:E:121:GLY:HA3	1:E:126:ASN:HB2	1.89	0.54
1:J:56:ASP:O	1:J:60:SER:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:LYS:HE2	1:J:124:PHE:HE1	1.73	0.53
1:A:92:TYR:HA	1:A:117:VAL:HG21	1.89	0.53
1:L:269:PRO:O	1:L:271:PRO:HD3	2.07	0.53
1:N:40:SER:HB2	1:N:267:GLU:OE2	2.08	0.53
1:J:273:ASN:O	1:J:274:ASP:OD1	2.26	0.53
1:I:188:THR:HG23	1:I:255:LYS:O	2.08	0.53
1:M:56:ASP:O	1:M:60:SER:HB2	2.08	0.53
1:G:56:ASP:O	1:G:60:SER:HB2	2.08	0.53
1:J:68:LYS:HZ1	1:O:83:SER:CB	2.21	0.53
1:I:272:TRP:HD1	1:J:33:ARG:HG3	1.74	0.53
1:D:16:ASN:OD1	1:D:53:GLU:HB2	2.08	0.53
1:A:56:ASP:O	1:A:60:SER:HB2	2.08	0.53
1:J:36:LEU:HD22	1:J:269:PRO:HB3	1.90	0.53
1:J:89:GLU:O	1:J:116:HIS:HA	2.09	0.53
1:I:56:ASP:O	1:I:60:SER:HB2	2.09	0.53
1:H:116:HIS:HE1	1:H:173:GLU:OE1	1.92	0.53
1:D:227:PRO:O	1:D:234:LYS:CB	2.56	0.53
1:G:239:ASN:ND2	1:G:239:ASN:N	2.52	0.53
1:E:227:PRO:HA	1:E:233:ALA:HB3	1.91	0.53
1:B:227:PRO:HA	1:B:233:ALA:HB3	1.90	0.53
1:A:24:LEU:HD12	1:A:24:LEU:N	2.23	0.53
1:B:73:TYR:CE1	1:B:109:PRO:HA	2.44	0.53
1:K:266:THR:HG22	1:L:279:TYR:CE1	2.43	0.53
1:A:167:ARG:O	1:A:171:MET:HG3	2.09	0.53
1:F:221:HIS:HB2	1:F:266:THR:HG23	1.91	0.53
1:G:198:ASN:O	1:G:201:THR:HG23	2.09	0.53
1:K:273:ASN:O	1:K:274:ASP:CG	2.47	0.53
1:D:52:ASN:HD21	1:D:194:ASP:H	1.55	0.53
1:B:22:THR:HG23	1:B:56:ASP:CG	2.29	0.53
1:E:162:HIS:O	1:E:163:ASP:C	2.47	0.53
1:C:286:LYS:HB3	1:D:259:GLN:HB3	1.90	0.52
1:B:124:PHE:HB2	1:B:155:ASP:OD2	2.10	0.52
1:C:89:GLU:O	1:C:116:HIS:HA	2.09	0.52
1:H:162:HIS:O	1:H:163:ASP:C	2.48	0.52
1:M:286:LYS:OXT	1:M:286:LYS:HG2	2.08	0.52
1:I:248:ILE:N	1:I:262:ASN:HD21	2.02	0.52
1:I:116:HIS:HE1	1:I:173:GLU:OE1	1.91	0.52
1:A:248:ILE:H	1:A:262:ASN:ND2	2.00	0.52
1:A:246:ASP:OD1	1:B:278:HIS:CD2	2.62	0.52
1:J:118:PHE:CE2	1:J:131:GLY:HA2	2.44	0.52
1:A:199:LYS:HE3	1:A:218:TYR:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:LYS:CE	1:K:222:ASN:HB3	2.40	0.52
1:J:8:THR:HG21	1:J:255:LYS:HZ1	1.75	0.52
1:G:86:ASP:HB2	1:G:113:LYS:O	2.10	0.52
1:D:285:SER:C	1:J:157:ARG:NH2	2.64	0.52
1:K:266:THR:HG22	1:L:279:TYR:CZ	2.45	0.52
1:C:214:ASN:HD21	1:C:252:LYS:HE3	1.74	0.52
1:B:69:LYS:HD3	1:C:93:SER:CB	2.36	0.52
1:C:228:GLN:HE21	1:E:202:PRO:CD	2.22	0.52
1:B:227:PRO:HA	1:B:233:ALA:CB	2.40	0.52
1:E:73:TYR:CD2	1:E:73:TYR:N	2.78	0.52
1:E:56:ASP:O	1:E:60:SER:HB2	2.09	0.52
1:N:56:ASP:O	1:N:60:SER:HB2	2.09	0.52
1:G:13:VAL:HB	1:G:49:VAL:HG22	1.90	0.52
1:F:56:ASP:O	1:F:60:SER:HB2	2.10	0.52
1:B:198:ASN:O	1:B:201:THR:HG23	2.10	0.52
1:C:228:GLN:NE2	1:E:202:PRO:CA	2.73	0.52
1:P:227:PRO:O	1:P:234:LYS:CB	2.58	0.52
1:B:227:PRO:O	1:B:234:LYS:CB	2.56	0.52
1:O:281:ILE:HG12	1:P:246:ASP:HB2	1.92	0.52
1:C:226:ASP:OD1	1:C:226:ASP:C	2.47	0.52
1:I:275:PHE:CE1	1:J:269:PRO:HG3	2.46	0.51
1:B:56:ASP:O	1:B:60:SER:HB2	2.10	0.51
1:M:227:PRO:O	1:M:234:LYS:CB	2.57	0.51
1:C:241:LYS:HZ1	1:E:198:ASN:ND2	2.08	0.51
1:C:162:HIS:O	1:C:163:ASP:C	2.48	0.51
1:F:239:ASN:HD22	1:F:239:ASN:N	2.06	0.51
1:N:162:HIS:O	1:N:163:ASP:C	2.48	0.51
1:K:89:GLU:O	1:K:116:HIS:HA	2.10	0.51
1:I:272:TRP:HE1	1:J:29:GLY:HA3	1.74	0.51
1:D:22:THR:HG23	1:D:56:ASP:CG	2.31	0.51
1:H:89:GLU:O	1:H:116:HIS:HA	2.11	0.51
1:C:198:ASN:O	1:C:201:THR:HG23	2.10	0.51
1:N:28:TRP:HB2	1:N:30:GLN:OE1	2.11	0.51
1:O:28:TRP:HB2	1:O:30:GLN:OE1	2.10	0.51
1:G:227:PRO:O	1:G:234:LYS:CB	2.56	0.51
1:G:167:ARG:O	1:G:171:MET:HG3	2.11	0.51
1:A:269:PRO:HG3	1:B:275:PHE:CZ	2.46	0.51
1:N:89:GLU:O	1:N:116:HIS:HA	2.10	0.51
1:G:270:LYS:HG3	1:H:32:LYS:HZ2	1.75	0.51
1:D:239:ASN:N	1:D:239:ASN:ND2	2.47	0.51
1:B:80:ARG:HD3	1:B:99:ASP:OD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:41:SER:HB2	1:O:267:GLU:OE1	2.11	0.51
1:E:278:HIS:CD2	1:F:246:ASP:OD1	2.62	0.51
1:I:98:GLU:HG3	1:I:99:ASP:H	1.75	0.51
1:M:162:HIS:O	1:M:163:ASP:C	2.48	0.51
1:P:56:ASP:O	1:P:60:SER:HB2	2.11	0.51
1:F:239:ASN:N	1:F:239:ASN:ND2	2.52	0.51
1:F:162:HIS:O	1:F:163:ASP:C	2.48	0.51
1:K:108:TYR:CD2	1:K:108:TYR:N	2.79	0.51
1:O:281:ILE:HG12	1:P:246:ASP:CB	2.41	0.51
1:B:13:VAL:HB	1:B:49:VAL:HG22	1.93	0.51
1:C:241:LYS:HE2	1:E:201:THR:CG2	2.41	0.50
1:H:98:GLU:HG3	1:H:99:ASP:H	1.75	0.50
1:E:78:LEU:HB2	1:E:133:VAL:CG2	2.41	0.50
1:G:239:ASN:N	1:G:239:ASN:HD22	2.06	0.50
1:C:17:VAL:CG2	1:C:19:MET:HG3	2.38	0.50
1:D:132:PHE:CD1	1:D:174:ILE:HG12	2.47	0.50
1:C:73:TYR:CE1	1:C:109:PRO:HA	2.46	0.50
1:F:188:THR:HG23	1:F:255:LYS:O	2.12	0.50
1:B:92:TYR:HA	1:B:117:VAL:HG21	1.94	0.50
1:C:282:LYS:HG3	1:D:13:VAL:HG22	1.93	0.50
1:M:248:ILE:N	1:M:262:ASN:HD21	2.01	0.50
1:I:15:HIS:CE1	1:J:280:PRO:HG3	2.47	0.50
1:A:212:ASN:O	1:A:252:LYS:HG2	2.12	0.50
1:D:73:TYR:CE1	1:D:109:PRO:HA	2.47	0.50
1:A:8:THR:HG21	1:A:255:LYS:HZ2	1.76	0.50
1:H:199:LYS:HE3	1:H:218:TYR:CE2	2.46	0.50
1:A:116:HIS:HE1	1:A:173:GLU:OE1	1.95	0.50
1:K:280:PRO:HG3	1:L:15:HIS:CE1	2.47	0.50
1:P:162:HIS:O	1:P:163:ASP:C	2.50	0.50
1:E:24:LEU:N	1:E:24:LEU:HD12	2.27	0.50
1:H:214:ASN:HD21	1:H:252:LYS:HE3	1.76	0.50
1:P:221:HIS:HD2	1:P:223:SER:H	1.59	0.50
1:M:199:LYS:HE3	1:M:218:TYR:CE2	2.47	0.50
1:E:227:PRO:HA	1:E:233:ALA:CB	2.42	0.50
1:F:16:ASN:OD1	1:F:53:GLU:HB2	2.11	0.50
1:A:239:ASN:N	1:A:239:ASN:ND2	2.57	0.50
1:G:227:PRO:HA	1:G:233:ALA:CB	2.42	0.49
1:B:118:PHE:CE2	1:B:131:GLY:HA2	2.47	0.49
1:K:13:VAL:HB	1:K:49:VAL:HG22	1.94	0.49
1:J:124:PHE:HB2	1:J:155:ASP:OD2	2.12	0.49
1:C:73:TYR:CD2	1:C:73:TYR:N	2.79	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:267:GLU:O	1:P:275:PHE:CE2	2.63	0.49
1:L:199:LYS:HE3	1:L:218:TYR:CE2	2.47	0.49
1:E:116:HIS:HE1	1:E:173:GLU:OE1	1.95	0.49
1:M:89:GLU:O	1:M:116:HIS:HA	2.12	0.49
1:O:155:ASP:N	1:O:163:ASP:OD2	2.40	0.49
1:G:227:PRO:HA	1:G:233:ALA:HB3	1.93	0.49
1:F:227:PRO:O	1:F:234:LYS:CB	2.58	0.49
1:N:221:HIS:HD2	1:N:223:SER:H	1.59	0.49
1:A:162:HIS:O	1:A:163:ASP:C	2.47	0.49
1:C:248:ILE:H	1:C:262:ASN:ND2	1.98	0.49
1:N:239:ASN:HD22	1:N:239:ASN:N	2.06	0.49
1:G:118:PHE:CE2	1:G:131:GLY:HA2	2.48	0.49
1:K:11:LYS:O	1:K:46:ASN:HB3	2.12	0.49
1:D:121:GLY:HA3	1:D:126:ASN:HB2	1.94	0.49
1:K:56:ASP:O	1:K:60:SER:HB2	2.12	0.49
1:D:286:LYS:CE	1:J:124:PHE:HE1	2.26	0.49
1:K:16:ASN:CA	1:K:52:ASN:HB2	2.39	0.49
1:K:239:ASN:HD22	1:K:239:ASN:N	2.03	0.49
1:M:214:ASN:HD21	1:M:252:LYS:HE3	1.77	0.49
1:G:11:LYS:O	1:G:46:ASN:HB3	2.12	0.49
1:C:24:LEU:HD12	1:C:24:LEU:N	2.27	0.49
1:A:282:LYS:HG3	1:B:13:VAL:HG22	1.95	0.49
1:A:274:ASP:OD2	1:B:268:LYS:NZ	2.46	0.49
1:H:11:LYS:O	1:H:46:ASN:HB3	2.13	0.49
1:K:52:ASN:HD21	1:K:194:ASP:H	1.61	0.49
1:M:239:ASN:ND2	1:M:239:ASN:N	2.58	0.49
1:N:198:ASN:O	1:N:201:THR:HG23	2.13	0.49
1:O:198:ASN:O	1:O:201:THR:HG23	2.13	0.49
1:B:24:LEU:N	1:B:24:LEU:HD12	2.28	0.49
1:O:227:PRO:HA	1:O:233:ALA:CB	2.43	0.48
1:O:227:PRO:HA	1:O:233:ALA:HB3	1.95	0.48
1:N:73:TYR:N	1:N:73:TYR:CD2	2.81	0.48
1:G:92:TYR:HA	1:G:117:VAL:HG21	1.95	0.48
1:I:221:HIS:HD2	1:I:223:SER:H	1.61	0.48
1:E:239:ASN:N	1:E:239:ASN:HD22	2.04	0.48
1:O:13:VAL:HA	1:P:281:ILE:O	2.13	0.48
1:D:239:ASN:N	1:D:239:ASN:HD22	2.01	0.48
1:C:227:PRO:O	1:C:234:LYS:CB	2.60	0.48
1:B:28:TRP:HB2	1:B:30:GLN:OE1	2.13	0.48
1:O:285:SER:OG	1:P:257:PRO:HB3	2.12	0.48
1:E:16:ASN:OD1	1:E:53:GLU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:227:PRO:O	1:O:234:LYS:CB	2.58	0.48
1:G:132:PHE:CD1	1:G:174:ILE:HG12	2.49	0.48
1:A:13:VAL:HB	1:A:49:VAL:HG22	1.96	0.48
1:D:284:TYR:O	1:J:157:ARG:NH2	2.44	0.48
1:N:13:VAL:HB	1:N:49:VAL:HG22	1.95	0.48
1:F:92:TYR:HA	1:F:117:VAL:HG21	1.95	0.48
1:D:108:TYR:HB3	1:D:109:PRO:CD	2.44	0.48
1:B:108:TYR:HB3	1:B:109:PRO:HD2	1.95	0.48
1:F:124:PHE:HB2	1:F:155:ASP:OD2	2.14	0.48
1:M:198:ASN:O	1:M:201:THR:HG23	2.14	0.48
1:G:278:HIS:HD2	1:H:246:ASP:OD1	1.97	0.48
1:L:214:ASN:HD21	1:L:252:LYS:HE3	1.79	0.48
1:J:68:LYS:HZ3	1:O:83:SER:HB3	1.76	0.48
1:C:283:ALA:HB3	1:D:248:ILE:HD12	1.95	0.48
1:H:212:ASN:O	1:H:252:LYS:HG2	2.14	0.48
1:M:172:LYS:O	1:M:176:ASP:HB2	2.13	0.48
