



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:07 PM GMT

PDB ID : 4N5Z
Title : Crystal structure of aerosol transmissible influenza H5 hemagglutinin mutant (N158D, N224K, Q226L and T318I) from the influenza virus A/Viet Nam/1203/2004 (H5N1)
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2013-10-10
Resolution : 2.95 Å(reported)

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

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

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

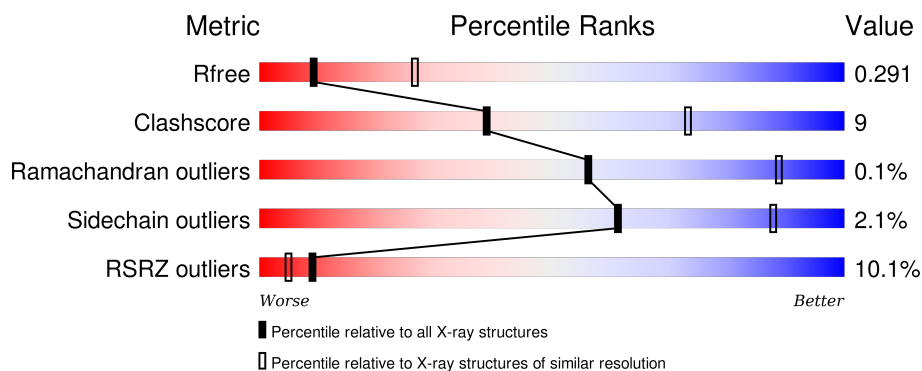
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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

Mol	Chain	Length	Quality of chain
1	A	334	<div> <div>2%</div> <div>62%</div> <div>33%</div> <div>..</div> </div>
1	C	334	<div> <div>3%</div> <div>63%</div> <div>32%</div> <div>..</div> </div>
1	E	334	<div> <div>2%</div> <div>72%</div> <div>23%</div> <div>..</div> </div>
1	G	334	<div> <div>%</div> <div>76%</div> <div>20%</div> <div>..</div> </div>
1	I	334	<div> <div>%</div> <div>69%</div> <div>26%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	334	
1	M	334	
1	O	334	
1	Q	334	
1	S	334	
1	U	334	
1	W	334	
1	Y	334	
1	a	334	
1	c	334	
2	B	181	
2	D	181	
2	F	181	
2	H	181	
2	J	181	
2	L	181	
2	N	181	
2	P	181	
2	R	181	
2	T	181	
2	V	181	
2	X	181	
2	Z	181	
2	b	181	
2	d	181	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	M	2001	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 60979 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	C	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	E	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	G	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	I	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	K	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	M	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	O	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	Q	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	S	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	U	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	W	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	Y	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	a	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			
1	c	324	Total	C	N	O	S	0	1	0
			2574	1630	442	487	15			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
A	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
A	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
A	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
A	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
A	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
A	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
A	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
C	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
C	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
C	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
C	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
C	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
C	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
C	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
C	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
E	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
E	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
E	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
E	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
E	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
E	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
E	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
E	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
G	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
G	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
G	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
G	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
G	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
G	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
G	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
G	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
I	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
I	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
I	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
I	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
I	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
I	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
I	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
I	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
K	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
K	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
K	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
K	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
K	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
K	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
K	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
K	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
M	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
M	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
M	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
M	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
M	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
M	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
M	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
M	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
O	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
O	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
O	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
O	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
O	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
O	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
O	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
O	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
Q	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
Q	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
Q	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
Q	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
Q	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
Q	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
Q	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
Q	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
S	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
S	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
S	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
S	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
S	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
S	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
S	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
S	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
U	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
U	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
U	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
U	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
U	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
U	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
U	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
U	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
W	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
W	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
W	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
W	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
W	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
W	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
W	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
W	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
Y	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
Y	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
Y	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
Y	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
Y	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
Y	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
Y	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
Y	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
a	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
a	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
a	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
a	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
a	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
a	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
a	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
a	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33
c	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
c	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
c	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
c	10	GLY	-	EXPRESSION TAG	UNP Q6DQ33
c	158	ASP	ASN	ENGINEERED MUTATION	UNP Q6DQ33
c	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
c	226	LEU	GLN	ENGINEERED MUTATION	UNP Q6DQ33
c	318	ILE	THR	ENGINEERED MUTATION	UNP Q6DQ33

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	D	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	H	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	J	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	L	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	N	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	P	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	R	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	T	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	V	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	X	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	Z	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	b	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			
2	d	177	Total	C	N	O	S	0	0	0
			1433	889	251	285	8			

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
B	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
B	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
B	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
B	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
B	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
B	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
D	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
D	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
D	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
D	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
D	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
D	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
D	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
F	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
F	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
F	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
F	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
F	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
F	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
F	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
H	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
H	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
H	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
H	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
H	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
H	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
H	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
J	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
J	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
J	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
J	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
J	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
J	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
J	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
L	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
L	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
L	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
L	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
L	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
L	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
L	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
N	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
N	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
N	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
N	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
N	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
N	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
N	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
P	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
P	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
P	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
P	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
P	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
P	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
P	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
R	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
R	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
R	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
R	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
R	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
R	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
R	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
T	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
T	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
T	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
T	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
T	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
T	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
T	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
V	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
V	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
V	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
V	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
V	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
V	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
V	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
X	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
X	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
X	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
X	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
X	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
X	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
X	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
Z	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
Z	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
Z	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
Z	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
Z	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
Z	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
Z	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
b	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
b	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
b	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
b	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
b	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
b	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
b	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33
d	175	SER	-	EXPRESSION TAG	UNP Q6DQ33
d	176	GLY	-	EXPRESSION TAG	UNP Q6DQ33
d	177	ARG	-	EXPRESSION TAG	UNP Q6DQ33
d	178	LEU	-	EXPRESSION TAG	UNP Q6DQ33
d	179	VAL	-	EXPRESSION TAG	UNP Q6DQ33
d	180	PRO	-	EXPRESSION TAG	UNP Q6DQ33
d	181	ARG	-	EXPRESSION TAG	UNP Q6DQ33

- Molecule 3 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			39	22	2	15		
3	C	3	Total	C	N	O	0	0
			39	22	2	15		
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	G	3	Total	C	N	O	0	0
			39	22	2	15		
3	I	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	M	3	Total	C	N	O	0	0
			39	22	2	15		
3	O	3	Total	C	N	O	0	0
			39	22	2	15		
3	Q	3	Total	C	N	O	0	0
			39	22	2	15		
3	S	3	Total	C	N	O	0	0
			39	22	2	15		
3	U	3	Total	C	N	O	0	0
			39	22	2	15		
3	W	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

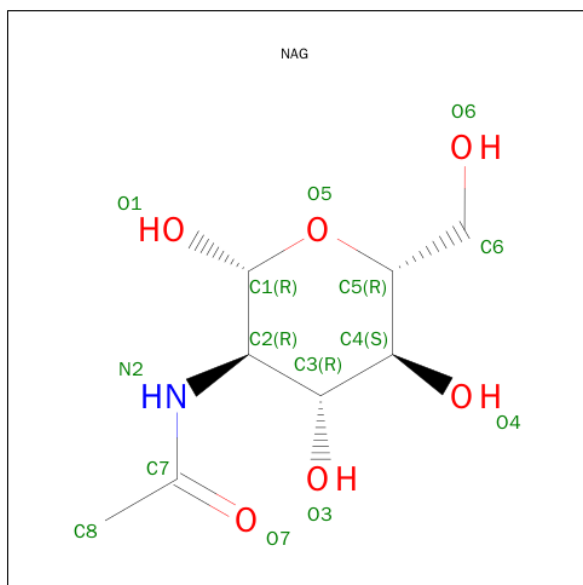
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	U	2	Total	C	N	O	0	0
			28	16	2	10		
4	W	2	Total	C	N	O	0	0
			28	16	2	10		
4	Y	2	Total	C	N	O	0	0
			28	16	2	10		
4	c	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

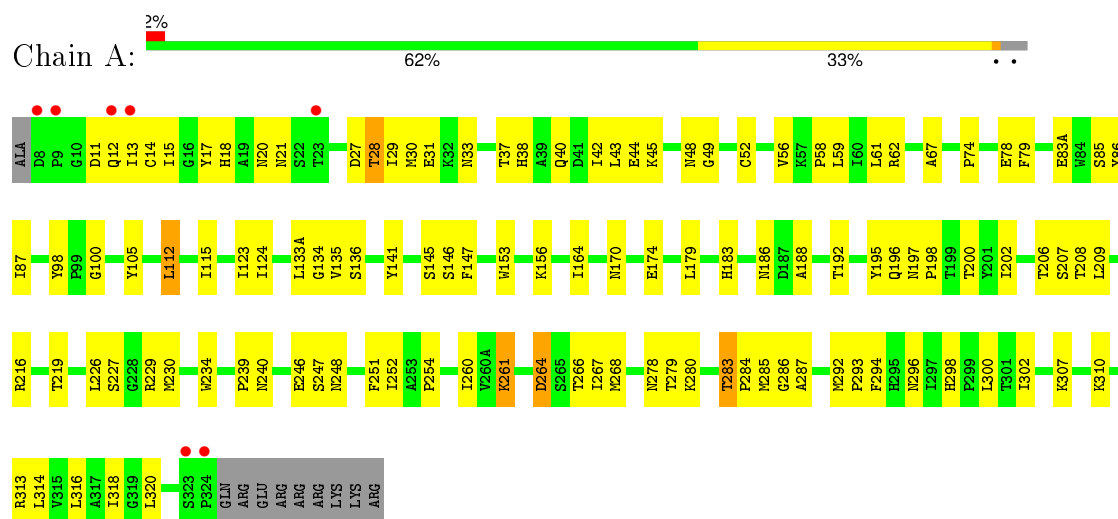
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	M	1	Total	C	N	O	0	0
			14	8	1	5		
5	O	1	Total	C	N	O	0	0
			14	8	1	5		
5	Y	1	Total	C	N	O	0	0
			14	8	1	5		
5	a	1	Total	C	N	O	0	0
			14	8	1	5		
5	c	1	Total	C	N	O	0	0
			14	8	1	5		

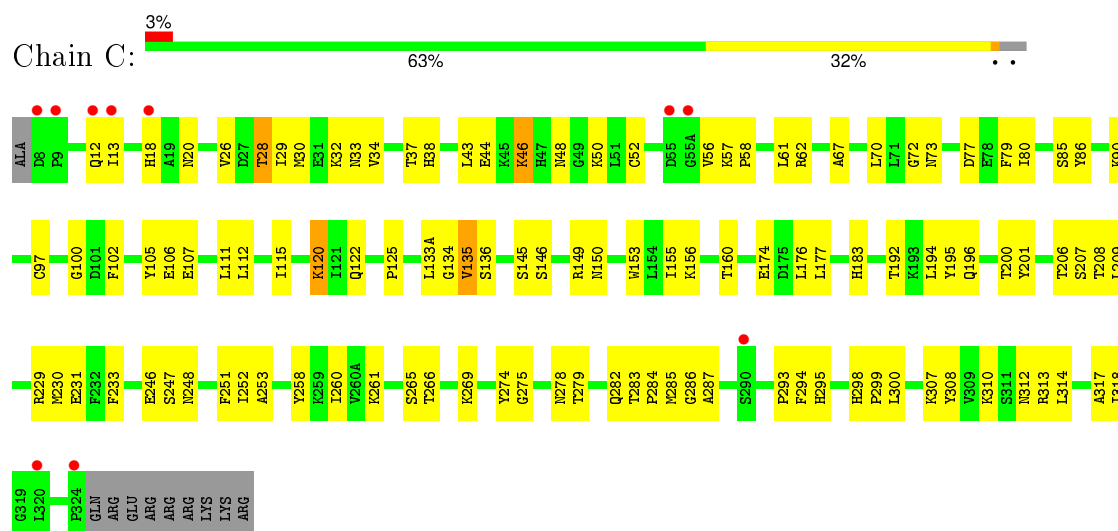
3 Residue-property plots

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: Hemagglutinin HA1 chain

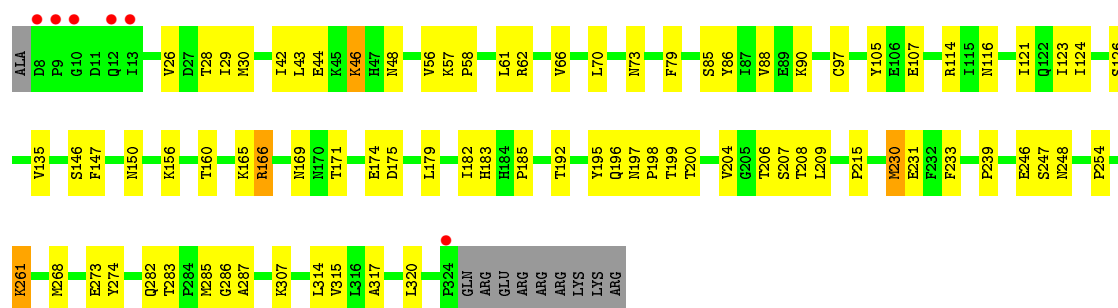


• Molecule 1: Hemagglutinin HA1 chain

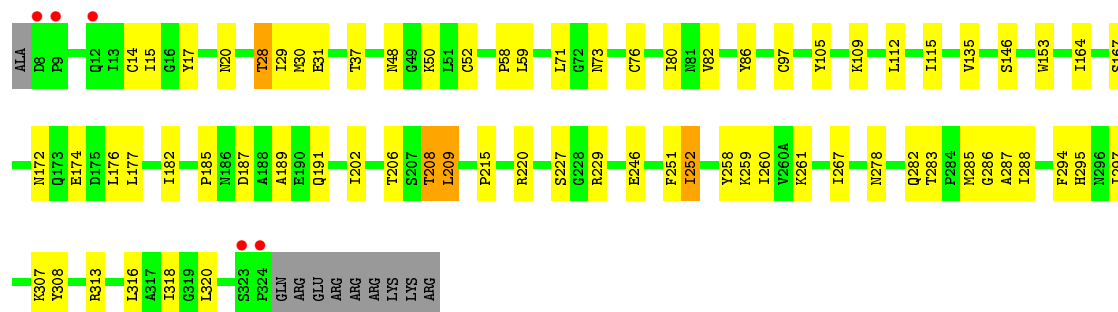
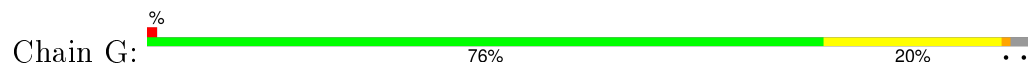