1:M:188:THR:HG23	1:M:255:LYS:O	2.13	0.48
1:K:35:ASP:HA	1:K:66:ASN:ND2	2.29	0.48
1:O:154:GLU:CA	1:O:163:ASP:OD2	2.51	0.48
1:J:188:THR:HG23	1:J:255:LYS:O	2.14	0.48
1:F:24:LEU:HD12	1:F:24:LEU:N	2.29	0.48
1:J:239:ASN:HD22	1:J:239:ASN:N	2.05	0.47
1:H:239:ASN:N	1:H:239:ASN:HD22	2.10	0.47
1:J:248:ILE:N	1:J:262:ASN:HD21	2.01	0.47
1:G:281:ILE:CD1	1:H:264:VAL:HG22	2.44	0.47
1:G:73:TYR:N	1:G:73:TYR:CD2	2.83	0.47
1:B:121:GLY:HA3	1:B:126:ASN:HB2	1.97	0.47
1:I:199:LYS:HB2	1:I:244:HIS:HB3	1.96	0.47
1:M:280:PRO:HG3	1:N:15:HIS:CE1	2.49	0.47
1:O:265:VAL:O	1:P:280:PRO:HD2	2.14	0.47
1:O:282:LYS:HG3	1:P:13:VAL:HG22	1.96	0.47
1:J:162:HIS:O	1:J:163:ASP:C	2.51	0.47
1:D:285:SER:C	1:J:157:ARG:CZ	2.83	0.47
1:B:69:LYS:HB3	1:B:69:LYS:HE2	1.74	0.47
1:E:239:ASN:N	1:E:239:ASN:ND2	2.51	0.47
1:E:275:PHE:CE1	1:F:269:PRO:HG3	2.49	0.47
1:P:124:PHE:HB2	1:P:155:ASP:OD2	2.13	0.47
1:I:199:LYS:HE3	1:I:218:TYR:CE2	2.49	0.47
1:B:11:LYS:O	1:B:46:ASN:HB3	2.14	0.47
1:I:232:ILE:HG22	1:J:277:ASP:HB3	1.95	0.47
1:P:198:ASN:O	1:P:201:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:TYR:CE1	1:A:109:PRO:HA	2.49	0.47
1:K:199:LYS:HE3	1:K:218:TYR:CE2	2.49	0.47
1:C:123:GLY:C	1:C:125:ASP:H	2.17	0.47
1:M:13:VAL:HB	1:M:49:VAL:HG22	1.96	0.47
1:M:265:VAL:O	1:N:280:PRO:HD2	2.14	0.47
1:H:226:ASP:OD1	1:H:226:ASP:C	2.53	0.47
1:I:272:TRP:CD1	1:J:33:ARG:HG3	2.49	0.47
1:C:228:GLN:HG2	1:E:202:PRO:HG3	1.96	0.47
1:B:108:TYR:HB3	1:B:109:PRO:CD	2.45	0.47
1:B:8:THR:HG21	1:B:255:LYS:HZ1	1.76	0.47
1:P:214:ASN:HD21	1:P:252:LYS:HE3	1.80	0.47
1:N:222:ASN:HB3	1:O:199:LYS:HE2	1.96	0.47
1:C:283:ALA:CB	1:D:248:ILE:HD12	2.44	0.47
1:C:188:THR:HG23	1:C:255:LYS:O	2.15	0.47
1:A:144:VAL:HG22	1:A:145:HIS:N	2.28	0.47
1:N:145:HIS:CE1	1:N:183:ILE:HD13	2.50	0.47
1:K:269:PRO:O	1:K:271:PRO:HD3	2.15	0.47
1:L:239:ASN:HD22	1:L:239:ASN:N	2.10	0.47
1:M:145:HIS:CE1	1:M:183:ILE:HD13	2.50	0.47
1:K:227:PRO:O	1:K:234:LYS:CB	2.58	0.47
1:I:8:THR:HG21	1:I:255:LYS:CE	2.45	0.47
1:G:124:PHE:HB2	1:G:155:ASP:OD2	2.14	0.47
1:N:270:LYS:HA	1:N:271:PRO:HD3	1.64	0.47
1:H:145:HIS:CE1	1:H:183:ILE:HD13	2.50	0.47
1:E:92:TYR:HA	1:E:117:VAL:HG21	1.95	0.47
1:N:199:LYS:HB2	1:N:244:HIS:HB3	1.96	0.47
1:M:16:ASN:OD1	1:M:53:GLU:HB2	2.14	0.47
1:E:275:PHE:O	1:F:33:ARG:HD2	2.14	0.47
1:J:239:ASN:N	1:J:239:ASN:ND2	2.51	0.46
1:F:89:GLU:O	1:F:116:HIS:HA	2.15	0.46
1:B:145:HIS:CE1	1:B:183:ILE:HD13	2.50	0.46
1:N:214:ASN:HD21	1:N:252:LYS:HE3	1.80	0.46
1:K:272:TRP:CZ2	1:L:29:GLY:CA	2.98	0.46
1:E:69:LYS:HD2	1:H:93:SER:CB	2.28	0.46
1:K:73:TYR:N	1:K:73:TYR:CD2	2.83	0.46
1:P:188:THR:HG23	1:P:255:LYS:O	2.16	0.46
1:F:118:PHE:CE2	1:F:131:GLY:HA2	2.50	0.46
1:D:198:ASN:HB3	1:D:201:THR:HG21	1.97	0.46
1:E:124:PHE:HB2	1:E:155:ASP:OD2	2.15	0.46
1:C:13:VAL:HB	1:C:49:VAL:HG22	1.97	0.46
1:B:35:ASP:OD1	1:B:62:LYS:HE3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:52:ASN:ND2	1:K:194:ASP:N	2.61	0.46
1:G:89:GLU:O	1:G:116:HIS:HA	2.15	0.46
1:P:13:VAL:HB	1:P:49:VAL:HG22	1.98	0.46
1:I:214:ASN:HD21	1:I:252:LYS:HE3	1.80	0.46
1:D:285:SER:C	1:J:157:ARG:HH12	2.19	0.46
1:I:73:TYR:CD2	1:I:73:TYR:N	2.83	0.46
1:N:35:ASP:HA	1:N:66:ASN:ND2	2.31	0.46
1:E:221:HIS:HD2	1:E:223:SER:H	1.64	0.46
1:J:17:VAL:CG2	1:J:19:MET:HG3	2.36	0.46
1:O:275:PHE:CZ	1:P:269:PRO:HD3	2.49	0.46
1:K:278:HIS:CG	1:L:16:ASN:HB3	2.50	0.46
1:J:8:THR:HG21	1:J:255:LYS:CE	2.46	0.46
1:D:172:LYS:O	1:D:176:ASP:HB2	2.15	0.46
1:O:56:ASP:O	1:O:60:SER:HB2	2.15	0.46
1:A:265:VAL:O	1:B:280:PRO:HD2	2.16	0.46
1:I:145:HIS:CE1	1:I:183:ILE:HD13	2.51	0.46
1:A:221:HIS:HB2	1:A:266:THR:CG2	2.45	0.46
1:P:239:ASN:N	1:P:239:ASN:HD22	2.07	0.46
1:I:239:ASN:N	1:I:239:ASN:HD22	2.12	0.46
1:L:124:PHE:HB2	1:L:155:ASP:OD2	2.15	0.46
1:I:261:VAL:O	1:J:283:ALA:HA	2.15	0.46
1:M:32:LYS:HZ2	1:N:272:TRP:HZ3	1.60	0.46
1:C:228:GLN:NE2	1:E:202:PRO:N	2.64	0.46
1:F:227:PRO:HA	1:F:233:ALA:CB	2.45	0.46
1:K:188:THR:HG23	1:K:255:LYS:O	2.16	0.46
1:A:78:LEU:O	1:A:99:ASP:HB2	2.16	0.46
1:C:269:PRO:HD2	1:D:273:ASN:O	2.15	0.46
1:O:199:LYS:HB2	1:O:244:HIS:HB3	1.98	0.46
1:C:69:LYS:HE2	1:C:69:LYS:HB3	1.74	0.46
1:C:228:GLN:NE2	1:E:202:PRO:CD	2.79	0.46
1:O:275:PHE:CE2	1:P:269:PRO:HD3	2.51	0.46
1:O:16:ASN:HB3	1:P:278:HIS:CG	2.51	0.46
1:B:239:ASN:N	1:B:239:ASN:ND2	2.51	0.46
1:A:8:THR:HG21	1:A:255:LYS:CE	2.46	0.46
1:N:126:ASN:C	1:N:128:SER:H	2.19	0.46
1:E:13:VAL:HB	1:E:49:VAL:HG22	1.96	0.46
1:B:17:VAL:HG21	1:B:19:MET:HE3	1.98	0.46
1:B:73:TYR:CD2	1:B:73:TYR:N	2.83	0.46
1:C:160:ALA:CB	1:E:239:ASN:HB3	2.45	0.46
1:J:73:TYR:CD2	1:J:73:TYR:N	2.83	0.46
1:I:124:PHE:HB2	1:I:155:ASP:OD2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ASP:OD1	1:C:62:LYS:HE3	2.15	0.46
1:K:278:HIS:HD2	1:L:246:ASP:OD1	1.99	0.46
1:C:8:THR:HG21	1:C:255:LYS:CE	2.46	0.46
1:K:265:VAL:HG12	1:K:267:GLU:H	1.81	0.46
1:A:123:GLY:C	1:A:125:ASP:H	2.19	0.46
1:H:227:PRO:O	1:H:234:LYS:CB	2.64	0.45
1:D:11:LYS:O	1:D:46:ASN:HB3	2.15	0.45
1:P:199:LYS:HB2	1:P:244:HIS:HB3	1.98	0.45
1:K:272:TRP:NE1	1:L:29:GLY:HA3	2.31	0.45
1:K:239:ASN:ND2	1:K:239:ASN:N	2.50	0.45
1:N:108:TYR:HB3	1:N:109:PRO:CD	2.47	0.45
1:B:8:THR:HG21	1:B:255:LYS:CE	2.46	0.45
1:D:163:ASP:O	1:D:167:ARG:HG3	2.16	0.45
1:C:274:ASP:CG	1:D:268:LYS:HZ2	2.20	0.45
1:J:49:VAL:HB	1:J:105:VAL:HG22	1.98	0.45
1:F:198:ASN:O	1:F:201:THR:HG23	2.15	0.45
1:I:162:HIS:O	1:I:163:ASP:C	2.55	0.45
1:N:69:LYS:HE2	1:N:69:LYS:HB3	1.75	0.45
1:M:24:LEU:N	1:M:24:LEU:HD12	2.31	0.45
1:O:246:ASP:OD1	1:P:278:HIS:CD2	2.68	0.45
1:N:188:THR:HG23	1:N:255:LYS:O	2.16	0.45
1:O:8:THR:HG21	1:O:255:LYS:HZ1	1.80	0.45
1:H:239:ASN:N	1:H:239:ASN:ND2	2.58	0.45
1:J:212:ASN:O	1:J:252:LYS:HG2	2.17	0.45
1:K:132:PHE:CD1	1:K:174:ILE:HG12	2.51	0.45
1:C:241:LYS:HG2	1:E:201:THR:HG22	1.99	0.45
1:O:284:TYR:CE2	1:P:261:VAL:HB	2.52	0.45
1:N:124:PHE:HB2	1:N:155:ASP:OD2	2.15	0.45
1:K:78:LEU:HB2	1:K:133:VAL:CG2	2.46	0.45
1:C:239:ASN:ND2	1:C:239:ASN:N	2.60	0.45
1:J:35:ASP:HA	1:J:66:ASN:ND2	2.31	0.45
1:M:73:TYR:CD2	1:M:73:TYR:N	2.85	0.45
1:L:145:HIS:HB2	1:L:189:VAL:HG22	1.99	0.45
1:C:221:HIS:HD2	1:C:223:SER:H	1.65	0.45
1:E:11:LYS:O	1:E:46:ASN:HB3	2.16	0.45
1:O:11:LYS:O	1:O:46:ASN:HB3	2.17	0.45
1:P:73:TYR:N	1:P:73:TYR:CD2	2.85	0.45
1:H:8:THR:HG21	1:H:255:LYS:HZ1	1.81	0.45
1:M:36:LEU:HD22	1:M:269:PRO:HB3	1.99	0.45
1:N:22:THR:HG23	1:N:56:ASP:CG	2.37	0.45
1:F:247:TYR:HA	1:F:262:ASN:ND2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:8:THR:HG21	1:H:255:LYS:CE	2.47	0.45
1:D:132:PHE:HB3	1:D:149:THR:HB	1.98	0.45
1:H:199:LYS:HB2	1:H:244:HIS:HB3	1.98	0.45
1:E:35:ASP:OD1	1:E:62:LYS:HE3	2.16	0.45
1:M:78:LEU:HB2	1:M:133:VAL:CG2	2.46	0.45
1:D:286:LYS:CD	1:J:124:PHE:CE1	3.00	0.45
1:F:93:SER:HB2	1:G:69:LYS:CD	2.33	0.45
1:D:108:TYR:HB3	1:D:109:PRO:HD2	1.99	0.45
1:A:122:CYS:HB3	1:A:152:GLN:NE2	2.31	0.45
1:B:198:ASN:HB3	1:B:201:THR:HG21	1.98	0.45
1:A:214:ASN:HD21	1:A:252:LYS:HE3	1.82	0.45
1:E:89:GLU:O	1:E:116:HIS:HA	2.17	0.45
1:K:269:PRO:HD2	1:L:273:ASN:O	2.17	0.45
1:N:123:GLY:C	1:N:125:ASP:H	2.20	0.45
1:P:35:ASP:OD1	1:P:62:LYS:HE3	2.17	0.45
1:K:214:ASN:HD21	1:K:252:LYS:HE3	1.81	0.45
1:O:172:LYS:O	1:O:176:ASP:HB2	2.17	0.45
1:P:172:LYS:O	1:P:176:ASP:HB2	2.17	0.45
1:K:172:LYS:O	1:K:176:ASP:HB2	2.17	0.45
1:A:118:PHE:CE2	1:A:131:GLY:CA	2.97	0.45
1:C:199:LYS:HB2	1:C:244:HIS:HB3	1.99	0.45
1:G:214:ASN:HD21	1:G:252:LYS:HE3	1.82	0.45
1:K:52:ASN:HD21	1:K:193:GLY:CA	2.29	0.44
1:O:8:THR:HG21	1:O:255:LYS:CE	2.47	0.44
1:A:13:VAL:HA	1:B:281:ILE:O	2.17	0.44
1:B:126:ASN:C	1:B:128:SER:H	2.20	0.44
1:H:172:LYS:O	1:H:176:ASP:HB2	2.16	0.44
1:A:259:GLN:H	1:B:285:SER:HB3	1.81	0.44
1:M:123:GLY:C	1:M:125:ASP:H	2.20	0.44
1:J:68:LYS:HZ1	1:O:83:SER:HB3	1.80	0.44
1:E:268:LYS:HA	1:E:269:PRO:HD3	1.63	0.44
1:O:239:ASN:N	1:O:239:ASN:HD22	2.11	0.44
1:L:279:TYR:HA	1:L:280:PRO:HD3	1.82	0.44
1:A:124:PHE:HB2	1:A:155:ASP:OD2	2.16	0.44
1:I:123:GLY:C	1:I:125:ASP:H	2.21	0.44
1:D:86:ASP:HB2	1:D:113:LYS:O	2.17	0.44
1:F:123:GLY:C	1:F:125:ASP:H	2.20	0.44
1:G:108:TYR:HB3	1:G:109:PRO:CD	2.47	0.44
1:D:227:PRO:HA	1:D:233:ALA:HB3	1.99	0.44
1:H:124:PHE:HB2	1:H:155:ASP:OD2	2.17	0.44
1:A:144:VAL:HG22	1:A:145:HIS:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:145:HIS:HB2	1:H:189:VAL:HG22	1.98	0.44
1:D:195:LEU:O	1:D:197:VAL:HG23	2.17	0.44
1:B:132:PHE:CD1	1:B:174:ILE:HG12	2.52	0.44
1:F:195:LEU:O	1:F:197:VAL:HG23	2.18	0.44
1:N:132:PHE:CD1	1:N:174:ILE:HG12	2.52	0.44
1:A:198:ASN:O	1:A:201:THR:HG23	2.17	0.44
1:F:73:TYR:N	1:F:73:TYR:CD2	2.85	0.44
1:D:227:PRO:HA	1:D:233:ALA:CB	2.47	0.44
1:F:8:THR:HG21	1:F:255:LYS:CE	2.47	0.44
1:K:28:TRP:HA	1:L:272:TRP:HZ2	1.82	0.44
1:P:22:THR:HG23	1:P:56:ASP:CG	2.37	0.44
1:B:49:VAL:HB	1:B:105:VAL:HG22	2.00	0.44
1:J:13:VAL:HB	1:J:49:VAL:HG22	2.00	0.44
1:E:272:TRP:HB2	1:F:36:LEU:CD1	2.47	0.44
1:M:264:VAL:HG22	1:N:281:ILE:CD1	2.47	0.44
1:B:52:ASN:HD21	1:B:194:ASP:H	1.60	0.44
1:B:35:ASP:HA	1:B:66:ASN:ND2	2.32	0.44
1:A:35:ASP:HA	1:A:66:ASN:ND2	2.33	0.44
1:D:284:TYR:HB2	1:J:157:ARG:NH1	2.32	0.44
1:K:150:HIS:CD2	1:K:194:ASP:HB3	2.53	0.44
1:H:73:TYR:N	1:H:73:TYR:CD2	2.86	0.44
1:I:52:ASN:HD21	1:I:193:GLY:CA	2.31	0.44
1:E:126:ASN:C	1:E:128:SER:H	2.21	0.44
1:G:49:VAL:HB	1:G:105:VAL:HG22	1.99	0.44
1:J:199:LYS:HB2	1:J:244:HIS:HB3	2.00	0.44
1:C:195:LEU:O	1:C:197:VAL:HG23	2.18	0.44
1:D:221:HIS:HD2	1:D:223:SER:H	1.65	0.44
1:A:226:ASP:OD1	1:A:226:ASP:C	2.56	0.44
1:O:16:ASN:OD1	1:O:53:GLU:HB2	2.18	0.44
1:F:172:LYS:O	1:F:176:ASP:HB2	2.18	0.44
1:O:241:LYS:HA	1:O:242:PRO:HD3	1.86	0.44
1:H:35:ASP:OD1	1:H:62:LYS:HE3	2.18	0.44
1:I:172:LYS:O	1:I:176:ASP:HB2	2.18	0.44
1:F:69:LYS:HE2	1:F:69:LYS:HB3	1.80	0.44
1:G:16:ASN:OD1	1:G:53:GLU:HB2	2.18	0.44
1:A:28:TRP:O	1:A:29:GLY:C	2.56	0.44
1:O:13:VAL:HB	1:O:49:VAL:HG22	1.99	0.44
1:F:214:ASN:HD21	1:F:252:LYS:HE3	1.83	0.44
1:E:214:ASN:HD21	1:E:252:LYS:HE3	1.82	0.44
1:H:69:LYS:HB3	1:H:69:LYS:HE2	1.80	0.44
1:F:248:ILE:N	1:F:262:ASN:HD21	2.09	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:8:THR:HG21	1:N:255:LYS:CE	2.47	0.44
1:I:227:PRO:O	1:I:234:LYS:CB	2.65	0.44
1:B:86:ASP:HB2	1:B:113:LYS:O	2.18	0.44
1:L:198:ASN:O	1:L:201:THR:HG23	2.17	0.44
1:P:92:TYR:HA	1:P:117:VAL:HG21	2.00	0.44
1:F:132:PHE:HB3	1:F:149:THR:HB	1.99	0.44
1:I:24:LEU:HD12	1:I:24:LEU:N	2.33	0.44
1:M:221:HIS:HD2	1:M:223:SER:H	1.65	0.44
1:N:227:PRO:O	1:N:234:LYS:CB	2.63	0.43
1:G:132:PHE:HB3	1:G:149:THR:HB	1.98	0.43
1:O:96:VAL:HG21	1:O:129:ASN:OD1	2.18	0.43
1:L:195:LEU:O	1:L:197:VAL:HG23	2.18	0.43
1:P:241:LYS:HA	1:P:242:PRO:HD3	1.84	0.43
1:C:264:VAL:HG22	1:D:281:ILE:CD1	2.48	0.43
1:P:35:ASP:HA	1:P:66:ASN:ND2	2.33	0.43
1:D:78:LEU:HB2	1:D:133:VAL:CG2	2.48	0.43
1:P:132:PHE:CD1	1:P:174:ILE:HG12	2.53	0.43
1:M:273:ASN:O	1:N:269:PRO:HD2	2.18	0.43
1:O:277:ASP:HB3	1:P:232:ILE:HG22	2.00	0.43
1:H:13:VAL:HB	1:H:49:VAL:HG22	1.98	0.43
1:I:226:ASP:C	1:I:226:ASP:OD1	2.56	0.43
1:C:78:LEU:HD21	1:C:131:GLY:N	2.32	0.43
1:G:198:ASN:HB3	1:G:201:THR:HG21	2.00	0.43
1:I:195:LEU:O	1:I:197:VAL:HG23	2.19	0.43
1:O:132:PHE:CD1	1:O:174:ILE:HG12	2.53	0.43
1:G:221:HIS:HD2	1:G:223:SER:H	1.66	0.43
1:A:17:VAL:CG2	1:A:19:MET:HG3	2.36	0.43
1:K:108:TYR:HB3	1:K:109:PRO:CD	2.49	0.43
1:L:89:GLU:O	1:L:116:HIS:HA	2.18	0.43
1:E:145:HIS:CE1	1:E:183:ILE:HD13	2.53	0.43
1:O:273:ASN:OD1	1:P:271:PRO:HG2	2.18	0.43
1:C:16:ASN:OD1	1:C:53:GLU:HB2	2.18	0.43
1:A:121:GLY:CA	1:A:126:ASN:HB2	2.48	0.43
1:N:78:LEU:O	1:N:99:ASP:HB2	2.19	0.43
1:O:89:GLU:O	1:O:116:HIS:HA	2.18	0.43
1:J:214:ASN:HD21	1:J:252:LYS:HE3	1.81	0.43
1:F:145:HIS:HB2	1:F:189:VAL:HG22	1.99	0.43
1:E:69:LYS:HE2	1:E:69:LYS:HB3	1.86	0.43
1:J:227:PRO:O	1:J:234:LYS:CB	2.63	0.43
1:M:8:THR:HG21	1:M:255:LYS:HZ2	1.83	0.43
1:K:13:VAL:HG22	1:L:282:LYS:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:199:LYS:HB2	1:M:244:HIS:HB3	1.99	0.43
1:G:199:LYS:HE3	1:G:218:TYR:CE2	2.53	0.43
1:C:281:ILE:HG12	1:D:246:ASP:HB2	2.00	0.43
1:P:11:LYS:O	1:P:46:ASN:HB3	2.19	0.43
1:F:241:LYS:HA	1:F:242:PRO:HD3	1.85	0.43
1:B:16:ASN:CA	1:B:52:ASN:HB2	2.40	0.43
1:J:108:TYR:HB3	1:J:109:PRO:CD	2.49	0.43
1:C:78:LEU:O	1:C:99:ASP:HB2	2.18	0.43
1:C:281:ILE:HG12	1:D:246:ASP:CB	2.48	0.43
1:A:11:LYS:O	1:A:46:ASN:HB3	2.18	0.43
1:M:11:LYS:O	1:M:46:ASN:HB3	2.19	0.43
1:F:35:ASP:HA	1:F:66:ASN:ND2	2.34	0.43
1:F:199:LYS:HB2	1:F:244:HIS:HB3	2.01	0.43
1:O:124:PHE:HB2	1:O:155:ASP:OD2	2.18	0.43
1:N:16:ASN:OD1	1:N:53:GLU:HB2	2.18	0.43
1:M:227:PRO:HA	1:M:233:ALA:CB	2.49	0.43
1:C:78:LEU:HB2	1:C:133:VAL:CG2	2.48	0.43
1:L:8:THR:HG21	1:L:255:LYS:CE	2.48	0.43
1:L:8:THR:HG21	1:L:255:LYS:HZ1	1.80	0.43
1:P:126:ASN:C	1:P:128:SER:H	2.22	0.43
1:G:275:PHE:O	1:H:33:ARG:HD2	2.18	0.43
1:F:198:ASN:HB3	1:F:201:THR:HG21	2.00	0.43
1:H:123:GLY:C	1:H:125:ASP:H	2.22	0.43
1:K:16:ASN:OD1	1:K:53:GLU:HB2	2.19	0.43
1:E:15:HIS:O	1:E:17:VAL:HG13	2.19	0.43
1:B:188:THR:HG23	1:B:255:LYS:O	2.18	0.43
1:L:49:VAL:HB	1:L:105:VAL:HG22	2.00	0.43
1:C:199:LYS:HE3	1:C:218:TYR:CE2	2.53	0.43
1:N:199:LYS:HE3	1:N:218:TYR:CE2	2.54	0.43
1:A:35:ASP:OD1	1:A:62:LYS:HE3	2.19	0.43
1:O:213:VAL:HB	1:O:249:PHE:HB3	2.01	0.43
1:E:281:ILE:CD1	1:F:264:VAL:HG22	2.49	0.43
1:K:198:ASN:O	1:K:201:THR:HG23	2.19	0.43
1:L:123:GLY:C	1:L:125:ASP:H	2.22	0.43
1:A:181:LYS:O	1:A:181:LYS:HG3	2.18	0.43
1:I:275:PHE:HE2	1:J:267:GLU:HG2	1.83	0.43
1:P:16:ASN:OD1	1:P:53:GLU:HB2	2.19	0.43
1:M:8:THR:HG21	1:M:255:LYS:CE	2.49	0.43
1:D:188:THR:HG23	1:D:255:LYS:O	2.19	0.43
1:F:126:ASN:C	1:F:128:SER:H	2.22	0.43
1:H:170:GLN:O	1:H:173:GLU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:145:HIS:CE1	1:O:183:ILE:HD13	2.53	0.43
1:P:195:LEU:O	1:P:197:VAL:HG23	2.19	0.43
1:J:28:TRP:O	1:J:29:GLY:C	2.54	0.42
1:G:33:ARG:O	1:G:37:ILE:HG13	2.19	0.42
1:B:52:ASN:HD21	1:B:193:GLY:CA	2.32	0.42
1:I:268:LYS:NZ	1:J:274:ASP:OD1	2.48	0.42
1:D:72:PRO:HB2	1:D:73:TYR:CD2	2.54	0.42
1:H:52:ASN:HD21	1:H:194:ASP:H	1.63	0.42
1:E:271:PRO:HG3	1:F:273:ASN:OD1	2.19	0.42
1:H:122:CYS:O	1:H:126:ASN:HB3	2.19	0.42
1:H:132:PHE:CD1	1:H:174:ILE:HG12	2.54	0.42
1:N:172:LYS:O	1:N:176:ASP:HB2	2.19	0.42
1:D:183:ILE:HA	1:D:184:PRO:HD3	1.91	0.42
1:L:16:ASN:OD1	1:L:53:GLU:HB2	2.19	0.42
1:B:60:SER:CB	1:B:80:ARG:HH12	2.31	0.42
1:F:8:THR:HG21	1:F:255:LYS:HZ1	1.82	0.42
1:P:49:VAL:HB	1:P:105:VAL:HG22	2.00	0.42
1:I:11:LYS:O	1:I:46:ASN:HB3	2.19	0.42
1:C:11:LYS:O	1:C:46:ASN:HB3	2.20	0.42
1:K:69:LYS:HE2	1:K:69:LYS:HB3	1.81	0.42
1:O:52:ASN:HD21	1:O:193:GLY:CA	2.32	0.42
1:M:269:PRO:HG3	1:N:275:PHE:CD1	2.54	0.42
1:O:49:VAL:HB	1:O:105:VAL:HG22	2.01	0.42
1:K:145:HIS:CE1	1:K:183:ILE:HD13	2.55	0.42
1:A:270:LYS:HA	1:A:271:PRO:HD3	1.72	0.42
1:L:52:ASN:HD21	1:L:193:GLY:CA	2.31	0.42
1:L:73:TYR:N	1:L:73:TYR:CD2	2.86	0.42
1:O:269:PRO:HG3	1:P:275:PHE:CZ	2.54	0.42
1:D:8:THR:HG21	1:D:255:LYS:CE	2.50	0.42
1:A:227:PRO:O	1:A:234:LYS:CB	2.65	0.42
1:G:28:TRP:O	1:G:29:GLY:C	2.56	0.42
1:H:28:TRP:O	1:H:29:GLY:C	2.57	0.42
1:M:198:ASN:HB3	1:M:201:THR:HG21	2.00	0.42
1:I:145:HIS:HB2	1:I:189:VAL:HG22	2.01	0.42
1:J:35:ASP:OD1	1:J:62:LYS:HE3	2.18	0.42
1:A:198:ASN:HB3	1:A:201:THR:HG21	2.01	0.42
1:O:123:GLY:C	1:O:125:ASP:H	2.22	0.42
1:D:24:LEU:HD12	1:D:24:LEU:N	2.34	0.42
1:I:275:PHE:CE2	1:J:267:GLU:HG2	2.55	0.42
1:M:248:ILE:H	1:M:262:ASN:ND2	2.02	0.42
1:I:265:VAL:O	1:J:280:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:ASN:OD1	1:C:199:LYS:N	2.53	0.42
1:O:285:SER:O	1:O:286:LYS:O	2.37	0.42
1:A:145:HIS:CE1	1:A:183:ILE:HD13	2.54	0.42
1:I:213:VAL:HG11	1:I:249:PHE:HB2	2.02	0.42
1:H:24:LEU:N	1:H:24:LEU:HD12	2.34	0.42
1:J:52:ASN:HD21	1:J:194:ASP:H	1.66	0.42
1:L:122:CYS:O	1:L:126:ASN:HB3	2.19	0.42
1:M:124:PHE:HB2	1:M:155:ASP:OD2	2.19	0.42
1:E:172:LYS:O	1:E:176:ASP:HB2	2.19	0.42
1:J:211:LEU:HD23	1:J:211:LEU:HA	1.85	0.42
1:O:188:THR:HG23	1:O:255:LYS:O	2.19	0.42