• Molecule 1: Hemagglutinin HA1 chain

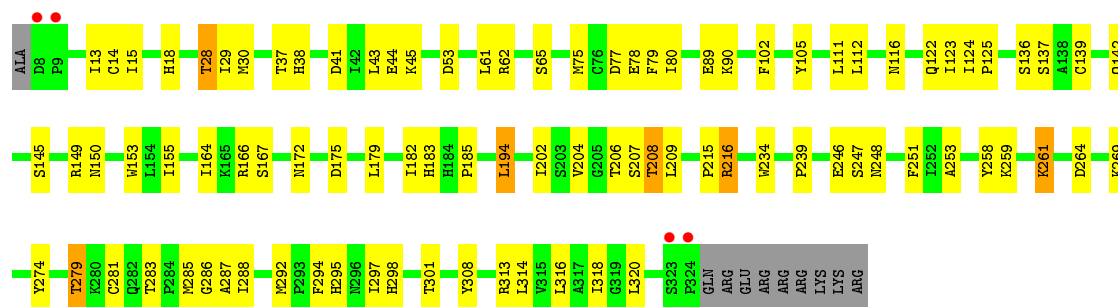




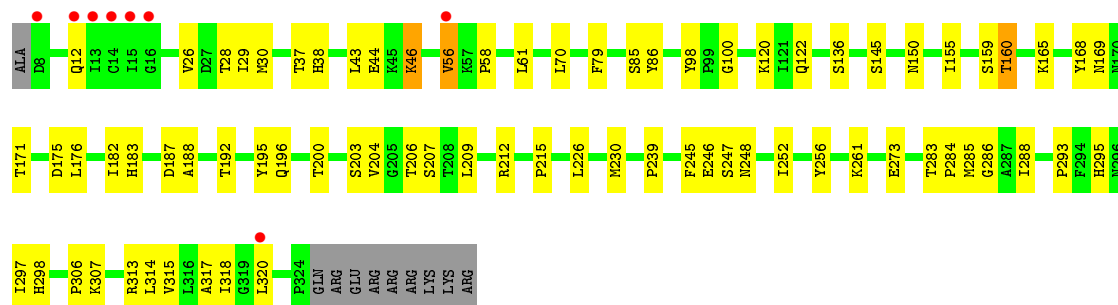
• Molecule 1: Hemagglutinin HA1 chain



• Molecule 1: Hemagglutinin HA1 chain



• Molecule 1: Hemagglutinin HA1 chain



Chain M:

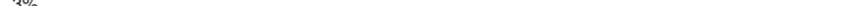
4% 71% 25%

ALA D8 P9 G10 D11 Q12 I13 I15 I16 I21 S22 T28 I29 M30 T37 R38 A39 Q40 L43 H47 D55 G55A V56 A57 P58 L61 R62 L70 N73 C76 D77 E78 F79 V82 P83 E83A Y86 Q97 G100 D101 F102 Y105 V106 R114 I121 K125A S133 L133A G134 V135 S136 S137 A138 C139 P140 S145 M150 W153 K156 M172 Q173 E174 L179 W180 G181 I182 H183 M186 E190 Q191 T192 Y195 Q196 T200 Y201 I202 S203 T206 S207 T208 L209 P215 T219 L226

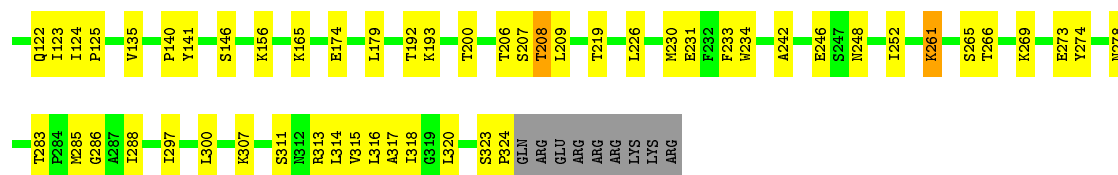
Chain O: 

Chain Q:

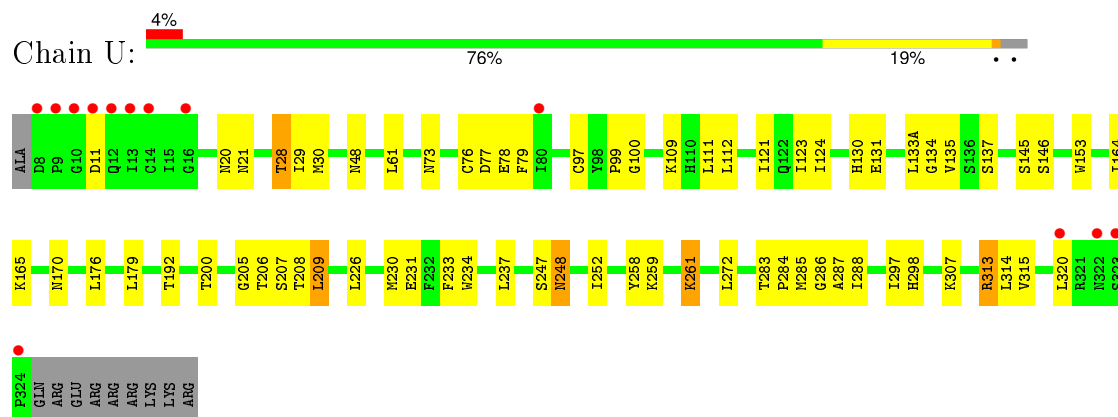
2% 72% 22%

Chain S: 

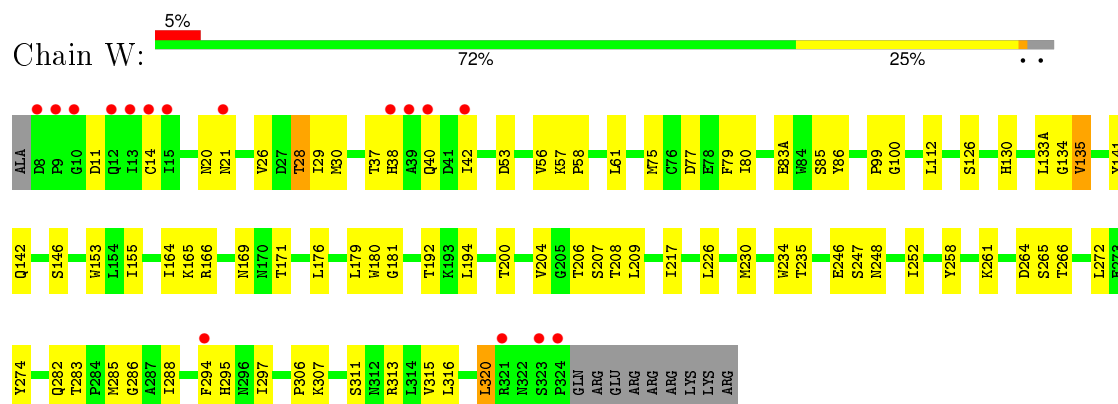
ALA D8 P9 G10 D11 Q12 I13 V26 D27 T28 I29 M30 E31 K32 N33 V34 A39 Q40 L43 E44 K46 G49 D55 G55A V56 K57 L61 A67 N73 P74 M75 C76 D77 E78 F79 E83A E84 S85 K90 D101 Y105 L112 I115 N116 F117



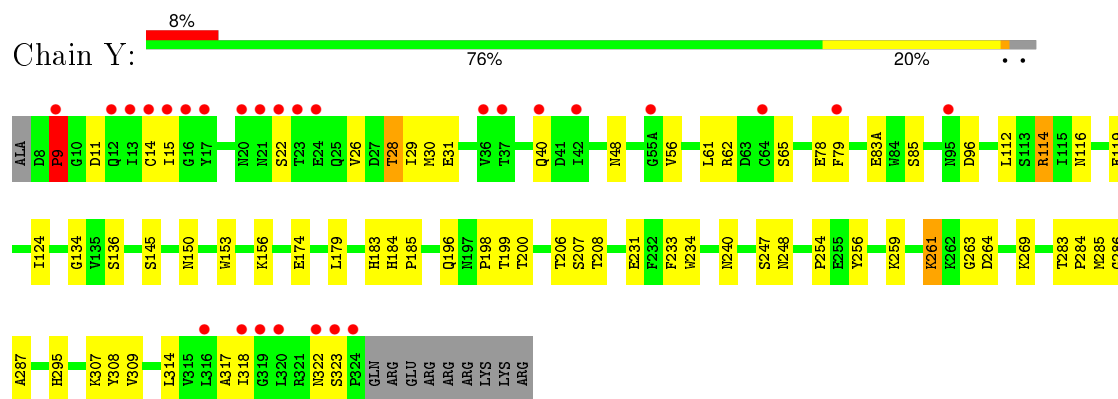
• Molecule 1: Hemagglutinin HA1 chain



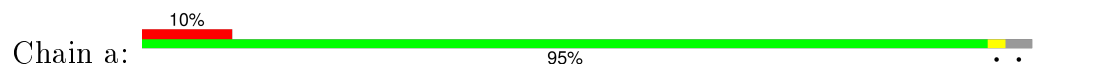
• Molecule 1: Hemagglutinin HA1 chain



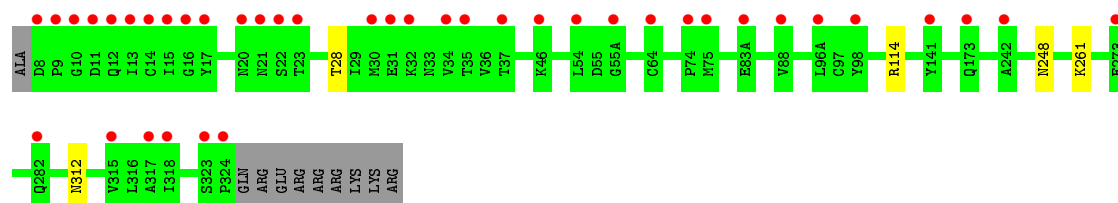
• Molecule 1: Hemagglutinin HA1 chain



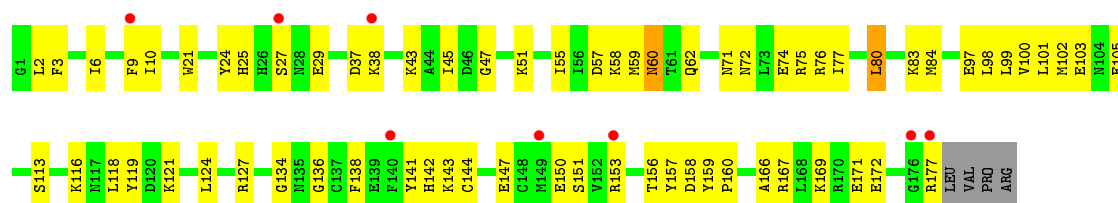
• Molecule 1: Hemagglutinin HA1 chain



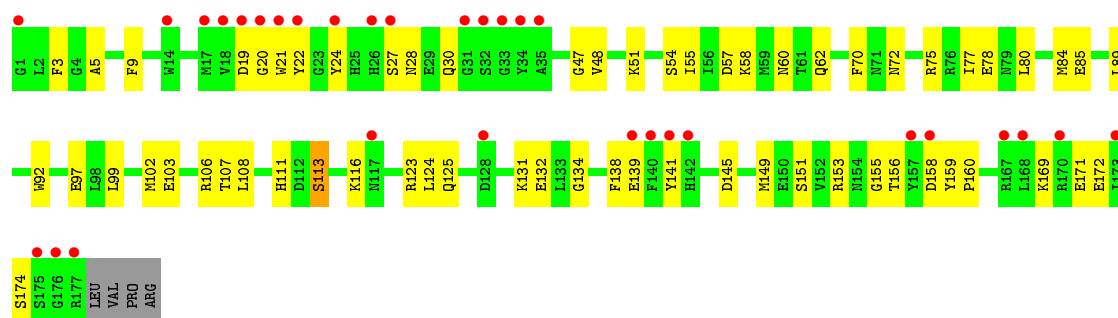
- Molecule 1: Hemagglutinin HA1 chain



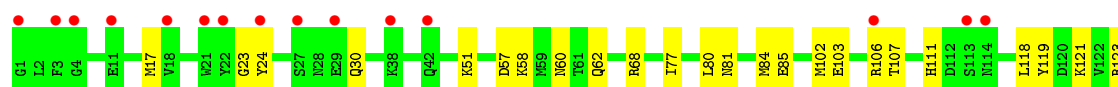
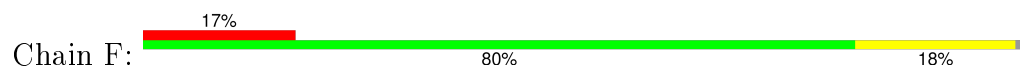
- Molecule 2: Hemagglutinin

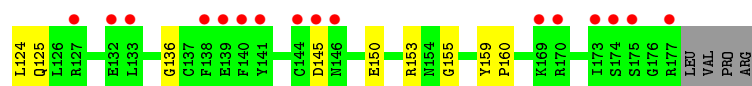


- Molecule 2: Hemagglutinin

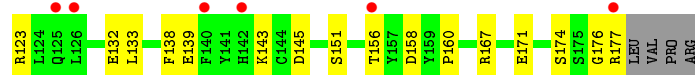


- Molecule 2: Hemagglutinin

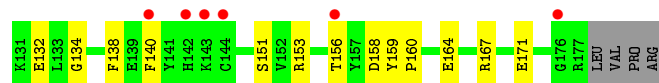




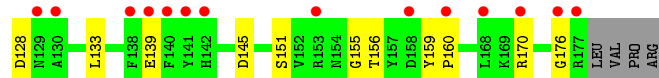
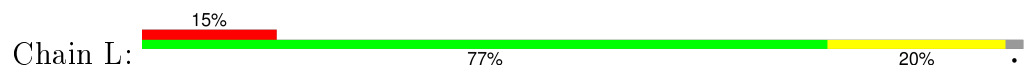
• Molecule 2: Hemagglutinin



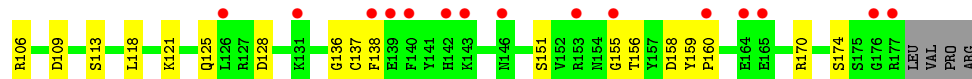
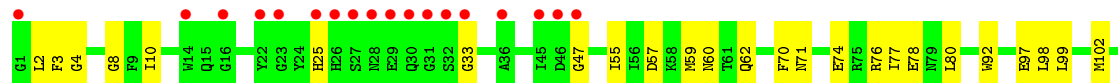
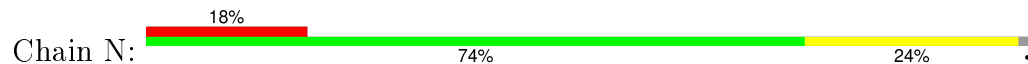
• Molecule 2: Hemagglutinin



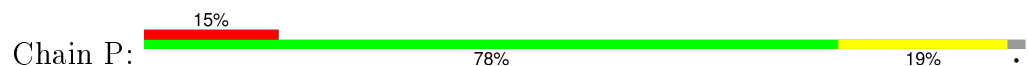
• Molecule 2: Hemagglutinin

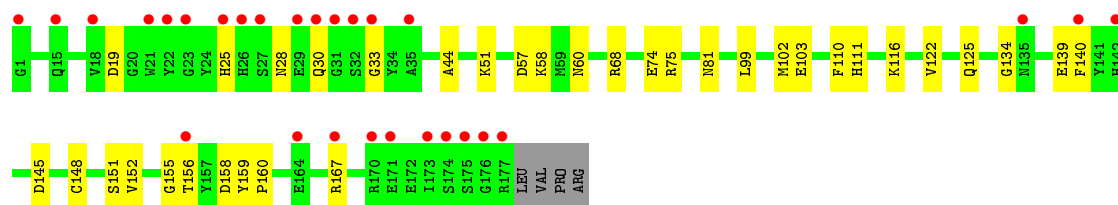


• Molecule 2: Hemagglutinin

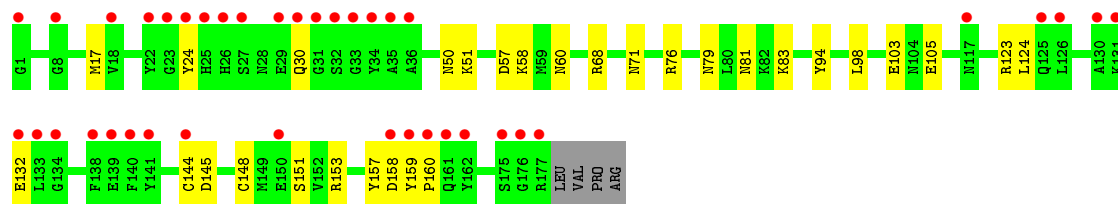
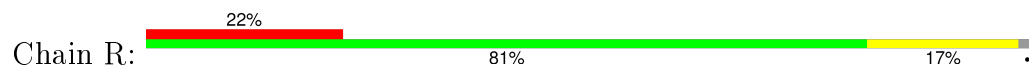


• Molecule 2: Hemagglutinin

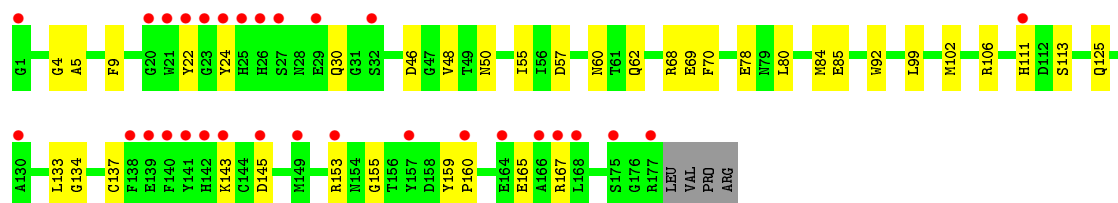
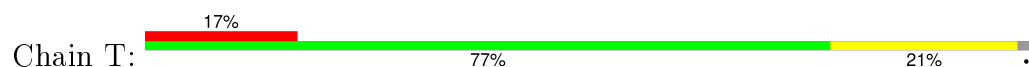




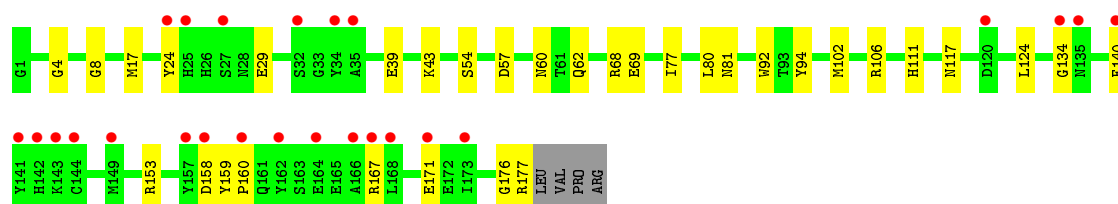
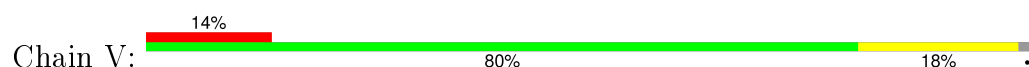
• Molecule 2: Hemagglutinin



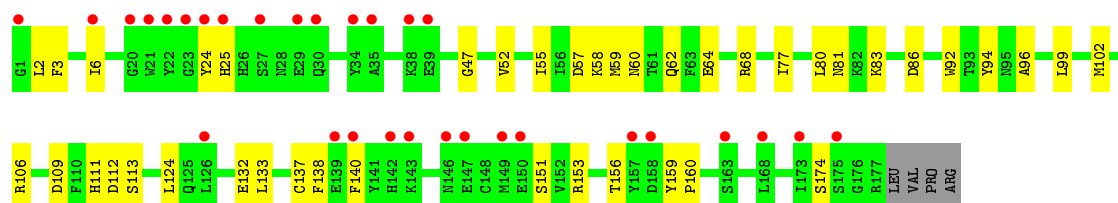
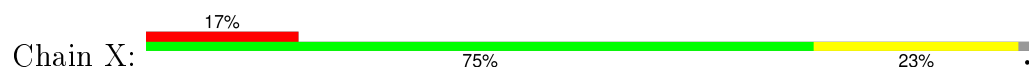
• Molecule 2: Hemagglutinin



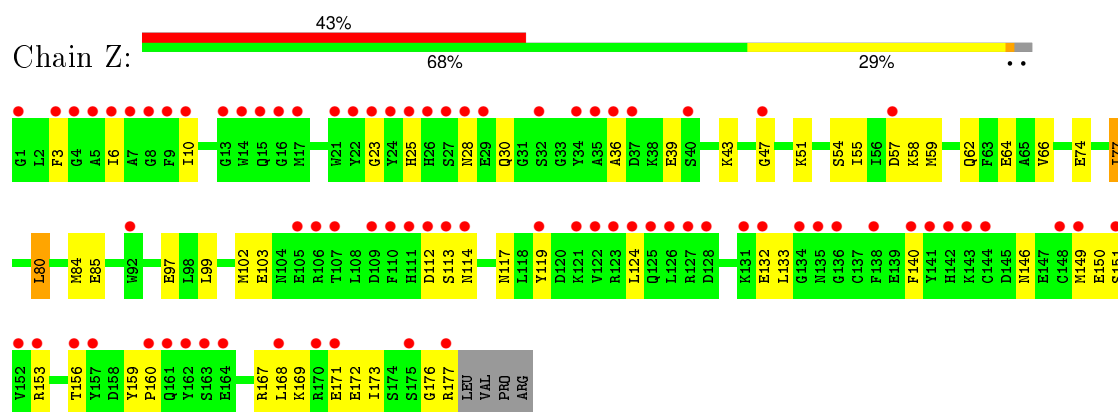
• Molecule 2: Hemagglutinin



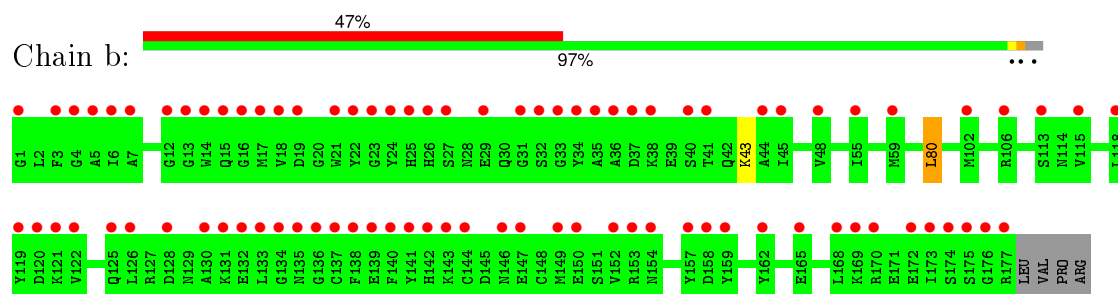
• Molecule 2: Hemagglutinin



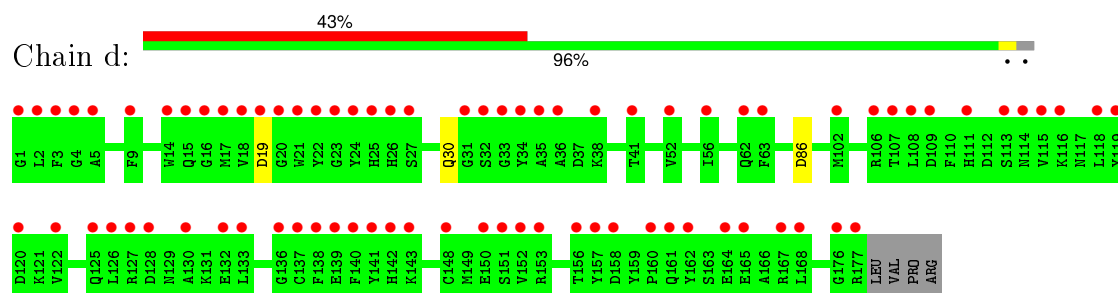
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	117.24Å 118.94Å 273.41Å 88.43° 89.68° 60.26°	Depositor
Resolution (Å)	47.75 – 2.95 48.12 – 2.95	Depositor EDS
% Data completeness (in resolution range)	87.7 (47.75-2.95) 87.4 (48.12-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.96Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.233 , 0.281 0.245 , 0.291	Depositor DCC
R_{free} test set	11870 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	63.6	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 51.6	EDS
Estimated twinning fraction	0.013 for k,-h+k,l 0.013 for h-k,h,l 0.055 for -h+k,-h,l 0.055 for -k,h-k,l 0.067 for h,h-k,-l 0.027 for -k,-h,-l 0.012 for -h,-k,l 0.026 for -h+k,k,-l 0.017 for h-k,-k,-l 0.011 for -h,-h+k,-l 0.010 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 236037 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	60979	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.66	0/2640	0.83	0/3585
1	C	0.56	0/2640	0.75	1/3585 (0.0%)
1	E	0.59	0/2640	0.76	0/3585
1	G	0.68	1/2640 (0.0%)	0.86	6/3585 (0.2%)
1	I	0.69	1/2640 (0.0%)	0.87	2/3585 (0.1%)
1	K	0.61	0/2640	0.75	1/3585 (0.0%)
1	M	0.66	0/2640	0.80	0/3585
1	O	0.64	0/2640	0.79	1/3585 (0.0%)
1	Q	0.64	0/2640	0.82	1/3585 (0.0%)
1	S	0.57	0/2640	0.75	0/3585
1	U	0.57	0/2640	0.74	1/3585 (0.0%)
1	W	0.58	1/2640 (0.0%)	0.74	0/3585
1	Y	0.46	0/2640	0.65	1/3585 (0.0%)
1	a	0.44	0/2640	0.64	0/3585
1	c	0.44	0/2640	0.63	0/3585
2	B	0.50	0/1460	0.69	1/1961 (0.1%)
2	D	0.41	0/1460	0.56	0/1961
2	F	0.40	0/1460	0.56	0/1961
2	H	0.49	0/1460	0.64	0/1961
2	J	0.50	0/1460	0.67	0/1961
2	L	0.42	0/1460	0.54	0/1961
2	N	0.42	0/1460	0.61	0/1961
2	P	0.44	0/1460	0.60	0/1961
2	R	0.44	0/1460	0.57	0/1961
2	T	0.39	0/1460	0.57	0/1961
2	V	0.42	0/1460	0.58	0/1961
2	X	0.40	0/1460	0.59	0/1961
2	Z	0.35	0/1460	0.60	1/1961 (0.1%)
2	b	0.33	0/1460	0.56	1/1961 (0.1%)
2	d	0.36	0/1460	0.55	0/1961
All	All	0.54	3/61500 (0.0%)	0.71	17/83190 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Y	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	W	135	VAL	CB-CG2	-5.53	1.41	1.52
1	I	139	CYS	CB-SG	-5.52	1.72	1.81
1	G	153	TRP	CB-CG	5.50	1.60	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	166	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	Y	9	PRO	CA-N-CD	-7.79	100.59	111.50
1	G	229	ARG	NE-CZ-NH2	-7.40	116.60	120.30
2	Z	80	LEU	CA-CB-CG	7.16	131.78	115.30
1	G	229	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	U	209	LEU	CA-CB-CG	6.60	130.49	115.30
2	b	80	LEU	CA-CB-CG	6.20	129.56	115.30
1	G	252	ILE	CG1-CB-CG2	-5.68	98.90	111.40
1	G	80	ILE	CG1-CB-CG2	-5.51	99.28	111.40
1	G	177	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	I	112	LEU	CB-CG-CD2	-5.33	101.94	111.00
1	G	209	LEU	CA-CB-CG	5.30	127.50	115.30
1	K	212	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	O	241	ASP	CB-CG-OD1	5.17	122.96	118.30
1	I	216	ARG	NE-CZ-NH1	-5.14	117.73	120.30
2	B	80	LEU	CB-CG-CD2	-5.14	102.25	111.00
1	C	229	ARG	NE-CZ-NH2	-5.08	117.76	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	Y	9	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2574	0	2525	96	0
1	C	2574	0	2525	90	0
1	E	2574	0	2525	58	0
1	G	2574	0	2525	46	0
1	I	2574	0	2525	59	0
1	K	2574	0	2525	55	0
1	M	2574	0	2525	56	0
1	O	2574	0	2524	45	0
1	Q	2574	0	2525	57	0
1	S	2574	0	2525	63	0
1	U	2574	0	2525	52	0
1	W	2574	0	2525	57	0
1	Y	2574	0	2525	47	0
1	a	2574	0	2526	0	0
1	c	2574	0	2525	0	0
2	B	1433	0	1340	65	0
2	D	1433	0	1340	60	0
2	F	1433	0	1340	23	0
2	H	1433	0	1340	39	0
2	J	1433	0	1340	37	0
2	L	1433	0	1340	28	0
2	N	1433	0	1340	34	0
2	P	1433	0	1340	24	0
2	R	1433	0	1340	22	0
2	T	1433	0	1340	32	0
2	V	1433	0	1340	26	0
2	X	1433	0	1340	29	0
2	Z	1433	0	1340	40	0
2	b	1433	0	1340	0	0
2	d	1433	0	1340	0	0
3	A	39	0	34	1	0
3	C	39	0	34	1	0
3	E	39	0	34	1	0
3	G	39	0	34	1	0
3	I	39	0	34	0	0
3	K	39	0	34	0	0
3	M	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	39	0	34	0	0
3	Q	39	0	34	0	0
3	S	39	0	34	1	0
3	U	39	0	34	0	0
3	W	39	0	34	0	0
4	A	28	0	25	0	0
4	E	28	0	25	0	0
4	G	28	0	25	1	0
4	I	28	0	25	1	0
4	O	28	0	25	0	0
4	Q	28	0	25	1	0
4	S	28	0	25	1	0
4	U	28	0	25	0	0
4	W	28	0	25	1	0
4	Y	28	0	25	1	0
4	c	28	0	25	0	0
5	C	14	0	13	0	0
5	K	14	0	13	0	0
5	M	14	0	13	0	0
5	O	14	0	13	0	0
5	Y	14	0	13	1	0
5	a	14	0	13	0	0
5	c	14	0	13	0	0
All	All	60979	0	58749	1073	0