1:L:13:VAL:HB	1:L:49:VAL:HG22	2.02	0.42
1:P:89:GLU:O	1:P:116:HIS:HA	2.19	0.42
1:F:132:PHE:CD1	1:F:174:ILE:HG12	2.55	0.42
1:L:11:LYS:O	1:L:46:ASN:HB3	2.19	0.42
1:L:172:LYS:O	1:L:176:ASP:HB2	2.19	0.42
1:K:272:TRP:CE2	1:L:29:GLY:HA3	2.55	0.42
1:E:49:VAL:HB	1:E:105:VAL:HG22	2.02	0.42
1:E:279:TYR:HA	1:E:280:PRO:HD3	1.89	0.42
1:D:285:SER:O	1:J:156:SER:HB2	2.20	0.42
1:I:269:PRO:C	1:I:271:PRO:HD3	2.39	0.42
1:L:227:PRO:O	1:L:234:LYS:CB	2.61	0.42
1:D:118:PHE:CG	1:D:170:GLN:HG2	2.55	0.42
1:O:281:ILE:CG1	1:P:246:ASP:HB2	2.50	0.42
1:C:61:ASP:O	1:C:62:LYS:C	2.57	0.42
1:L:143:ASN:HD22	1:L:143:ASN:HA	1.65	0.42
1:D:285:SER:HA	1:J:157:ARG:HH22	1.73	0.42
1:E:69:LYS:NZ	1:H:93:SER:HB2	2.34	0.42
1:G:69:LYS:HB3	1:G:69:LYS:HE2	1.76	0.42
1:A:73:TYR:CD2	1:A:73:TYR:N	2.88	0.42
1:A:239:ASN:HD22	1:A:239:ASN:N	2.09	0.42
1:J:111:LYS:HE2	1:J:111:LYS:HB3	1.90	0.42
1:F:221:HIS:HD2	1:F:223:SER:H	1.68	0.42
1:K:269:PRO:C	1:K:271:PRO:HD3	2.40	0.42
1:A:201:THR:HB	1:A:202:PRO:CD	2.50	0.42
1:F:13:VAL:HB	1:F:49:VAL:HG22	2.02	0.42
1:H:132:PHE:HB3	1:H:149:THR:HB	2.02	0.42
1:H:221:HIS:HB2	1:H:266:THR:HG23	2.02	0.42
1:L:51:PHE:CE1	1:L:63:LEU:HD21	2.55	0.42
1:M:211:LEU:HA	1:M:211:LEU:HD23	1.90	0.42
1:D:248:ILE:N	1:D:262:ASN:HD21	2.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:VAL:O	1:A:118:PHE:C	2.57	0.41
1:E:122:CYS:O	1:E:126:ASN:HB3	2.20	0.41
1:C:267:GLU:HG2	1:D:275:PHE:HE2	1.85	0.41
1:K:49:VAL:HB	1:K:105:VAL:HG22	2.02	0.41
1:B:145:HIS:ND1	1:B:183:ILE:HD13	2.35	0.41
1:O:132:PHE:HB3	1:O:149:THR:HB	2.02	0.41
1:D:145:HIS:CE1	1:D:183:ILE:HD13	2.55	0.41
1:L:92:TYR:HA	1:L:117:VAL:HG21	2.02	0.41
1:L:213:VAL:HB	1:L:249:PHE:HB3	2.02	0.41
1:P:145:HIS:HB2	1:P:189:VAL:HG22	2.02	0.41
1:N:24:LEU:HD12	1:N:24:LEU:N	2.35	0.41
1:P:24:LEU:HD12	1:P:24:LEU:N	2.35	0.41
1:D:284:TYR:CG	1:J:157:ARG:NE	2.87	0.41
1:B:52:ASN:ND2	1:B:194:ASP:N	2.63	0.41
1:P:108:TYR:HB3	1:P:109:PRO:CD	2.50	0.41
1:G:188:THR:HG23	1:G:255:LYS:O	2.19	0.41
1:I:122:CYS:HB3	1:I:152:GLN:NE2	2.35	0.41
1:N:78:LEU:HB2	1:N:133:VAL:CG2	2.50	0.41
1:O:266:THR:HG22	1:P:279:TYR:CZ	2.54	0.41
1:M:241:LYS:HA	1:M:242:PRO:HD3	1.80	0.41
1:B:213:VAL:HB	1:B:249:PHE:HB3	2.03	0.41
1:B:214:ASN:HD21	1:B:252:LYS:HE3	1.85	0.41
1:I:268:LYS:HA	1:I:269:PRO:HD2	1.93	0.41
1:O:52:ASN:HD21	1:O:194:ASP:H	1.64	0.41
1:P:52:ASN:HD21	1:P:193:GLY:CA	2.33	0.41
1:A:283:ALA:CB	1:B:248:ILE:HD12	2.50	0.41
1:P:8:THR:HG21	1:P:255:LYS:CE	2.50	0.41
1:D:126:ASN:C	1:D:128:SER:H	2.22	0.41
1:A:221:HIS:HB2	1:A:266:THR:HG21	2.01	0.41
1:N:36:LEU:HD22	1:N:269:PRO:HB3	2.02	0.41
1:G:199:LYS:HB2	1:G:244:HIS:HB3	2.02	0.41
1:D:49:VAL:HB	1:D:105:VAL:HG22	2.01	0.41
1:N:219:ALA:HB2	1:O:217:LEU:HD22	2.02	0.41
1:B:51:PHE:CE1	1:B:63:LEU:HD21	2.55	0.41
1:P:227:PRO:HA	1:P:233:ALA:CB	2.50	0.41
1:K:268:LYS:NZ	1:L:274:ASP:OD1	2.53	0.41
1:E:22:THR:HG23	1:E:56:ASP:CG	2.41	0.41
1:G:278:HIS:CD2	1:H:246:ASP:OD1	2.73	0.41
1:J:198:ASN:HB3	1:J:201:THR:HG21	2.02	0.41
1:C:77:VAL:HG11	1:C:80:ARG:NH2	2.35	0.41
1:G:172:LYS:O	1:G:176:ASP:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LYS:O	1:B:176:ASP:HB2	2.20	0.41
1:D:284:TYR:CG	1:J:157:ARG:CZ	3.03	0.41
1:L:248:ILE:H	1:L:262:ASN:ND2	2.06	0.41
1:N:8:THR:HG21	1:N:255:LYS:HZ2	1.82	0.41
1:P:212:ASN:O	1:P:252:LYS:HG2	2.21	0.41
1:B:132:PHE:HB3	1:B:149:THR:HB	2.02	0.41
1:E:281:ILE:O	1:F:13:VAL:HA	2.21	0.41
1:N:11:LYS:O	1:N:46:ASN:HB3	2.20	0.41
1:H:195:LEU:O	1:H:197:VAL:HG23	2.20	0.41
1:H:143:ASN:HA	1:H:143:ASN:HD22	1.65	0.41
1:O:275:PHE:CZ	1:P:269:PRO:HG3	2.56	0.41
1:E:227:PRO:O	1:E:234:LYS:CB	2.58	0.41
1:N:73:TYR:CE1	1:N:109:PRO:HA	2.55	0.41
1:C:122:CYS:HB3	1:C:152:GLN:NE2	2.34	0.41
1:E:28:TRP:O	1:E:29:GLY:C	2.58	0.41
1:K:28:TRP:HA	1:L:272:TRP:CZ2	2.55	0.41
1:K:92:TYR:HA	1:K:117:VAL:HG21	2.02	0.41
1:M:35:ASP:HA	1:M:66:ASN:ND2	2.35	0.41
1:J:126:ASN:C	1:J:128:SER:H	2.24	0.41
1:E:8:THR:HG21	1:E:255:LYS:CE	2.51	0.41
1:G:163:ASP:O	1:G:167:ARG:HG3	2.21	0.41
1:K:29:GLY:HA3	1:L:272:TRP:HE1	1.85	0.41
1:O:170:GLN:O	1:O:173:GLU:HB2	2.20	0.41
1:P:199:LYS:HE3	1:P:218:TYR:CE2	2.56	0.41
1:O:213:VAL:HG11	1:O:249:PHE:HB2	2.03	0.41
1:O:145:HIS:HB2	1:O:189:VAL:HG22	2.02	0.41
1:H:241:LYS:HA	1:H:242:PRO:HD3	1.86	0.41
1:J:78:LEU:HB2	1:J:133:VAL:CG2	2.51	0.41
1:M:132:PHE:CD1	1:M:174:ILE:HG12	2.55	0.41
1:J:268:LYS:HA	1:J:269:PRO:HD3	1.81	0.41
1:D:52:ASN:HD21	1:D:193:GLY:CA	2.33	0.41
1:E:16:ASN:CA	1:E:52:ASN:HB2	2.42	0.41
1:A:61:ASP:O	1:A:62:LYS:C	2.59	0.41
1:I:69:LYS:HB3	1:I:69:LYS:HE2	1.78	0.41
1:M:189:VAL:HG12	1:M:189:VAL:O	2.21	0.41
1:D:285:SER:C	1:J:157:ARG:HH22	2.23	0.41
1:M:52:ASN:HD21	1:M:193:GLY:CA	2.34	0.41
1:J:279:TYR:HA	1:J:280:PRO:HD3	1.85	0.41
1:G:52:ASN:HD21	1:G:193:GLY:CA	2.33	0.41
1:H:121:GLY:CA	1:H:126:ASN:HB2	2.50	0.41
1:B:36:LEU:HD23	1:B:36:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:8:THR:HG21	1:K:255:LYS:HZ2	1.81	0.41
1:O:126:ASN:C	1:O:128:SER:H	2.24	0.41
1:H:78:LEU:O	1:H:99:ASP:HB2	2.21	0.41
1:B:28:TRP:O	1:B:29:GLY:C	2.57	0.41
1:L:145:HIS:CE1	1:L:183:ILE:HD13	2.56	0.41
1:J:199:LYS:HE3	1:J:218:TYR:CE2	2.55	0.41
1:H:35:ASP:HA	1:H:66:ASN:ND2	2.36	0.41
1:P:78:LEU:HB2	1:P:133:VAL:CG2	2.51	0.41
1:J:24:LEU:N	1:J:24:LEU:HD12	2.35	0.41
1:H:74:GLN:HG2	1:H:105:VAL:HG12	2.02	0.41
1:B:221:HIS:HD2	1:B:223:SER:H	1.69	0.41
1:K:246:ASP:OD1	1:L:278:HIS:HD2	2.04	0.41
1:C:92:TYR:CD2	1:C:92:TYR:C	2.94	0.41
1:J:227:PRO:HA	1:J:233:ALA:CB	2.51	0.41
1:G:275:PHE:CZ	1:H:269:PRO:HG3	2.56	0.41
1:D:28:TRP:O	1:D:29:GLY:C	2.57	0.41
1:K:35:ASP:HA	1:K:66:ASN:HD21	1.86	0.41
1:C:246:ASP:OD1	1:D:278:HIS:HD2	2.04	0.41
1:J:16:ASN:OD1	1:J:53:GLU:HB2	2.21	0.40
1:I:213:VAL:HB	1:I:249:PHE:HB3	2.03	0.40
1:I:35:ASP:OD1	1:I:62:LYS:HE3	2.22	0.40
1:I:92:TYR:HA	1:I:117:VAL:HG21	2.03	0.40
1:P:213:VAL:HB	1:P:249:PHE:HB3	2.03	0.40
1:J:226:ASP:C	1:J:226:ASP:OD1	2.59	0.40
1:D:150:HIS:CD2	1:D:194:ASP:HB3	2.56	0.40
1:I:150:HIS:CD2	1:I:194:ASP:HB3	2.56	0.40
1:M:126:ASN:C	1:M:128:SER:H	2.24	0.40
1:G:8:THR:HG21	1:G:255:LYS:CE	2.51	0.40
1:G:22:THR:HG23	1:G:56:ASP:CG	2.41	0.40
1:A:22:THR:HG23	1:A:56:ASP:CG	2.42	0.40
1:F:145:HIS:CE1	1:F:183:ILE:HD13	2.56	0.40
1:G:241:LYS:HA	1:G:242:PRO:HD3	1.89	0.40
1:C:276:SER:HB3	1:C:278:HIS:O	2.21	0.40
1:H:52:ASN:HD21	1:H:193:GLY:CA	2.34	0.40
1:C:227:PRO:HA	1:C:233:ALA:CB	2.52	0.40
1:A:273:ASN:O	1:B:269:PRO:HD2	2.21	0.40
1:G:8:THR:HG21	1:G:255:LYS:HZ1	1.83	0.40
1:M:198:ASN:OD1	1:M:199:LYS:N	2.55	0.40
1:E:13:VAL:HA	1:F:281:ILE:O	2.20	0.40
1:F:212:ASN:O	1:F:252:LYS:HG2	2.21	0.40
1:O:78:LEU:HB2	1:O:133:VAL:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ASP:OD1	1:D:62:LYS:HE3	2.21	0.40
1:J:92:TYR:HA	1:J:117:VAL:HG21	2.02	0.40
1:M:195:LEU:O	1:M:197:VAL:HG23	2.21	0.40
1:A:195:LEU:O	1:A:197:VAL:HG23	2.21	0.40
1:P:183:ILE:HA	1:P:184:PRO:HD3	1.94	0.40
1:L:78:LEU:HB2	1:L:133:VAL:CG2	2.51	0.40
1:E:213:VAL:HB	1:E:249:PHE:HB3	2.03	0.40
1:L:24:LEU:HD12	1:L:24:LEU:N	2.36	0.40
1:I:268:LYS:HZ3	1:J:274:ASP:CG	2.25	0.40
1:J:52:ASN:O	1:J:53:GLU:C	2.59	0.40
1:I:8:THR:HG21	1:I:255:LYS:HZ2	1.82	0.40
1:K:122:CYS:O	1:K:126:ASN:HB3	2.22	0.40
1:C:239:ASN:HD22	1:C:239:ASN:N	2.12	0.40
1:G:265:VAL:O	1:H:280:PRO:HD2	2.22	0.40
1:I:278:HIS:CD2	1:J:246:ASP:OD1	2.71	0.40
1:I:198:ASN:OD1	1:I:199:LYS:N	2.54	0.40
1:D:78:LEU:HB2	1:D:133:VAL:HG22	2.04	0.40
1:N:241:LYS:HA	1:N:242:PRO:HD3	1.79	0.40
1:P:123:GLY:C	1:P:125:ASP:H	2.25	0.40
1:K:123:GLY:C	1:K:125:ASP:H	2.25	0.40
1:J:69:LYS:HB3	1:J:69:LYS:HE2	1.71	0.40
1:H:16:ASN:OD1	1:H:53:GLU:HB2	2.22	0.40
1:I:126:ASN:C	1:I:128:SER:H	2.24	0.40
1:A:264:VAL:HG22	1:B:281:ILE:CD1	2.51	0.40
1:E:13:VAL:HG22	1:F:282:LYS:HG3	2.03	0.40
1:J:172:LYS:O	1:J:176:ASP:HB2	2.20	0.40
1:O:221:HIS:HD2	1:O:223:SER:H	1.69	0.40
1:G:285:SER:HA	1:H:259:GLN:O	2.22	0.40
1:E:132:PHE:HB3	1:E:149:THR:HB	2.03	0.40

All (6) 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:E:61:ASP:OD1	1:G:92:TYR:OH[2_645]	1.84	0.36
1:B:92:TYR:OH	1:D:61:ASP:OD2[2_555]	1.86	0.34
1:E:92:TYR:OH	1:G:61:ASP:OD2[2_645]	2.05	0.15
1:A:89:GLU:OE1	1:B:87:LYS:NZ[2_545]	2.09	0.11
1:B:61:ASP:OD1	1:D:82:GLN:N[2_555]	2.10	0.10
1:L:140:ASN:ND2	1:M:165:LYS:NZ[1_454]	2.19	0.01

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	278/306 (91%)	261 (94%)	15 (5%)	2 (1%)	26	68
1	B	278/306 (91%)	260 (94%)	17 (6%)	1 (0%)	39	78
1	C	278/306 (91%)	257 (92%)	18 (6%)	3 (1%)	17	58
1	D	278/306 (91%)	259 (93%)	19 (7%)	0	100	100
1	E	278/306 (91%)	255 (92%)	23 (8%)	0	100	100
1	F	278/306 (91%)	258 (93%)	20 (7%)	0	100	100
1	G	278/306 (91%)	259 (93%)	19 (7%)	0	100	100
1	H	278/306 (91%)	256 (92%)	21 (8%)	1 (0%)	39	78
1	I	278/306 (91%)	257 (92%)	19 (7%)	2 (1%)	26	68
1	J	278/306 (91%)	256 (92%)	21 (8%)	1 (0%)	39	78
1	K	278/306 (91%)	256 (92%)	21 (8%)	1 (0%)	39	78
1	L	278/306 (91%)	259 (93%)	18 (6%)	1 (0%)	39	78
1	M	278/306 (91%)	259 (93%)	18 (6%)	1 (0%)	39	78
1	N	278/306 (91%)	257 (92%)	21 (8%)	0	100	100
1	O	278/306 (91%)	258 (93%)	19 (7%)	1 (0%)	39	78
1	P	278/306 (91%)	257 (92%)	21 (8%)	0	100	100
All	All	4448/4896 (91%)	4124 (93%)	310 (7%)	14 (0%)	46	82