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 9.

All (1073) 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:192:THR:HG21	1:S:192:THR:HG21	1.34	1.08
1:I:283:THR:HG22	1:I:285:MET:H	1.26	1.00
1:Q:283:THR:HG22	1:Q:285:MET:H	1.25	1.00
1:G:283:THR:HG22	1:G:285:MET:H	1.27	0.99
1:U:206:THR:HG22	1:U:208:THR:H	1.25	0.98
1:O:283:THR:HG22	1:O:285:MET:H	1.29	0.97
1:S:283:THR:HG22	1:S:285:MET:H	1.35	0.90
1:U:283:THR:HG22	1:U:285:MET:H	1.38	0.89
1:A:206:THR:HG22	1:A:208:THR:H	1.37	0.87
1:A:283:THR:HG22	1:A:285:MET:H	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:166:ARG:HH11	1:Q:166:ARG:HG3	1.41	0.85
1:E:166:ARG:HG3	1:E:166:ARG:HH11	1.43	0.84
1:Y:283:THR:HG22	1:Y:285:MET:H	1.41	0.84
1:G:206:THR:HG22	1:G:208:THR:H	1.41	0.84
1:E:283:THR:HG22	1:E:285:MET:H	1.43	0.83
1:M:283:THR:HG22	1:M:285:MET:H	1.42	0.83
1:W:283:THR:HG22	1:W:285:MET:H	1.44	0.83
1:W:206:THR:HG22	1:W:208:THR:H	1.43	0.82
1:C:283:THR:HG22	1:C:285:MET:H	1.52	0.80
1:I:206:THR:HG22	1:I:208:THR:H	1.44	0.80
1:W:134:GLY:HA3	1:W:153:TRP:HB3	1.64	0.79
1:A:29:ILE:HD11	2:B:102:MET:HG2	1.97	0.78
1:W:206:THR:HB	1:W:209:LEU:H	1.48	0.77
1:K:283:THR:HG22	1:K:285:MET:H	1.50	0.77
1:A:12:GLN:HB2	2:B:27:SER:HB3	2.63	0.76
1:A:61:LEU:HA	1:A:79:PHE:CZ	2.38	0.76
1:S:29:ILE:HD11	2:T:102:MET:HG2	1.67	0.75
1:C:12:GLN:HB2	2:D:27:SER:HB3	3.50	0.75
1:S:206:THR:HB	1:S:209:LEU:H	1.51	0.75
1:K:192:THR:CG2	1:S:192:THR:HG21	2.16	0.74
1:S:43:LEU:HB2	1:S:314:LEU:HB2	1.69	0.74
1:I:29:ILE:HD11	2:J:102:MET:HG2	1.70	0.74
1:K:70:LEU:O	1:K:150:ASN:ND2	2.21	0.74
1:U:131:GLU:HB3	1:U:133(A):LEU:HD23	1.69	0.74
1:K:29:ILE:HD11	2:L:102:MET:HA	1.70	0.74
1:C:192:THR:HG21	1:W:192:THR:HG21	1.70	0.74
1:S:61:LEU:HA	1:S:79:PHE:CZ	2.23	0.73
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.84	0.73
1:E:70:LEU:O	1:E:150:ASN:ND2	2.20	0.73
1:I:279:THR:HB	1:I:281:CYS:H	1.54	0.73
1:C:312:ASN:OD1	1:C:312:ASN:N	3.76	0.73
2:N:174:SER:O	2:P:167:ARG:NH1	2.21	0.73
1:I:283:THR:HB	1:I:286:GLY:O	1.89	0.73
2:B:134:GLY:HA2	2:D:124:LEU:HD22	197.37	0.73
2:B:141:TYR:O	2:B:169:LYS:HG2	2.72	0.72
1:K:44:GLU:OE1	1:K:46:LYS:HG3	1.90	0.72
2:T:30:GLN:HE22	2:T:145:ASP:HB2	1.53	0.71
2:X:62:GLN:HG3	2:X:92:TRP:CG	2.25	0.71
1:I:61:LEU:HA	1:I:79:PHE:CZ	2.26	0.71
1:E:43:LEU:HB2	1:E:314:LEU:HB2	1.73	0.71
2:D:84:MET:HE2	2:D:85:GLU:HG2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:134:GLY:HA3	1:Y:153:TRP:HB3	1.70	0.71
1:C:57:LYS:HE2	1:C:274:TYR:CZ	2.25	0.71
1:U:76:CYS:O	1:U:78:GLU:N	2.21	0.71
1:C:156:LYS:HD2	1:C:196:GLN:HB2	2.28	0.71
2:N:106:ARG:HH22	2:R:105:GLU:HG2	1.56	0.71
1:E:192:THR:HG21	1:U:192:THR:HG21	1.72	0.71
1:M:83(A):GLU:OE1	1:M:261:LYS:NZ	2.24	0.71
1:C:134:GLY:HA3	1:C:153:TRP:HB3	2.24	0.71
1:A:30:MET:HG2	2:H:47:GLY:O	1.90	0.70
1:K:12:GLN:HB2	2:L:27:SER:HB3	1.73	0.70
1:C:80:ILE:O	1:C:120:LYS:NZ	2.25	0.70
2:Z:173:ILE:HG23	2:Z:177:ARG:HE	1.57	0.70
2:D:134:GLY:HA2	2:Z:124:LEU:HD22	255.11	0.69
1:U:61:LEU:HA	1:U:79:PHE:CZ	2.28	0.69
1:S:32:LYS:NZ	2:V:54:SER:OG	2.27	0.68
1:Q:283:THR:HB	1:Q:286:GLY:O	1.93	0.68
1:Y:62:ARG:NH1	1:Y:78:GLU:OE2	2.26	0.68
2:L:57:ASP:O	2:L:60:ASN:HB2	1.94	0.68
1:Y:307:LYS:NZ	2:Z:64:GLU:OE2	2.26	0.68
2:T:55:ILE:HG12	2:T:99:LEU:HD21	1.75	0.67
1:S:206:THR:HG22	1:S:208:THR:H	1.57	0.67
1:U:206:THR:HB	1:U:209:LEU:H	1.59	0.67
1:I:62:ARG:O	1:I:90:LYS:HD2	1.95	0.67
1:Y:61:LEU:HA	1:Y:79:PHE:CZ	2.29	0.67
2:D:19:ASP:N	2:D:19:ASP:OD1	2.75	0.67
2:B:29:GLU:OE1	2:B:143:LYS:NZ	2.24	0.66
1:Y:26:VAL:HG21	1:Y:317:ALA:HB2	1.76	0.66
2:D:106:ARG:HG2	2:F:106:ARG:HH22	1.61	0.66
1:G:182:ILE:HD11	1:G:215:PRO:HD3	1.78	0.66
1:Y:314:LEU:HD21	2:Z:97:GLU:HG2	1.77	0.66
2:R:30:GLN:HE22	2:R:145:ASP:HB2	1.59	0.66
2:D:57:ASP:O	2:D:60:ASN:HB2	1.96	0.66
1:G:29:ILE:HD11	2:H:102:MET:HG2	1.78	0.66
1:G:288:ILE:HD11	1:G:297:ILE:HG13	1.78	0.66
2:J:54:SER:O	2:J:58:LYS:HG2	1.96	0.65
1:S:135:VAL:HG22	1:S:146:SER:HA	1.78	0.65
2:J:126:LEU:HD13	2:J:140:PHE:HE1	1.61	0.65
1:U:28:THR:HG23	1:U:30:MET:H	1.61	0.65
1:I:13:ILE:HG22	2:J:138:PHE:HB2	1.79	0.65
1:M:100:GLY:HA3	1:M:230:MET:O	1.97	0.65
1:I:77:ASP:OD2	1:I:149:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:165:LYS:HE2	1:S:246:GLU:OE2	1.97	0.64
1:A:43:LEU:HD23	1:A:45:LYS:HE3	2.65	0.64
1:O:22:SER:O	1:O:322:ASN:ND2	2.31	0.64
1:I:30:MET:HG2	2:B:47:GLY:O	1.96	0.64
1:S:230:MET:SD	1:S:252:ILE:HD11	2.38	0.64
2:F:30:GLN:HE22	2:F:145:ASP:HA	1.60	0.64
1:M:12:GLN:HG3	2:N:138:PHE:O	1.98	0.64
1:G:307:LYS:HE3	2:H:60:ASN:O	1.97	0.64
2:P:28:ASN:ND2	2:P:30:GLN:OE1	2.31	0.64
1:C:307:LYS:NZ	2:D:60:ASN:O	3.23	0.64
1:G:318:ILE:HG23	2:H:48:VAL:HG11	1.79	0.64
2:F:84:MET:HE2	2:F:85:GLU:HG2	1.77	0.64
1:K:100:GLY:HA3	1:K:230:MET:O	1.97	0.64
2:L:84:MET:HE2	2:L:85:GLU:HG2	1.80	0.64
1:O:28:THR:HG23	1:O:30:MET:H	1.63	0.64
2:L:133:LEU:HD21	2:L:139:GLU:HB2	1.80	0.64
1:K:183:HIS:ND1	1:K:195:TYR:OH	2.30	0.64
1:E:44:GLU:OE1	1:E:46:LYS:HG3	1.99	0.63
1:Y:9:PRO:HD2	1:Y:9:PRO:O	1.96	0.63
2:H:29:GLU:OE1	2:H:143:LYS:NZ	2.28	0.63
1:Q:283:THR:HG22	1:Q:285:MET:N	2.08	0.63
1:Q:18:HIS:ND1	2:R:17:MET:O	2.27	0.63
1:O:156:LYS:HD2	1:O:196:GLN:HB2	1.80	0.63
2:J:151:SER:O	2:J:156:THR:N	2.32	0.63
1:W:29:ILE:HD11	2:X:102:MET:HG2	1.80	0.63
1:M:283:THR:HB	1:M:286:GLY:O	1.99	0.62
1:Y:150:ASN:HA	1:Y:256:TYR:HD2	1.63	0.62
1:G:59:LEU:HD13	1:G:82:VAL:HG11	1.81	0.62
1:W:126:SER:HB2	1:W:166:ARG:HH22	1.62	0.62
1:M:12:GLN:HE21	2:N:137:CYS:HB3	1.63	0.62
2:J:57:ASP:O	2:J:60:ASN:HB2	1.98	0.62
2:T:4:GLY:HA3	2:V:117:ASN:ND2	2.15	0.62
2:B:3:PHE:CE2	2:B:113:SER:HB2	2.76	0.62
1:W:200:THR:HA	1:W:248:ASN:OD1	2.00	0.62
1:E:56:VAL:HB	1:E:85:SER:HB3	1.82	0.62
1:O:116:ASN:HB2	1:O:261:LYS:HG2	1.82	0.61
2:Z:149:MET:O	2:Z:153:ARG:HG3	1.99	0.61
1:Y:200:THR:HA	1:Y:248:ASN:OD1	2.00	0.61
1:K:283:THR:HB	1:K:286:GLY:O	2.01	0.61
1:A:135:VAL:HG23	1:A:146:SER:HA	3.74	0.61
2:T:68:ARG:NH2	2:X:83:LYS:HG3	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:VAL:HA	1:C:313:ARG:NH2	2.14	0.61
1:Q:65:SER:OG	1:Q:96:ASP:HA	2.00	0.61
2:B:72:ASN:OD1	2:B:75:ARG:NH2	2.55	0.61
2:N:99:LEU:HD13	2:R:98:LEU:HD21	1.82	0.61
1:C:196:GLN:HE22	1:M:192:THR:HG21	94.90	0.61
1:C:26:VAL:HG21	1:C:317:ALA:HB2	2.41	0.61
2:D:72:ASN:OD1	2:D:75:ARG:NH1	3.22	0.61
2:F:57:ASP:O	2:F:60:ASN:HB2	2.00	0.61
1:O:29:ILE:HD11	2:P:102:MET:HG2	1.83	0.61
1:M:29:ILE:HD11	2:N:102:MET:HA	1.82	0.61
1:W:265:SER:OG	1:W:266:THR:N	2.34	0.61
1:O:283:THR:HB	1:O:286:GLY:O	2.00	0.60
1:E:192:THR:CG2	1:U:192:THR:HG21	2.31	0.60
2:Z:84:MET:HE2	2:Z:85:GLU:HG2	1.82	0.60
2:D:151:SER:O	2:D:156:THR:N	2.34	0.60
1:A:13:ILE:HG22	2:B:138:PHE:HB2	2.15	0.60
2:V:24:TYR:CD2	2:V:153:ARG:HG2	2.36	0.60
1:W:288:ILE:HD11	1:W:297:ILE:HG13	1.82	0.60
2:H:151:SER:O	2:H:156:THR:N	2.34	0.60
1:C:100:GLY:HA3	1:C:230:MET:O	2.02	0.60
2:N:57:ASP:O	2:N:60:ASN:HB2	2.02	0.60
1:A:17:TYR:CZ	2:B:6:ILE:HG23	2.37	0.60
1:Q:28:THR:HG23	1:Q:30:MET:H	1.67	0.60
1:A:183:HIS:ND1	1:A:195:TYR:OH	2.72	0.60