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	J	270	LYS
1	K	271	PRO
1	C	271	PRO
1	C	40	SER
1	I	271	PRO
1	A	40	SER

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Mol	Chain	Res	Type
1	A	271	PRO
1	L	40	SER
1	H	40	SER
1	C	123	GLY
1	M	123	GLY
1	I	123	GLY
1	O	270	LYS
1	B	26	PRO

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	250/274 (91%)	239 (96%)	11 (4%)	35	72
1	B	250/274 (91%)	239 (96%)	11 (4%)	35	72
1	C	250/274 (91%)	243 (97%)	7 (3%)	51	82
1	D	250/274 (91%)	240 (96%)	10 (4%)	38	74
1	E	250/274 (91%)	241 (96%)	9 (4%)	42	77
1	F	250/274 (91%)	239 (96%)	11 (4%)	35	72
1	G	250/274 (91%)	243 (97%)	7 (3%)	51	82
1	H	250/274 (91%)	242 (97%)	8 (3%)	46	80
1	I	250/274 (91%)	240 (96%)	10 (4%)	38	74
1	J	250/274 (91%)	240 (96%)	10 (4%)	38	74
1	K	250/274 (91%)	240 (96%)	10 (4%)	38	74
1	L	250/274 (91%)	239 (96%)	11 (4%)	35	72
1	M	250/274 (91%)	243 (97%)	7 (3%)	51	82
1	N	250/274 (91%)	239 (96%)	11 (4%)	35	72
1	O	250/274 (91%)	242 (97%)	8 (3%)	46	80
1	P	250/274 (91%)	240 (96%)	10 (4%)	38	74
All	All	4000/4384 (91%)	3849 (96%)	151 (4%)	40	75