1:M:174:GLU:HG3	1:M:259:LYS:HB3	1.82	0.60
1:M:55:ASP:O	1:M:278:ASN:ND2	2.34	0.60
1:Y:322:ASN:OD1	1:Y:323:SER:N	2.35	0.60
2:Z:55:ILE:HG12	2:Z:99:LEU:HD21	1.84	0.59
1:I:316:LEU:HD23	2:J:100:VAL:HG13	1.82	0.59
1:K:284:PRO:HG2	1:K:298:HIS:CE1	2.37	0.59
1:E:204:VAL:HG12	1:E:209:LEU:HD23	1.85	0.59
1:S:283:THR:HB	1:S:286:GLY:O	2.03	0.59
1:W:14:CYS:HB2	2:X:25:HIS:HB3	1.85	0.59
2:B:167:ARG:NH1	2:B:171:GLU:OE2	2.75	0.59
1:A:48:ASN:HD21	1:A:287:ALA:HB3	2.58	0.59
1:C:318:ILE:HG23	2:D:48:VAL:HG11	1.84	0.59
1:E:200:THR:HA	1:E:248:ASN:OD1	2.03	0.59
2:B:55:ILE:HG12	2:B:99:LEU:HD21	2.04	0.59
1:A:179:LEU:HD23	1:A:234:TRP:HB3	2.25	0.59
1:M:37:THR:HG22	1:M:38:HIS:CD2	2.37	0.58
1:U:288:ILE:HD11	1:U:297:ILE:HG13	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:166:ARG:HG3	1:Q:166:ARG:NH1	2.16	0.58
2:B:2:LEU:HG	2:D:3:PHE:HZ	164.42	0.58
1:S:49:GLY:HA2	1:S:285:MET:O	2.03	0.58
1:E:126:SER:OG	1:E:166:ARG:NH2	2.35	0.58
1:S:90:LYS:NZ	1:S:273:GLU:OE2	2.35	0.58
1:S:28:THR:HG23	1:S:30:MET:H	1.68	0.58
1:M:134:GLY:HA3	1:M:153:TRP:HB3	1.83	0.58
2:B:124:LEU:HD22	2:J:134:GLY:HA2	1.85	0.58
2:B:169:LYS:HG3	2:B:177:ARG:NH2	17.20	0.58
1:Y:156:LYS:HD2	1:Y:196:GLN:HB2	1.86	0.58
1:K:61:LEU:HA	1:K:79:PHE:CZ	2.39	0.57
1:Q:40:GLN:HB2	1:Q:318:ILE:HD11	1.85	0.57
2:R:57:ASP:O	2:R:60:ASN:HB2	2.05	0.57
1:G:187:ASP:OD2	1:G:189:ALA:HB3	2.05	0.57
1:C:28:THR:HG22	1:C:30:MET:H	1.69	0.57
1:W:28:THR:HG23	1:W:30:MET:H	1.68	0.57
1:C:48:ASN:HD21	1:C:287:ALA:HB3	1.88	0.57
1:W:180:TRP:HZ3	1:W:235:THR:HG22	1.69	0.57
1:O:320:LEU:HD23	2:P:111:HIS:HB3	1.85	0.57
2:T:24:TYR:CD2	2:T:153:ARG:HG2	2.39	0.57
1:W:56:VAL:HB	1:W:85:SER:HB3	1.86	0.57
1:U:231:GLU:HG2	1:U:233:PHE:CE1	2.39	0.57
1:W:61:LEU:HA	1:W:79:PHE:CZ	2.39	0.57
1:I:14:CYS:HB2	2:J:25:HIS:HB3	1.85	0.57
1:I:37:THR:HG22	1:I:38:HIS:CD2	2.39	0.57
2:Z:167:ARG:O	2:Z:171:GLU:HG2	2.05	0.57
1:E:179:LEU:O	1:E:254:PRO:HB3	2.05	0.57
1:Y:28:THR:HG22	1:Y:30:MET:H	1.70	0.57
1:K:318:ILE:HG23	2:L:48:VAL:HG11	1.87	0.56
2:N:10:ILE:HG12	2:N:136:GLY:HA3	1.86	0.56
2:T:106:ARG:HG3	2:V:106:ARG:HH22	1.70	0.56
1:E:166:ARG:HG3	1:E:166:ARG:NH1	2.12	0.56
1:U:231:GLU:HG2	1:U:233:PHE:HE1	1.70	0.56
1:A:141:TYR:OH	1:U:261:LYS:HD2	61.47	0.56
1:S:123:ILE:HG13	1:S:124:ILE:HG13	1.86	0.56
1:C:61:LEU:HA	1:C:79:PHE:CZ	2.50	0.56
1:E:156:LYS:HD2	1:E:196:GLN:HB2	1.86	0.56
4:I:2004:NAG:H4	4:I:2005:NAG:H4	1.86	0.56
2:H:53:ASN:O	2:H:57:ASP:HB2	2.05	0.56
1:U:100:GLY:HA3	1:U:230:MET:O	2.05	0.56
2:B:151:SER:O	2:B:156:THR:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:70:LEU:O	1:M:150:ASN:ND2	2.39	0.56
1:S:26:VAL:HG21	1:S:317:ALA:HB2	1.88	0.56
1:S:318:ILE:HG23	2:T:48:VAL:HG11	1.88	0.56
1:M:311:SER:HB3	2:N:97:GLU:OE2	2.05	0.56
1:S:269:LYS:HE3	2:T:69:GLU:OE1	2.06	0.56
1:O:100:GLY:HA3	1:O:230:MET:O	2.06	0.56
1:W:307:LYS:NZ	2:X:64:GLU:OE2	2.38	0.56
1:W:83(A):GLU:OE1	1:W:261:LYS:NZ	2.38	0.56
1:A:206:THR:HB	1:A:209:LEU:HB3	1.88	0.56
1:W:135:VAL:HG23	1:W:146:SER:HA	1.88	0.56
1:Q:166:ARG:HH11	1:Q:166:ARG:CG	2.15	0.56
2:P:122:VAL:HA	2:P:125:GLN:HE21	1.70	0.56
1:I:202:ILE:HD11	1:I:251:PHE:HA	1.88	0.56
1:M:73:ASN:ND2	1:M:97:CYS:HB3	2.21	0.56
2:B:127:ARG:NH1	2:Z:133:LEU:O	85.50	0.55
1:G:283:THR:HB	1:G:286:GLY:O	2.06	0.55
1:C:115:ILE:HD13	1:C:260:ILE:HG12	2.06	0.55
1:U:130:HIS:CE1	1:U:164:ILE:HG12	2.41	0.55
3:E:2001:NAG:O3	3:E:2002:NAG:O5	2.24	0.55
1:I:279:THR:HG21	1:I:287:ALA:HB1	1.88	0.55
2:P:28:ASN:HD22	2:P:145:ASP:HA	1.71	0.55
2:Z:51:LYS:HD3	2:Z:103:GLU:HB3	1.88	0.55
1:W:180:TRP:CZ3	1:W:235:THR:HG22	2.41	0.55
1:K:183:HIS:HB2	1:K:252:ILE:HD11	1.89	0.55
2:N:76:ARG:NH1	2:P:74:GLU:OE1	2.39	0.55
2:Z:169:LYS:HD2	2:Z:172:GLU:OE1	2.06	0.55
1:Y:48:ASN:ND2	1:Y:287:ALA:HB3	2.22	0.55
1:U:123:ILE:HG13	1:U:124:ILE:HG13	1.88	0.55
2:X:55:ILE:HG12	2:X:99:LEU:HD21	1.88	0.55
2:J:53:ASN:O	2:J:57:ASP:HB2	2.06	0.55
2:P:125:GLN:OE1	2:P:155:GLY:HA2	2.07	0.55
1:U:73:ASN:HD21	1:U:97:CYS:HB3	1.72	0.55
1:I:294:PHE:HZ	2:J:59:MET:HG3	1.70	0.55
1:K:26:VAL:HG12	1:K:315:VAL:HG12	1.89	0.55
1:A:56:VAL:HB	1:A:85:SER:HB3	1.89	0.55
2:X:68:ARG:NH1	2:X:81:ASN:OD1	2.40	0.55
1:I:283:THR:HG22	1:I:285:MET:N	2.10	0.54
1:C:192:THR:CG2	1:W:192:THR:HG21	2.35	0.54
1:I:62:ARG:NH1	1:I:78:GLU:OE2	2.39	0.54
1:U:48:ASN:HD21	1:U:287:ALA:HB3	1.73	0.54
2:T:62:GLN:HG3	2:T:92:TRP:CG	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ILE:O	1:A:246:GLU:HA	2.07	0.54
2:D:70:PHE:CD2	2:D:78:GLU:HA	3.55	0.54
1:I:179:LEU:HD23	1:I:234:TRP:HB3	1.88	0.54
2:D:106:ARG:CG	2:F:106:ARG:HH22	2.19	0.54
1:Q:61:LEU:HA	1:Q:79:PHE:CZ	2.42	0.54
1:M:182:ILE:HD11	1:M:215:PRO:HD3	1.89	0.54
1:K:188:ALA:O	1:K:192:THR:HG22	2.07	0.54
2:J:9:PHE:CE1	2:J:10:ILE:HG13	2.41	0.54
1:W:133(A):LEU:O	1:W:135:VAL:HG12	2.06	0.54
2:F:77:ILE:HA	2:F:80:LEU:HB3	1.88	0.54
1:A:29:ILE:HD11	2:B:102:MET:HA	1.90	0.54
2:L:30:GLN:HE22	2:L:145:ASP:HB2	1.72	0.54
1:O:251:PHE:CE2	1:O:253:ALA:HB2	2.43	0.54
1:C:265:SER:OG	1:C:266:THR:N	2.40	0.54
1:K:204:VAL:HG22	1:K:245:PHE:HD1	1.72	0.54
1:Y:283:THR:HB	1:Y:286:GLY:O	2.08	0.54
1:E:247:SER:OG	1:E:248:ASN:N	2.41	0.54
1:Y:116:ASN:HB2	1:Y:261:LYS:HG2	1.90	0.54
4:W:2004:NAG:H3	4:W:2005:NAG:O7	2.08	0.54
1:A:58:PRO:HB3	1:A:86:TYR:CE1	2.43	0.54
1:M:73:ASN:HB3	1:M:76:CYS:SG	2.48	0.53
1:M:179:LEU:HD23	1:M:234:TRP:HB3	1.89	0.53
2:X:3:PHE:CE2	2:X:113:SER:HB2	2.43	0.53
1:W:283:THR:HB	1:W:286:GLY:O	2.08	0.53
1:E:57:LYS:HE2	1:E:274:TYR:CZ	2.43	0.53
1:U:29:ILE:HD11	2:V:102:MET:HG2	1.90	0.53
2:Z:54:SER:O	2:Z:58:LYS:HG2	2.08	0.53
1:K:98:TYR:CD2	1:K:230:MET:HE1	2.43	0.53
1:C:206:THR:HB	1:C:209:LEU:H	1.95	0.53
1:C:73:ASN:ND2	1:C:97:CYS:HB3	2.23	0.53
2:D:30:GLN:N	2:D:30:GLN:HE21	5.47	0.53
1:Q:135:VAL:HG22	1:Q:146:SER:HA	1.89	0.53
1:Q:204:VAL:HG12	1:Q:209:LEU:HD23	1.91	0.53
2:V:134:GLY:HA2	2:X:124:LEU:HD22	1.90	0.53
1:C:13:ILE:HG22	2:D:138:PHE:HB2	2.58	0.53
1:O:295:HIS:CE1	1:O:308:TYR:HD1	2.27	0.53
1:W:247:SER:OG	1:W:248:ASN:N	2.40	0.53
2:J:22:TYR:OH	2:J:111:HIS:ND1	2.24	0.53
1:A:48:ASN:ND2	1:A:287:ALA:HB3	2.98	0.53
2:D:51:LYS:HD3	2:D:103:GLU:HB3	1.91	0.53
2:B:169:LYS:HG3	2:B:177:ARG:HH22	17.95	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:62:ARG:HD3	1:O:273:GLU:OE1	2.08	0.53
1:C:18:HIS:HB2	2:D:21:TRP:HA	2.49	0.53
1:K:200:THR:HA	1:K:248:ASN:OD1	2.08	0.53
1:E:206:THR:HG22	1:E:208:THR:H	1.73	0.53
2:D:30:GLN:HE22	2:D:145:ASP:HA	3.74	0.53
1:Y:15:ILE:O	2:Z:10:ILE:HD13	2.09	0.53
1:K:288:ILE:HD11	1:K:297:ILE:HG13	1.91	0.53
2:Z:159:TYR:HB3	2:Z:160:PRO:HD3	1.90	0.53
1:C:29:ILE:HD11	2:D:102:MET:HG2	2.03	0.53
2:Z:150:GLU:OE2	2:Z:153:ARG:HD2	2.08	0.53
1:C:52:CYS:HB3	1:C:278:ASN:HA	1.91	0.53
2:T:134:GLY:HA2	2:V:124:LEU:HD22	1.91	0.53
1:U:99:PRO:HD2	1:U:226:LEU:HD12	1.91	0.52
1:K:206:THR:HG22	1:K:207:SER:N	2.24	0.52
1:M:43:LEU:HB2	1:M:314:LEU:HB2	1.91	0.52
2:T:143:LYS:HG3	2:T:165:GLU:OE2	2.10	0.52
1:S:288:ILE:HD11	1:S:297:ILE:HG13	1.89	0.52
2:L:118:LEU:HD12	2:L:121:LYS:HD3	1.89	0.52
1:C:57:LYS:HE2	1:C:274:TYR:CE2	2.43	0.52
2:Z:168:LEU:O	2:Z:172:GLU:HG3	2.08	0.52
2:N:70:PHE:HD1	2:R:76:ARG:NH1	2.08	0.52
1:M:202:ILE:HA	1:M:247:SER:HB3	1.91	0.52
2:D:97:GLU:OE1	2:Z:58:LYS:NZ	185.29	0.52
1:M:200:THR:HG21	1:M:249:GLY:HA3	1.92	0.52
1:W:206:THR:HG22	1:W:207:SER:N	2.25	0.52
1:Y:48:ASN:HD21	1:Y:287:ALA:HB3	1.73	0.52
1:E:57:LYS:HE2	1:E:274:TYR:CE2	2.44	0.52
1:I:41:ASP:OD2	1:I:45:LYS:NZ	2.42	0.52
1:C:70:LEU:O	1:C:150:ASN:ND2	2.50	0.52
1:E:61:LEU:HA	1:E:79:PHE:CZ	2.45	0.52
2:J:62:GLN:HG3	2:J:92:TRP:CG	2.45	0.52
1:A:62:ARG:NH1	1:A:78:GLU:OE2	2.48	0.52
1:S:57:LYS:HE2	1:S:274:TYR:CE2	2.45	0.52
1:Y:9:PRO:CD	1:Y:9:PRO:O	2.57	0.52
2:P:57:ASP:O	2:P:60:ASN:HB2	2.10	0.52
1:E:48:ASN:HD21	1:E:287:ALA:HB3	1.75	0.52
1:A:266:THR:HG22	1:A:302:ILE:HD12	2.58	0.52
1:U:283:THR:HB	1:U:286:GLY:O	2.10	0.52
2:J:130:ALA:HB2	2:J:140:PHE:HD1	1.74	0.52
1:C:176:LEU:HD23	1:C:258:TYR:O	2.10	0.52
1:Q:231:GLU:HG2	1:Q:233:PHE:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:169:LYS:O	2:D:172:GLU:HB3	2.38	0.52
1:U:30:MET:HG2	2:X:47:GLY:O	2.10	0.52
1:C:43:LEU:HB2	1:C:314:LEU:HB2	1.92	0.52
1:O:169:ASN:O	1:O:171:THR:HG23	2.10	0.52
2:T:84:MET:HE2	2:T:85:GLU:HG2	1.92	0.51
1:Q:279:THR:HG21	1:Q:287:ALA:HB1	1.91	0.51
2:H:85:GLU:O	2:H:89:LEU:HG	2.09	0.51
1:Y:231:GLU:HG2	1:Y:233:PHE:CE1	2.44	0.51
1:Q:83(A):GLU:OE1	1:Q:261:LYS:NZ	2.43	0.51
1:C:48:ASN:ND2	1:C:287:ALA:HB3	2.30	0.51
2:V:57:ASP:O	2:V:60:ASN:HB2	2.10	0.51
1:K:136:SER:O	1:K:145:SER:HB2	2.10	0.51
2:R:24:TYR:CD2	2:R:153:ARG:HG2	2.45	0.51
2:T:133:LEU:HD12	2:T:137:CYS:HB2	1.92	0.51
1:Y:40:GLN:HB2	1:Y:318:ILE:HD11	1.92	0.51
2:B:2:LEU:O	2:H:113:SER:OG	2.21	0.51
1:Q:313:ARG:NH2	1:Q:315:VAL:HG21	2.24	0.51
2:T:57:ASP:O	2:T:60:ASN:HB2	2.11	0.51
1:O:61:LEU:HA	1:O:79:PHE:CZ	2.45	0.51
1:G:164:ILE:O	1:G:246:GLU:HA	2.10	0.51
2:X:59:MET:HE1	2:X:96:ALA:HB2	1.92	0.51
2:T:4:GLY:HA3	2:V:117:ASN:HD21	1.76	0.51
1:G:320:LEU:H	1:G:320:LEU:HD23	1.75	0.51
2:B:158:ASP:OD1	2:B:160:PRO:HD2	2.19	0.51
2:H:132:GLU:HG3	2:H:138:PHE:CE1	2.45	0.51
2:R:24:TYR:CE2	2:R:153:ARG:HG2	2.45	0.51
1:A:136:SER:O	1:A:145:SER:HB2	2.31	0.51
1:I:288:ILE:HD11	1:I:297:ILE:HG13	1.93	0.51
2:P:51:LYS:HD3	2:P:103:GLU:HB3	1.93	0.51
1:Y:29:ILE:HD11	2:Z:102:MET:HG2	1.93	0.51
2:T:22:TYR:OH	2:T:111:HIS:ND1	2.36	0.51
1:K:120:LYS:HG2	1:K:256:TYR:HB3	1.93	0.51
2:R:123:ARG:HD2	2:R:132:GLU:OE2	2.11	0.51
1:C:283:THR:HB	1:C:286:GLY:O	2.10	0.50
1:Q:28:THR:HG22	1:Q:31:GLU:H	1.74	0.50
1:O:206:THR:HG22	1:O:207:SER:N	2.25	0.50
2:V:176:GLY:O	2:V:177:ARG:HG3	2.11	0.50
1:C:247:SER:OG	1:C:248:ASN:N	2.41	0.50
1:A:268:MET:HG2	1:A:284:PRO:HG3	1.93	0.50
1:A:49:GLY:HA2	1:A:285:MET:O	2.11	0.50
1:S:231:GLU:HG2	1:S:233:PHE:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:136:SER:O	1:I:145:SER:HB2	2.10	0.50
1:K:58:PRO:HB3	1:K:86:TYR:CE1	2.46	0.50
1:W:100:GLY:HA3	1:W:230:MET:O	2.11	0.50
1:G:316:LEU:HD23	2:H:100:VAL:HG13	1.92	0.50
2:L:151:SER:O	2:L:156:THR:N	2.43	0.50
1:M:179:LEU:O	1:M:254:PRO:HB3	2.11	0.50
2:T:159:TYR:HB3	2:T:160:PRO:HD3	1.93	0.50
1:S:55:ASP:O	1:S:278:ASN:ND2	2.43	0.50
1:Y:206:THR:HG22	1:Y:208:THR:H	1.76	0.50
2:B:151:SER:HA	2:B:156:THR:HB	2.01	0.50
1:A:83(A):GLU:OE1	1:A:261:LYS:NZ	2.83	0.50
2:L:54:SER:O	2:L:58:LYS:HG2	2.12	0.50
1:G:185:PRO:HG2	1:G:191:GLN:OE1	2.12	0.50
1:E:320:LEU:HB3	2:F:111:HIS:CG	2.47	0.50
1:Q:245:PHE:CD2	1:Q:251:PHE:HZ	2.30	0.50
1:A:28:THR:OG1	2:B:105:GLU:HB2	2.62	0.50
2:D:3:PHE:CE2	2:D:113:SER:HB2	2.71	0.50
1:Q:100:GLY:HA3	1:Q:230:MET:O	2.11	0.50
2:N:158:ASP:OD1	2:N:160:PRO:HD2	2.12	0.50
1:K:43:LEU:HB2	1:K:314:LEU:HB2	1.94	0.50
2:N:71:ASN:OD1	2:N:74:GLU:HG3	2.12	0.50
1:U:135:VAL:HG23	1:U:146:SER:HA	1.94	0.50
1:E:206:THR:HG22	1:E:207:SER:N	2.27	0.50
2:H:176:GLY:O	2:H:177:ARG:HG3	2.10	0.50
2:Z:3:PHE:CE1	2:Z:113:SER:HB2	2.47	0.50
2:B:118:LEU:HD12	2:B:121:LYS:HD3	3.88	0.50
2:B:105:GLU:HB3	2:D:106:ARG:HH22	150.34	0.50
2:X:62:GLN:HG3	2:X:92:TRP:CD2	2.47	0.49
1:S:77:ASP:OD2	1:S:141:TYR:HE1	1.95	0.49
1:Y:119:GLU:HB3	1:Y:259:LYS:HB2	1.92	0.49
1:A:156:LYS:HD2	1:A:196:GLN:HB2	2.16	0.49
2:P:68:ARG:NH1	2:P:81:ASN:OD1	2.45	0.49
1:A:87:ILE:HD12	1:A:267:ILE:HG12	2.72	0.49
1:E:147:PHE:HE1	1:E:230:MET:HE2	1.77	0.49
2:J:159:TYR:HB3	2:J:160:PRO:HD3	1.94	0.49
1:I:183:HIS:O	1:I:185:PRO:HD3	2.11	0.49
1:U:284:PRO:HG2	1:U:298:HIS:CE1	2.46	0.49
1:W:130:HIS:CE1	1:W:164:ILE:HG12	2.47	0.49
1:I:53:ASP:OD1	1:I:274:TYR:OH	2.20	0.49
1:W:204:VAL:HG12	1:W:209:LEU:HD23	1.94	0.49
1:E:48:ASN:ND2	1:E:287:ALA:HB3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:170:ASN:HB2	1:O:237:LEU:HD23	1.93	0.49
2:V:167:ARG:O	2:V:171:GLU:HG2	2.12	0.49
1:G:206:THR:HB	1:G:209:LEU:H	1.76	0.49
1:C:295:HIS:CE1	1:C:308:TYR:HD1	2.60	0.49
1:A:240:ASN:O	3:A:2001:NAG:H82	2.12	0.49
2:L:41:THR:O	2:L:45:ILE:HG13	2.12	0.49
1:M:105:TYR:CE2	1:M:109:LYS:HE3	2.48	0.49
1:E:165:LYS:HE2	1:E:246:GLU:OE2	2.12	0.49
2:H:158:ASP:OD1	2:H:160:PRO:HD2	2.13	0.49
1:Q:266:THR:HG22	1:Q:302:ILE:HD12	1.94	0.49
1:G:48:ASN:O	1:G:50:LYS:HG3	2.13	0.49
2:D:159:TYR:HB3	2:D:160:PRO:HD3	1.95	0.49
1:A:283:THR:HB	1:A:286:GLY:O	2.17	0.49
1:E:26:VAL:HG12	1:E:315:VAL:HG12	1.94	0.49
2:B:102:MET:HE2	2:Z:102:MET:HE1	83.76	0.49
2:B:105:GLU:HB3	2:H:106:ARG:HH22	1.76	0.49
1:C:200:THR:HA	1:C:248:ASN:OD1	2.17	0.49
1:Q:206:THR:HG22	1:Q:208:THR:H	1.77	0.49
1:K:203:SER:OG	1:K:246:GLU:HB3	2.13	0.49
1:A:206:THR:CG2	1:A:207:SER:N	2.75	0.49
1:U:135:VAL:HG23	1:U:146:SER:CA	2.43	0.49
1:A:202:ILE:HD11	1:A:251:PHE:HA	1.94	0.49
2:D:97:GLU:HB3	2:Z:58:LYS:NZ	186.56	0.49
1:M:22:SER:O	1:M:322:ASN:ND2	2.45	0.49
4:Y:2002:NAG:O3	4:Y:2003:NAG:H2	2.13	0.49
2:V:159:TYR:HB3	2:V:160:PRO:HD3	1.94	0.49
1:O:37:THR:HG22	1:O:38:HIS:CE1	2.48	0.49
1:S:61:LEU:HA	1:S:79:PHE:HZ	1.73	0.49
1:O:73:ASN:HD21	1:O:97:CYS:HB3	1.76	0.49
2:D:125:GLN:OE1	2:D:155:GLY:HA2	2.12	0.49
2:V:39:GLU:O	2:V:43:LYS:HB2	2.13	0.49
1:S:206:THR:HG22	1:S:207:SER:N	2.28	0.49
1:C:30:MET:HG2	2:Z:47:GLY:O	208.65	0.49
1:W:135:VAL:HG23	1:W:146:SER:CA	2.43	0.49
1:A:100:GLY:HA3	1:A:230:MET:O	2.14	0.49
1:I:182:ILE:HD11	1:I:215:PRO:HD3	1.94	0.49
2:T:46:ASP:O	2:T:50:ASN:ND2	2.46	0.49
1:W:176:LEU:HD23	1:W:258:TYR:O	2.12	0.49
1:Q:230:MET:SD	1:Q:252:ILE:HD11	2.53	0.48
2:N:159:TYR:HB3	2:N:160:PRO:HD3	1.95	0.48
1:K:30:MET:HG2	2:D:47:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:251:PHE:CE2	1:C:253:ALA:HB2	2.48	0.48
2:H:51:LYS:HZ2	2:H:107:THR:HG1	1.54	0.48
1:O:102:PHE:HE1	1:O:234:TRP:CD1	2.31	0.48
1:C:160:THR:HG22	1:S:165:LYS:NZ	2.28	0.48
2:H:30:GLN:HE22	2:H:145:ASP:HA	1.78	0.48
1:A:264:ASP:OD1	1:A:264:ASP:N	2.45	0.48
2:B:71:ASN:OD1	2:B:74:GLU:HG3	2.16	0.48
1:G:294:PHE:HZ	2:H:59:MET:HG3	1.78	0.48
1:Q:43:LEU:HB2	1:Q:314:LEU:HB2	1.95	0.48
1:W:57:LYS:HE2	1:W:274:TYR:CE2	2.49	0.48
1:C:231:GLU:HG2	1:C:233:PHE:HE1	2.68	0.48
2:T:113:SER:OG	2:X:2:LEU:O	2.21	0.48
1:S:206:THR:HB	1:S:209:LEU:CB	2.43	0.48