All (151) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	SER
1	A	61	ASP
1	A	83	SER
1	A	99	ASP
1	A	107	LYS
1	A	120	SER
1	A	126	ASN
1	A	162	HIS
1	A	163	ASP
1	A	239	ASN
1	A	286	LYS
1	B	60	SER
1	B	61	ASP
1	B	80	ARG
1	B	83	SER
1	B	120	SER
1	B	126	ASN
1	B	162	HIS
1	B	163	ASP
1	B	201	THR
1	B	239	ASN
1	B	246	ASP
1	C	60	SER
1	C	61	ASP
1	C	83	SER
1	C	120	SER
1	C	126	ASN
1	C	162	HIS
1	C	239	ASN
1	D	60	SER
1	D	83	SER
1	D	99	ASP
1	D	107	LYS
1	D	120	SER
1	D	126	ASN
1	D	162	HIS
1	D	163	ASP
1	D	239	ASN
1	D	286	LYS
1	E	60	SER
1	E	61	ASP
1	E	83	SER

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Mol	Chain	Res	Type
1	E	99	ASP
1	E	120	SER
1	E	126	ASN
1	E	162	HIS
1	E	163	ASP
1	E	239	ASN
1	F	60	SER
1	F	61	ASP
1	F	83	SER
1	F	99	ASP
1	F	120	SER
1	F	124	PHE
1	F	126	ASN
1	F	162	HIS
1	F	163	ASP
1	F	239	ASN
1	F	266	THR
1	G	60	SER
1	G	83	SER
1	G	120	SER
1	G	126	ASN
1	G	162	HIS
1	G	163	ASP
1	G	239	ASN
1	H	60	SER
1	H	61	ASP
1	H	83	SER
1	H	99	ASP
1	H	120	SER
1	H	126	ASN
1	H	162	HIS
1	H	239	ASN
1	I	60	SER
1	I	61	ASP
1	I	83	SER
1	I	99	ASP
1	I	120	SER
1	I	126	ASN
1	I	162	HIS
1	I	163	ASP
1	I	239	ASN
1	I	246	ASP

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Mol	Chain	Res	Type
1	J	60	SER
1	J	61	ASP
1	J	83	SER
1	J	99	ASP
1	J	120	SER
1	J	126	ASN
1	J	162	HIS
1	J	163	ASP
1	J	239	ASN
1	J	246	ASP
1	K	60	SER
1	K	61	ASP
1	K	83	SER
1	K	99	ASP
1	K	120	SER
1	K	126	ASN
1	K	162	HIS
1	K	163	ASP
1	K	239	ASN
1	K	266	THR
1	L	60	SER
1	L	61	ASP
1	L	83	SER
1	L	99	ASP
1	L	120	SER
1	L	126	ASN
1	L	162	HIS
1	L	163	ASP
1	L	239	ASN
1	L	266	THR
1	L	270	LYS
1	M	60	SER
1	M	61	ASP
1	M	83	SER
1	M	99	ASP
1	M	120	SER
1	M	126	ASN
1	M	239	ASN
1	N	60	SER
1	N	61	ASP
1	N	83	SER
1	N	99	ASP

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Mol	Chain	Res	Type
1	N	120	SER
1	N	126	ASN
1	N	162	HIS
1	N	163	ASP
1	N	239	ASN
1	N	246	ASP
1	N	286	LYS
1	O	60	SER
1	O	61	ASP
1	O	83	SER
1	O	99	ASP
1	O	120	SER
1	O	126	ASN
1	O	162	HIS
1	O	239	ASN
1	P	60	SER
1	P	61	ASP
1	P	83	SER
1	P	99	ASP
1	P	120	SER
1	P	126	ASN
1	P	162	HIS
1	P	163	ASP
1	P	239	ASN
1	P	267	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (184) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	74	GLN
1	A	116	HIS
1	A	140	ASN
1	A	143	ASN
1	A	150	HIS
1	A	214	ASN
1	A	239	ASN
1	A	244	HIS
1	A	262	ASN
1	B	52	ASN
1	B	74	GLN
1	B	82	GLN

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Mol	Chain	Res	Type
1	B	116	HIS
1	B	140	ASN
1	B	150	HIS
1	B	196	ASN
1	B	214	ASN
1	B	228	GLN
1	B	239	ASN
1	B	256	GLN
1	B	262	ASN
1	B	278	HIS
1	C	52	ASN
1	C	74	GLN
1	C	116	HIS
1	C	140	ASN
1	C	150	HIS
1	C	162	HIS
1	C	214	ASN
1	C	228	GLN
1	C	239	ASN
1	C	262	ASN
1	D	52	ASN
1	D	74	GLN
1	D	82	GLN
1	D	116	HIS
1	D	140	ASN
1	D	143	ASN
1	D	150	HIS
1	D	196	ASN
1	D	214	ASN
1	D	239	ASN
1	D	256	GLN
1	D	262	ASN
1	D	278	HIS
1	E	52	ASN
1	E	74	GLN
1	E	82	GLN
1	E	116	HIS
1	E	140	ASN
1	E	143	ASN
1	E	150	HIS
1	E	196	ASN
1	E	198	ASN

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Mol	Chain	Res	Type
1	E	214	ASN
1	E	239	ASN
1	E	256	GLN
1	E	262	ASN
1	E	278	HIS
1	F	52	ASN
1	F	74	GLN
1	F	82	GLN
1	F	116	HIS
1	F	140	ASN
1	F	150	HIS
1	F	196	ASN
1	F	214	ASN
1	F	239	ASN
1	F	262	ASN
1	G	52	ASN
1	G	74	GLN
1	G	82	GLN
1	G	116	HIS
1	G	140	ASN
1	G	143	ASN
1	G	150	HIS
1	G	196	ASN
1	G	214	ASN
1	G	239	ASN
1	G	262	ASN
1	G	278	HIS
1	H	52	ASN
1	H	74	GLN
1	H	82	GLN
1	H	116	HIS
1	H	140	ASN
1	H	150	HIS
1	H	214	ASN
1	H	239	ASN
1	H	262	ASN
1	I	52	ASN
1	I	74	GLN
1	I	82	GLN
1	I	116	HIS
1	I	140	ASN
1	I	143	ASN

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Mol	Chain	Res	Type
1	I	150	HIS
1	I	196	ASN
1	I	214	ASN
1	I	239	ASN
1	I	262	ASN
1	I	278	HIS
1	J	52	ASN
1	J	74	GLN
1	J	82	GLN
1	J	116	HIS
1	J	140	ASN
1	J	150	HIS
1	J	196	ASN
1	J	214	ASN
1	J	239	ASN
1	J	262	ASN
1	K	52	ASN
1	K	74	GLN
1	K	82	GLN
1	K	116	HIS
1	K	140	ASN
1	K	150	HIS
1	K	196	ASN
1	K	214	ASN
1	K	221	HIS
1	K	228	GLN
1	K	239	ASN
1	K	256	GLN
1	K	262	ASN
1	K	278	HIS
1	L	52	ASN
1	L	74	GLN
1	L	82	GLN
1	L	116	HIS
1	L	140	ASN
1	L	150	HIS
1	L	196	ASN
1	L	214	ASN
1	L	239	ASN
1	L	262	ASN
1	L	278	HIS
1	M	52	ASN

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Mol	Chain	Res	Type
1	M	74	GLN
1	M	82	GLN
1	M	116	HIS
1	M	140	ASN
1	M	150	HIS
1	M	214	ASN
1	M	239	ASN
1	M	262	ASN
1	M	278	HIS
1	N	52	ASN
1	N	74	GLN
1	N	82	GLN
1	N	116	HIS
1	N	140	ASN
1	N	143	ASN
1	N	150	HIS
1	N	196	ASN
1	N	214	ASN
1	N	239	ASN
1	N	262	ASN
1	N	278	HIS
1	O	52	ASN
1	O	74	GLN
1	O	82	GLN
1	O	116	HIS
1	O	140	ASN
1	O	150	HIS
1	O	196	ASN
1	O	214	ASN
1	O	239	ASN
1	O	256	GLN
1	O	262	ASN
1	P	52	ASN
1	P	74	GLN
1	P	82	GLN
1	P	116	HIS
1	P	140	ASN
1	P	143	ASN
1	P	150	HIS
1	P	196	ASN
1	P	214	ASN
1	P	239	ASN

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Mol	Chain	Res	Type
1	P	256	GLN
1	P	262	ASN
1	P	278	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	280/306 (91%)	-0.19	3 (1%) 82 83	28, 55, 104, 194	6 (2%)
1	B	280/306 (91%)	-0.23	2 (0%) 89 89	29, 55, 121, 196	5 (1%)
1	C	280/306 (91%)	-0.12	6 (2%) 67 67	32, 64, 123, 193	4 (1%)
1	D	280/306 (91%)	-0.03	10 (3%) 46 46	33, 66, 135, 234	3 (1%)
1	E	280/306 (91%)	0.16	13 (4%) 36 36	59, 94, 146, 213	6 (2%)
1	F	280/306 (91%)	0.25	21 (7%) 17 18	29, 107, 165, 221	5 (1%)
1	G	280/306 (91%)	0.11	12 (4%) 39 38	66, 102, 166, 232	5 (1%)
1	H	280/306 (91%)	0.21	16 (5%) 27 27	68, 110, 191, 245	5 (1%)
1	I	280/306 (91%)	0.03	7 (2%) 61 60	42, 97, 169, 224	5 (1%)
1	J	280/306 (91%)	0.73	36 (12%) 5 4	45, 133, 205, 260	4 (1%)
1	K	280/306 (91%)	0.03	4 (1%) 78 79	40, 92, 147, 214	5 (1%)
1	L	280/306 (91%)	0.43	29 (10%) 8 8	44, 119, 196, 267	6 (2%)
1	M	280/306 (91%)	0.22	8 (2%) 55 56	77, 113, 171, 222	4 (1%)
1	N	280/306 (91%)	0.38	20 (7%) 19 19	28, 116, 165, 232	3 (1%)
1	O	280/306 (91%)	0.92	52 (18%) 2 2	43, 157, 228, 279	5 (1%)
1	P	280/306 (91%)	1.57	91 (32%) 1 1	88, 216, 285, 318	6 (2%)
All	All	4480/4896 (91%)	0.28	330 (7%) 17 18	28, 101, 210, 318	77 (1%)

All (330) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	129	ASN	10.0
1	P	95	THR	8.4
1	P	182	ASN	7.9
1	P	148	GLY	7.7
1	M	141	GLY	7.2