1:A:17:TYR:CE2	2:B:6:ILE:HA	2.48	0.48
1:K:295:HIS:CD2	1:K:306:PRO:HG2	2.48	0.48
2:P:159:TYR:HB3	2:P:160:PRO:HD3	1.96	0.48
1:A:206:THR:HG22	1:A:207:SER:N	2.28	0.48
1:C:206:THR:HG22	1:C:207:SER:N	2.30	0.48
2:V:62:GLN:HG3	2:V:92:TRP:CD2	2.49	0.48
1:A:200:THR:HA	1:A:248:ASN:OD1	2.48	0.48
1:M:183:HIS:ND1	1:M:195:TYR:OH	2.24	0.48
2:B:98:LEU:HD21	2:D:99:LEU:HD13	136.00	0.48
2:L:77:ILE:HA	2:L:80:LEU:HB3	1.96	0.48
1:A:192:THR:HG21	1:O:196:GLN:HE22	77.04	0.48
4:G:2004:NAG:H4	4:G:2005:NAG:O3	2.14	0.48
2:H:167:ARG:O	2:H:171:GLU:HG3	2.14	0.48
1:M:186:ASN:HB2	1:M:190:GLU:OE2	2.13	0.48
1:O:11:ASP:C	2:P:140:PHE:HD2	2.17	0.48
1:Q:134:GLY:HA3	1:Q:153:TRP:HB3	1.96	0.48
1:K:204:VAL:HG22	1:K:245:PHE:CD1	2.48	0.48
1:K:136:SER:C	1:K:145:SER:HB2	2.34	0.48
1:Q:195:TYR:O	1:Q:197:ASN:N	2.46	0.48
1:U:134:GLY:HA3	1:U:153:TRP:HB3	1.94	0.48
1:U:11:ASP:HB2	2:V:140:PHE:HD2	1.79	0.48
1:C:37:THR:HG22	1:C:38:HIS:CD2	2.49	0.48
2:D:134:GLY:HA2	2:F:124:LEU:HD22	1.96	0.48
1:W:42:ILE:O	1:W:294:PHE:HB2	2.13	0.48
2:N:128:ASP:O	2:N:170:ARG:NH1	2.47	0.48
1:I:28:THR:HG23	1:I:30:MET:H	1.79	0.47
1:A:124:ILE:HD12	1:A:254:PRO:HG2	1.96	0.47
1:E:116:ASN:HB2	1:E:261:LYS:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:68:ARG:NH1	2:F:81:ASN:OD1	2.46	0.47
2:Z:173:ILE:CG2	2:Z:177:ARG:HE	2.26	0.47
2:Z:149:MET:HB2	2:Z:153:ARG:HH21	1.79	0.47
1:O:206:THR:HB	1:O:209:LEU:HB2	1.96	0.47
1:E:62:ARG:O	1:E:90:LYS:HD2	2.14	0.47
2:F:118:LEU:HD12	2:F:121:LYS:HD3	1.96	0.47
2:D:131:LYS:HB3	2:D:139:GLU:HB3	1.96	0.47
1:E:42:ILE:HG13	1:E:314:LEU:HB3	1.96	0.47
1:A:202:ILE:HG12	1:A:247:SER:OG	2.15	0.47
2:V:68:ARG:NH1	2:V:81:ASN:OD1	2.47	0.47
2:R:159:TYR:HB3	2:R:160:PRO:HD3	1.97	0.47
1:G:135:VAL:HG23	1:G:146:SER:HA	1.96	0.47
1:I:44:GLU:HB2	1:I:292:MET:HG3	1.97	0.47
1:C:308:TYR:HD2	2:D:89:LEU:HD22	1.88	0.47
1:G:73:ASN:ND2	1:G:97:CYS:HB3	2.29	0.47
4:Q:2004:NAG:O3	4:Q:2005:NAG:H2	2.14	0.47
2:H:116:LYS:HZ1	2:J:116:LYS:HZ1	1.63	0.47
1:C:298:HIS:CE1	1:C:300:LEU:HB2	2.49	0.47
1:E:147:PHE:CE1	1:E:230:MET:HE2	2.49	0.47
2:T:80:LEU:HD13	2:V:81:ASN:OD1	2.15	0.47
2:D:171:GLU:HA	2:D:174:SER:HB2	1.96	0.47
2:N:98:LEU:HD21	2:P:99:LEU:HD13	1.96	0.47
2:J:164:GLU:OE2	2:J:167:ARG:NE	2.46	0.47
1:U:109:LYS:HD3	2:V:69:GLU:OE2	2.15	0.47
2:L:84:MET:CE	2:L:85:GLU:HG2	2.44	0.47
1:Y:247:SER:OG	1:Y:248:ASN:N	2.44	0.47
1:I:251:PHE:CE2	1:I:253:ALA:HB2	2.49	0.47
1:K:247:SER:OG	1:K:248:ASN:N	2.45	0.47
2:D:62:GLN:HG3	2:D:92:TRP:CG	2.50	0.47
1:Q:105:TYR:CE2	1:Q:109:LYS:HE3	2.50	0.47
2:X:6:ILE:HG13	2:X:112:ASP:HA	1.97	0.47
1:Q:295:HIS:CE1	1:Q:308:TYR:HD1	2.32	0.47
2:P:25:HIS:HA	2:P:33:GLY:O	2.14	0.47
1:A:206:THR:HB	1:A:209:LEU:H	1.78	0.47
1:M:172:ASN:HB3	1:M:174:GLU:OE2	2.14	0.47
1:Q:116:ASN:HB2	1:Q:261:LYS:HG2	1.97	0.47
1:O:73:ASN:ND2	1:O:97:CYS:HB3	2.29	0.47
2:D:55:ILE:HG12	2:D:99:LEU:HD21	1.96	0.47
2:F:150:GLU:OE2	2:F:153:ARG:HD2	2.15	0.47
1:E:28:THR:HG23	1:E:30:MET:H	1.80	0.47
1:O:266:THR:HG22	1:O:302:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:77:ASP:OD2	1:W:141:TYR:HE1	1.98	0.47
1:Q:247:SER:OG	1:Q:248:ASN:N	2.47	0.47
1:K:169:ASN:O	1:K:171:THR:HG23	2.14	0.47
2:B:83:LYS:HG3	2:H:68:ARG:HH21	1.79	0.47
1:Y:14:CYS:HB2	2:Z:25:HIS:HB3	1.97	0.47
1:W:179:LEU:HD23	1:W:234:TRP:HB3	1.96	0.47
1:S:116:ASN:HB2	1:S:261:LYS:HG2	1.96	0.47
2:L:159:TYR:HB3	2:L:160:PRO:HD3	1.95	0.47
1:A:44:GLU:HB2	1:A:292:MET:HG3	2.13	0.47
2:D:30:GLN:H	2:D:30:GLN:HE21	5.16	0.47
1:U:307:LYS:NZ	2:V:60:ASN:O	2.47	0.47
1:C:50:LYS:HD3	1:C:275:GLY:HA3	2.56	0.47
1:M:28:THR:HG23	1:M:30:MET:H	1.79	0.47
1:Q:62:ARG:NH2	1:Q:78:GLU:OE2	2.48	0.47
1:A:192:THR:HG21	1:O:196:GLN:NE2	77.14	0.46
1:A:133(A):LEU:O	1:A:135:VAL:HG12	5.24	0.46
1:S:56:VAL:HB	1:S:85:SER:HB3	1.97	0.46
1:E:307:LYS:HD2	2:F:62:GLN:HB3	1.97	0.46
2:B:37:ASP:OD1	2:B:38:LYS:N	3.08	0.46
1:A:314:LEU:HD22	2:B:100:VAL:HG21	2.54	0.46
1:C:282:GLN:NE2	1:C:283:THR:H	2.13	0.46
2:B:57:ASP:O	2:B:60:ASN:HB2	3.59	0.46
1:M:29:ILE:HD11	2:N:102:MET:HG2	1.96	0.46
2:Z:51:LYS:NZ	2:Z:103:GLU:O	2.46	0.46
2:B:159:TYR:HB3	2:B:160:PRO:HD3	1.99	0.46
2:Z:28:ASN:ND2	2:Z:146:ASN:OD1	2.44	0.46
2:D:54:SER:O	2:D:58:LYS:HG2	2.16	0.46
1:A:14:CYS:O	2:B:24:TYR:HA	2.15	0.46
2:D:141:TYR:O	2:D:169:LYS:HG2	2.63	0.46
1:A:197:ASN:HA	1:A:198:PRO:HD3	1.87	0.46
2:F:51:LYS:HD3	2:F:103:GLU:HB3	1.97	0.46
1:K:165:LYS:HE2	1:K:246:GLU:OE2	2.15	0.46
2:Z:151:SER:O	2:Z:156:THR:N	2.48	0.46
2:Z:119:TYR:OH	2:Z:132:GLU:OE1	2.28	0.46
1:K:182:ILE:HD11	1:K:215:PRO:HD3	1.96	0.46
1:I:150:ASN:ND2	1:I:258:TYR:OH	2.48	0.46
1:E:160:THR:HG21	1:W:165:LYS:HE3	1.97	0.46
1:I:43:LEU:HB2	1:I:314:LEU:HB2	1.97	0.46
1:I:153:TRP:O	1:I:155:ILE:HD12	2.15	0.46
2:B:21:TRP:HZ3	2:B:45:ILE:HG13	2.62	0.46
1:M:133:SER:O	1:M:133(A):LEU:HD23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LEU:HD21	1:A:296:ASN:ND2	3.43	0.46
1:W:164:ILE:O	1:W:246:GLU:HA	2.16	0.46
1:A:18:HIS:HB2	2:B:21:TRP:HA	1.97	0.46
2:H:62:GLN:HG3	2:H:92:TRP:CG	2.51	0.46
1:U:170:ASN:HB2	1:U:237:LEU:HD23	1.98	0.46
1:K:320:LEU:HB3	2:L:111:HIS:CD2	2.50	0.46
1:M:40:GLN:HB2	1:M:318:ILE:CD1	2.46	0.46
1:E:283:THR:HB	1:E:286:GLY:O	2.15	0.46
1:S:101:ASP:O	1:S:231:GLU:HA	2.16	0.46
1:K:320:LEU:HB3	2:L:111:HIS:CG	2.49	0.46
2:N:62:GLN:HG3	2:N:92:TRP:CG	2.51	0.46
2:B:147:GLU:HA	2:B:150:GLU:HB2	2.91	0.46
1:C:33:ASN:ND2	3:C:2002:NAG:O7	75.52	0.46
1:S:67:ALA:HB2	1:S:105:TYR:CE1	2.51	0.46
1:M:136:SER:C	1:M:145:SER:HB2	2.36	0.46
1:Q:192:THR:HG21	1:Y:196:GLN:HE22	1.81	0.46
2:B:151:SER:O	2:B:157:TYR:N	2.65	0.46
1:M:40:GLN:HB2	1:M:318:ILE:HD11	1.98	0.46
2:L:128:ASP:O	2:L:170:ARG:NH1	2.49	0.46
1:Y:11:ASP:HB2	2:Z:140:PHE:HB2	1.98	0.46
1:S:122:GLN:NE2	1:S:125:PRO:HA	2.31	0.46
1:O:236:ILE:HG23	1:O:236:ILE:HD12	1.72	0.46
1:C:230:MET:SD	1:C:252:ILE:HD11	2.55	0.46
1:E:206:THR:HB	1:E:209:LEU:H	1.81	0.46
1:W:53:ASP:OD1	1:W:57:LYS:HA	2.15	0.46
2:D:99:LEU:HD13	2:L:98:LEU:HD21	1.97	0.46
1:G:73:ASN:O	1:G:76:CYS:HB2	2.15	0.46
1:G:176:LEU:HD23	1:G:258:TYR:O	2.16	0.46
1:C:160:THR:HG22	1:S:165:LYS:HZ1	1.82	0.45
2:J:151:SER:HA	2:J:156:THR:HB	1.98	0.45
1:Q:245:PHE:CD2	1:Q:251:PHE:CZ	3.04	0.45
1:W:40:GLN:HB3	1:W:316:LEU:HB2	1.98	0.45
2:D:123:ARG:HD2	2:D:132:GLU:OE2	2.52	0.45
1:C:177:LEU:HB3	1:C:258:TYR:HB2	2.33	0.45
1:G:135:VAL:HG23	1:G:146:SER:CA	2.46	0.45
2:F:159:TYR:HB3	2:F:160:PRO:HD3	1.99	0.45
1:C:201:TYR:OH	1:C:246:GLU:OE1	2.28	0.45
1:Y:65:SER:OG	1:Y:96:ASP:HA	2.16	0.45
2:D:131:LYS:HB2	2:D:141:TYR:HE2	3.03	0.45
2:Z:173:ILE:HG23	2:Z:177:ARG:NE	2.28	0.45
1:G:182:ILE:HD11	1:G:215:PRO:CD	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:HIS:HD2	1:A:229:ARG:O	1.99	0.45
1:Q:206:THR:HB	1:Q:209:LEU:CB	2.47	0.45
2:D:58:LYS:HE2	2:L:101:LEU:CD1	2.46	0.45
1:A:40:GLN:OE1	1:A:318:ILE:HD11	2.16	0.45
2:B:51:LYS:HD3	2:B:103:GLU:HB3	2.11	0.45
1:U:61:LEU:HA	1:U:79:PHE:HZ	1.81	0.45
1:Q:62:ARG:O	1:Q:90:LYS:HD2	2.16	0.45
1:C:133(A):LEU:O	1:C:135:VAL:HG12	5.08	0.45
1:A:27:ASP:OD1	1:A:33:ASN:N	2.30	0.45