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Mol	Chain	Res	Type	RSRZ
1	P	160	ALA	6.8
1	O	79	GLY	6.6
1	J	159	GLY	6.2
1	O	148	GLY	6.2
1	P	152	GLN	6.0
1	G	124	PHE	6.0
1	P	133	VAL	5.7
1	P	181	LYS	5.7
1	O	155	ASP	5.7
1	N	157	ARG	5.7
1	P	193	GLY	5.4
1	P	93	SER	5.4
1	O	160	ALA	5.4
1	J	192	GLY	5.3
1	O	241	LYS	5.3
1	P	164	ARG	5.3
1	P	101	GLY	5.2
1	N	124	PHE	5.1
1	L	25	TYR	5.1
1	P	52	ASN	5.1
1	P	131	GLY	5.0
1	O	162	HIS	5.0
1	P	122	CYS	4.8
1	P	158	CYS	4.8
1	J	23	VAL	4.8
1	O	129	ASN	4.7
1	K	286	LYS	4.6
1	I	124	PHE	4.6
1	P	150	HIS	4.5
1	O	161	GLY	4.5
1	P	156	SER	4.5
1	P	91	SER	4.4
1	H	156	SER	4.3
1	P	214	ASN	4.3
1	N	7	ASP	4.3
1	O	193	GLY	4.3
1	P	88	THR	4.2
1	H	157	ARG	4.2
1	P	119	LYS	4.2
1	P	115	GLN	4.2
1	P	183	ILE	4.2
1	G	229	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	239	ASN	4.2
1	J	108	TYR	4.2
1	O	52	ASN	4.1
1	N	52	ASN	4.1
1	J	95	THR	4.1
1	J	9	ASP	4.0
1	J	24	LEU	4.0
1	P	89	GLU	4.0
1	L	160	ALA	4.0
1	P	102	VAL	4.0
1	O	194	ASP	4.0
1	E	194	ASP	3.9
1	O	97	ALA	3.9
1	H	239	ASN	3.9
1	M	140	ASN	3.8
1	N	91	SER	3.8
1	O	124	PHE	3.8
1	P	196	ASN	3.7
1	P	112	GLU	3.7
1	D	286	LYS	3.7
1	P	188	THR	3.7
1	H	182	ASN	3.7
1	G	8	THR	3.7
1	J	98	GLU	3.7
1	P	138	GLU	3.7
1	H	8	THR	3.7
1	P	24	LEU	3.7
1	P	19	MET	3.6
1	P	28	TRP	3.6
1	F	156	SER	3.6
1	I	157	ARG	3.6
1	G	52	ASN	3.6
1	P	117	VAL	3.6
1	H	141	GLY	3.5
1	L	239	ASN	3.5
1	P	147	ILE	3.5
1	J	145	HIS	3.5
1	L	193	GLY	3.5
1	L	192	GLY	3.5
1	P	155	ASP	3.5
1	O	157	ARG	3.5
1	P	53	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	N	8	THR	3.4
1	O	149	THR	3.4
1	P	15	HIS	3.4
1	H	160	ALA	3.4
1	J	91	SER	3.4
1	G	194	ASP	3.4
1	J	148	GLY	3.4
1	L	84	GLY	3.4
1	N	155	ASP	3.4
1	O	158	CYS	3.3
1	O	84	GLY	3.3
1	L	129	ASN	3.3
1	P	159	GLY	3.3
1	F	235	TYR	3.3
1	N	258	LYS	3.3
1	J	158	CYS	3.3
1	P	180	LYS	3.3
1	P	16	ASN	3.3
1	O	159	GLY	3.3
1	D	158	CYS	3.3
1	O	239	ASN	3.2
1	N	127	ASP	3.2
1	F	52	ASN	3.2
1	K	94	SER	3.2
1	G	205	LYS	3.2
1	M	52	ASN	3.2
1	J	8	THR	3.2
1	E	193	GLY	3.2
1	J	83	SER	3.2
1	J	200	GLY	3.2
1	L	161	GLY	3.2
1	P	136	LYS	3.1
1	M	156	SER	3.1
1	P	23	VAL	3.1
1	B	158	CYS	3.1
1	J	149	THR	3.1
1	N	150	HIS	3.1
1	O	83	SER	3.1
1	H	164	ARG	3.1
1	P	134	TYR	3.1
1	J	134	TYR	3.0
1	O	50	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	233	ALA	3.0
1	P	97	ALA	3.0
1	P	79	GLY	3.0
1	G	259	GLN	3.0
1	F	160	ALA	3.0
1	O	125	ASP	3.0
1	O	192	GLY	3.0
1	E	192	GLY	3.0
1	P	82	GLN	3.0
1	O	150	HIS	3.0
1	A	124	PHE	2.9
1	P	225	TRP	2.9
1	P	14	SER	2.9
1	N	193	GLY	2.9
1	L	86	ASP	2.9
1	O	25	TYR	2.9
1	C	238	PRO	2.9
1	G	193	GLY	2.9
1	H	124	PHE	2.9
1	L	52	ASN	2.9
1	P	108	TYR	2.9
1	J	193	GLY	2.9
1	P	54	ALA	2.9
1	D	52	ASN	2.9
1	J	71	TYR	2.9
1	N	158	CYS	2.9
1	E	229	SER	2.8
1	G	192	GLY	2.8
1	L	150	HIS	2.8
1	B	157	ARG	2.8
1	O	141	GLY	2.8
1	P	8	THR	2.8
1	L	157	ARG	2.8
1	L	94	SER	2.8
1	O	91	SER	2.8
1	O	14	SER	2.8
1	P	272	TRP	2.8
1	J	85	TRP	2.8
1	E	52	ASN	2.8
1	P	161	GLY	2.8
1	A	239	ASN	2.8
1	O	119	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	194	ASP	2.8
1	P	192	GLY	2.7
1	I	7	ASP	2.7
1	O	101	GLY	2.7
1	F	109	PRO	2.7
1	I	141	GLY	2.7
1	L	69	LYS	2.7
1	P	197	VAL	2.7
1	O	27	ASN	2.7
1	C	124	PHE	2.7
1	F	228	GLN	2.7
1	J	26	PRO	2.7
1	P	241	LYS	2.6
1	F	127	ASP	2.6
1	O	286	LYS	2.6
1	P	186	ASP	2.6
1	L	16	ASN	2.6
1	L	240	GLY	2.6
1	J	180	LYS	2.6
1	D	194	ASP	2.6
1	F	157	ARG	2.6
1	F	236	ASN	2.6
1	N	88	THR	2.6
1	L	92	TYR	2.6
1	O	28	TRP	2.6
1	P	96	VAL	2.6
1	P	143	ASN	2.6
1	F	15	HIS	2.6
1	L	53	GLU	2.6
1	F	193	GLY	2.6
1	N	16	ASN	2.6
1	E	158	CYS	2.6
1	G	156	SER	2.6
1	P	94	SER	2.6
1	P	7	ASP	2.5
1	P	205	LYS	2.5
1	I	97	ALA	2.5
1	P	190	TYR	2.5
1	C	286	LYS	2.5
1	O	200	GLY	2.5
1	P	31	TYR	2.5
1	P	194	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	157	ARG	2.5
1	P	157	ARG	2.5
1	F	14	SER	2.5
1	F	124	PHE	2.5
1	O	96	VAL	2.5
1	O	92	TYR	2.5
1	N	192	GLY	2.5
1	N	286	LYS	2.5
1	O	87	LYS	2.5
1	P	210	ASN	2.5
1	P	187	GLU	2.5
1	D	124	PHE	2.5
1	J	160	ALA	2.5
1	F	192	GLY	2.5
1	P	286	LYS	2.5
1	M	101	GLY	2.5
1	P	144	VAL	2.5
1	O	78	LEU	2.4
1	N	149	THR	2.4
1	C	140	ASN	2.4
1	P	118	PHE	2.4
1	O	8	THR	2.4
1	K	148	GLY	2.4
1	P	169	GLU	2.4
1	J	25	TYR	2.4
1	P	151	THR	2.4
1	F	16	ASN	2.4
1	D	157	ARG	2.4
1	L	89	GLU	2.4
1	P	75	THR	2.4
1	H	193	GLY	2.4
1	L	180	LYS	2.3
1	P	140	ASN	2.3
1	J	165	LYS	2.3
1	L	27	ASN	2.3
1	P	127	ASP	2.3
1	H	238	PRO	2.3
1	O	16	ASN	2.3
1	O	247	TYR	2.3
1	P	239	ASN	2.3
1	P	139	LYS	2.3
1	J	94	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	90	GLY	2.3
1	P	132	PHE	2.3
1	O	23	VAL	2.3
1	P	208	LEU	2.3
1	P	81	SER	2.3
1	P	235	TYR	2.3
1	N	194	ASP	2.3
1	P	206	ASP	2.3
1	L	14	SER	2.3
1	O	225	TRP	2.3
1	K	273	ASN	2.3
1	M	16	ASN	2.3
1	J	119	LYS	2.3
1	F	227	PRO	2.2
1	C	259	GLN	2.2
1	O	116	HIS	2.2
1	E	14	SER	2.2
1	L	22	THR	2.2
1	O	123	GLY	2.2
1	J	120	SER	2.2
1	L	140	ASN	2.2
1	G	286	LYS	2.2
1	H	16	ASN	2.2
1	N	169	GLU	2.2
1	O	24	LEU	2.2
1	E	15	HIS	2.2
1	G	7	ASP	2.2
1	J	164	ARG	2.2
1	E	286	LYS	2.2
1	O	69	LYS	2.2
1	P	120	SER	2.2
1	H	286	LYS	2.2
1	M	87	LYS	2.2
1	O	182	ASN	2.2
1	C	9	ASP	2.2
1	H	145	HIS	2.2
1	L	286	LYS	2.2
1	E	88	THR	2.2
1	J	238	PRO	2.1
1	O	205	LYS	2.1
1	J	14	SER	2.1
1	O	156	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	52	ASN	2.1
1	L	162	HIS	2.1
1	F	141	GLY	2.1
1	N	15	HIS	2.1
1	M	7	ASP	2.1
1	O	109	PRO	2.1
1	P	162	HIS	2.1
1	J	79	GLY	2.1
1	A	156	SER	2.1
1	F	194	ASP	2.1
1	L	155	ASP	2.1
1	J	100	GLY	2.1
1	J	101	GLY	2.1
1	J	96	VAL	2.1
1	P	121	GLY	2.1
1	O	209	LYS	2.1
1	I	186	ASP	2.1
1	H	227	PRO	2.1
1	D	233	ALA	2.1
1	D	259	GLN	2.1
1	D	192	GLY	2.1
1	E	246	ASP	2.0
1	P	57	ASN	2.0
1	F	246	ASP	2.0
1	F	238	PRO	2.0
1	J	157	ARG	2.0
1	P	184	PRO	2.0
1	D	155	ASP	2.0
1	P	107	LYS	2.0
1	L	119	LYS	2.0
1	P	50	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CL	B	287	1/1	0.98	0.18	0.38	57,57,57,57	0
2	CL	D	287	1/1	0.95	0.13	-1.67	56,56,56,56	0
2	CL	L	287	1/1	0.94	0.30	-	72,72,72,72	0
3	NA	C	287	1/1	0.88	0.37	-	38,38,38,38	0

6.5 Other polymers

There are no such residues in this entry.