2:T:68:ARG:HH22	2:X:83:LYS:HG3	1.79	0.45
1:K:56:VAL:HB	1:K:85:SER:HB3	1.98	0.45
2:T:5:ALA:HA	2:T:9:PHE:CE1	2.52	0.45
2:H:54:SER:O	2:H:58:LYS:HG2	2.16	0.45
1:M:102:PHE:HE1	1:M:234:TRP:CD1	2.35	0.45
2:L:42:GLN:HA	2:L:45:ILE:HD12	1.97	0.45
2:B:142:HIS:HD2	2:B:166:ALA:HB2	2.77	0.45
2:H:17:MET:SD	2:H:23:GLY:HA3	2.57	0.45
1:Y:56:VAL:HB	1:Y:85:SER:HB3	1.99	0.45
1:C:282:GLN:HE21	1:C:283:THR:H	1.64	0.45
1:A:320:LEU:HD13	2:B:6:ILE:HD13	1.99	0.45
1:Y:83(A):GLU:OE2	1:Y:261:LYS:NZ	2.49	0.45
1:W:77:ASP:O	1:W:80:ILE:HG13	2.16	0.45
2:N:125:GLN:OE1	2:N:155:GLY:HA2	2.16	0.45
1:C:58:PRO:HB3	1:C:86:TYR:CE1	2.50	0.45
1:G:28:THR:HG22	1:G:31:GLU:H	1.81	0.45
1:C:317:ALA:O	2:D:107:THR:HG21	2.17	0.45
1:Q:42:ILE:HG13	1:Q:314:LEU:HB3	1.98	0.45
1:S:179:LEU:HD23	1:S:234:TRP:HB3	1.99	0.45
1:E:182:ILE:HD11	1:E:215:PRO:HD3	1.98	0.45
2:F:119:TYR:CE1	2:F:136:GLY:HA2	2.51	0.45
1:G:71:LEU:HD23	1:G:71:LEU:HA	1.82	0.45
2:B:84:MET:SD	2:Z:84:MET:HG3	85.48	0.45
1:W:316:LEU:HD13	2:X:52:VAL:HG22	1.98	0.45
2:V:77:ILE:HA	2:V:80:LEU:HB3	1.99	0.45
1:U:179:LEU:HD23	1:U:234:TRP:HB3	1.99	0.45
1:I:175:ASP:OD1	1:I:239:PRO:HD3	2.16	0.45
1:Y:269:LYS:O	1:Y:284:PRO:HB3	2.17	0.45
2:Z:23:GLY:HA3	2:Z:36:ALA:HA	1.99	0.45
2:D:97:GLU:HB3	2:Z:58:LYS:HZ3	187.01	0.45
1:M:200:THR:HG22	1:M:248:ASN:OD1	2.17	0.45
1:W:37:THR:HG22	1:W:38:HIS:ND1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:THR:HG22	1:A:38:HIS:CD2	2.52	0.45
1:C:155:ILE:CD1	1:C:194:LEU:HD22	2.47	0.45
1:O:154:LEU:HA	1:O:154:LEU:HD23	1.75	0.45
1:O:83(A):GLU:OE1	1:O:261:LYS:NZ	2.49	0.44
2:J:9:PHE:CD1	2:J:10:ILE:HG13	2.52	0.44
2:L:28:ASN:ND2	2:L:30:GLN:OE1	2.50	0.44
1:Q:298:HIS:CE1	1:Q:300:LEU:HB2	2.52	0.44
1:G:20:ASN:ND2	1:G:37:THR:HG23	2.32	0.44
2:N:3:PHE:CE2	2:N:113:SER:HB2	2.51	0.44
1:I:206:THR:HB	1:I:209:LEU:H	1.81	0.44
1:C:77:ASP:O	1:C:80:ILE:HG13	2.30	0.44
2:N:55:ILE:HG12	2:N:99:LEU:CD2	2.48	0.44
1:C:206:THR:HB	1:C:209:LEU:HB2	2.26	0.44
2:H:167:ARG:NH1	2:H:171:GLU:OE2	2.50	0.44
1:C:298:HIS:HA	1:C:299:PRO:HD3	2.33	0.44
1:U:247:SER:OG	1:U:248:ASN:N	2.49	0.44
1:I:116:ASN:HB2	1:I:261:LYS:HG2	2.00	0.44
1:O:57:LYS:HE2	1:O:274:TYR:CE2	2.52	0.44
1:C:34:VAL:HG11	2:D:108:LEU:HD11	1.99	0.44
1:A:195:TYR:O	1:A:197:ASN:N	2.47	0.44
1:A:164:ILE:N	1:A:247:SER:O	2.74	0.44
1:Y:206:THR:HG22	1:Y:207:SER:N	2.33	0.44
2:T:125:GLN:OE1	2:T:155:GLY:HA2	2.17	0.44
1:K:37:THR:HG22	1:K:38:HIS:CD2	2.52	0.44
1:M:58:PRO:HB3	1:M:86:TYR:CE1	2.53	0.44
2:X:132:GLU:HG3	2:X:138:PHE:CE1	2.52	0.44
1:A:135:VAL:HG23	1:A:146:SER:CA	4.51	0.44
1:S:320:LEU:HB3	2:T:111:HIS:CG	2.52	0.44
1:A:200:THR:HG22	1:A:248:ASN:OD1	2.17	0.44
1:E:66:VAL:HB	1:E:105:TYR:OH	2.17	0.44
1:I:247:SER:OG	1:I:248:ASN:N	2.48	0.44
1:W:26:VAL:HG12	1:W:315:VAL:HG12	2.00	0.44
2:P:19:ASP:OD1	2:P:19:ASP:N	2.51	0.44
2:T:70:PHE:CE2	2:T:78:GLU:HA	2.53	0.44
1:K:283:THR:HG23	1:K:298:HIS:HB3	1.99	0.44
1:A:28:THR:HG22	1:A:31:GLU:O	2.35	0.44
2:N:70:PHE:HD2	2:N:78:GLU:HG3	1.81	0.44
1:K:122:GLN:HB2	1:K:256:TYR:CE1	2.52	0.44
2:X:159:TYR:HB3	2:X:160:PRO:HD3	2.00	0.44
2:D:24:TYR:CD2	2:D:153:ARG:HG2	2.53	0.44
1:C:122:GLN:NE2	1:C:125:PRO:HA	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:314:LEU:HA	1:S:314:LEU:HD23	1.89	0.44
1:E:107:GLU:OE1	2:D:75:ARG:HB2	2.18	0.44
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.99	0.44
1:A:307:LYS:HB3	2:B:62:GLN:NE2	3.17	0.44
1:U:206:THR:HG22	1:U:207:SER:N	2.33	0.44
1:Y:314:LEU:HA	1:Y:314:LEU:HD23	1.77	0.44
2:Z:6:ILE:HG13	2:Z:112:ASP:HA	2.00	0.44
1:G:295:HIS:CE1	1:G:308:TYR:HD1	2.35	0.44
1:E:123:ILE:HG13	1:E:124:ILE:HG13	1.99	0.44
1:Q:82:VAL:HA	1:Q:83:PRO:HD3	1.82	0.44
2:R:79:ASN:O	2:R:83:LYS:HG2	2.18	0.44
1:Y:28:THR:HG22	1:Y:31:GLU:H	1.83	0.44
1:I:288:ILE:HD11	1:I:297:ILE:CG1	2.48	0.44
2:J:158:ASP:OD1	2:J:160:PRO:HD2	2.18	0.44
1:O:236:ILE:HD13	1:O:236:ILE:HA	1.83	0.44
2:H:76:ARG:NH2	2:J:74:GLU:OE2	2.51	0.44
2:F:17:MET:SD	2:F:23:GLY:HA3	2.58	0.44
1:U:176:LEU:HD23	1:U:258:TYR:O	2.18	0.44
1:A:42:ILE:HB	1:A:293:PRO:HG2	1.99	0.44
1:W:295:HIS:ND1	1:W:297:ILE:HG12	2.33	0.44
2:X:2:LEU:HD13	2:X:109:ASP:OD2	2.18	0.44
2:F:24:TYR:CD2	2:F:153:ARG:HG2	2.53	0.44
2:T:167:ARG:NH2	2:X:174:SER:O	2.51	0.44
1:E:73:ASN:ND2	1:E:97:CYS:HB3	2.33	0.44
1:S:112:LEU:HD23	1:S:112:LEU:HA	1.68	0.44
1:S:112:LEU:HD23	1:S:115:ILE:HD12	1.99	0.44
1:M:61:LEU:HA	1:M:79:PHE:CZ	2.52	0.44
1:S:206:THR:HB	1:S:209:LEU:HB2	1.99	0.43
1:A:30:MET:HB2	2:B:105:GLU:OE1	2.88	0.43
1:K:175:ASP:OD1	1:K:239:PRO:HD3	2.18	0.43
1:C:106:GLU:HB3	2:B:76:ARG:HD3	91.53	0.43
2:V:4:GLY:O	2:V:8:GLY:HA3	2.18	0.43
1:E:183:HIS:ND1	1:E:195:TYR:OH	2.41	0.43
1:Q:156:LYS:HD2	1:Q:196:GLN:HB2	1.99	0.43
3:G:2001:NAG:H62	1:Q:259:LYS:NZ	2.33	0.43
1:M:206:THR:HG22	1:M:207:SER:N	2.33	0.43
1:S:219:THR:O	1:U:205:GLY:HA3	2.18	0.43
1:C:283:THR:HG23	1:C:284:PRO:HD2	2.01	0.43
2:B:169:LYS:O	2:B:177:ARG:NH2	16.09	0.43
1:Y:231:GLU:HG2	1:Y:233:PHE:HE1	1.83	0.43
1:C:20:ASN:HD21	1:C:37:THR:HG23	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:58:LYS:HD3	2:D:58:LYS:HA	2.58	0.43
1:S:323:SER:HA	1:S:324:PRO:HD2	1.90	0.43
1:G:30:MET:HG2	2:J:47:GLY:O	2.18	0.43
2:B:58:LYS:HA	2:B:58:LYS:HD3	1.74	0.43
1:W:99:PRO:HD2	1:W:226:LEU:HD12	2.00	0.43
1:S:226:LEU:HA	1:S:226:LEU:HD23	1.73	0.43
1:C:73:ASN:HD21	1:C:97:CYS:HB3	1.82	0.43
1:G:17:TYR:CE2	2:H:6:ILE:HA	2.54	0.43
1:Q:298:HIS:HE1	1:Q:300:LEU:HD12	1.83	0.43
1:A:98:TYR:CE2	1:A:226:LEU:HD13	3.06	0.43
1:I:89:GLU:O	1:I:269:LYS:HA	2.18	0.43
1:E:231:GLU:HG2	1:E:233:PHE:CE1	2.54	0.43
1:G:58:PRO:HB3	1:G:86:TYR:CE1	2.52	0.43
1:W:194:LEU:HA	1:W:194:LEU:HD23	1.79	0.43
1:A:112:LEU:HD23	1:A:112:LEU:HA	2.56	0.43
1:U:133(A):LEU:O	1:U:135:VAL:HG12	2.18	0.43
1:E:314:LEU:HD23	1:E:314:LEU:HA	1.72	0.43
2:N:55:ILE:HG12	2:N:99:LEU:HD21	1.99	0.43
2:Z:58:LYS:HD2	2:Z:58:LYS:HA	1.79	0.43
1:K:206:THR:HB	1:K:209:LEU:H	1.82	0.43
1:E:26:VAL:HG12	1:E:315:VAL:CG1	2.47	0.43
1:I:44:GLU:HB2	1:I:292:MET:HB2	1.99	0.43
1:A:314:LEU:HD23	1:A:314:LEU:HA	2.21	0.43
4:S:2004:NAG:H3	4:S:2005:NAG:H2	2.00	0.43
1:G:172:ASN:CG	1:G:259:LYS:HD3	2.38	0.43
1:O:12:GLN:HG2	2:P:139:GLU:HA	2.00	0.43
1:I:172:ASN:CG	1:I:259:LYS:HD3	2.39	0.43
2:D:131:LYS:HB2	2:D:141:TYR:CE2	3.00	0.43
2:B:172:GLU:HG2	2:B:177:ARG:HG2	8.25	0.43
1:W:295:HIS:CD2	1:W:306:PRO:HG2	2.53	0.43
1:M:15:ILE:O	2:N:10:ILE:HD13	2.18	0.43
2:H:123:ARG:HD2	2:H:132:GLU:OE2	2.19	0.43
1:O:206:THR:HG22	1:O:207:SER:H	1.83	0.43
1:U:121:ILE:HG21	1:U:259:LYS:HE2	1.99	0.43
2:Z:114:ASN:HA	2:Z:117:ASN:HB2	2.00	0.43
1:O:67:ALA:HB3	1:O:96:ASP:OD1	2.18	0.43
1:E:58:PRO:HB3	1:E:86:TYR:CZ	2.54	0.43
1:S:200:THR:HG22	1:S:248:ASN:OD1	2.18	0.43
1:O:133(A):LEU:HD23	1:O:133(A):LEU:HA	1.69	0.43
2:F:58:LYS:HD3	2:F:58:LYS:HA	1.74	0.43
1:A:28:THR:HG23	1:A:30:MET:H	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:THR:CG2	1:E:207:SER:N	2.82	0.43
1:C:20:ASN:ND2	1:C:37:THR:HG23	2.34	0.43
1:A:40:GLN:HB2	1:A:318:ILE:HD11	2.22	0.43
2:T:70:PHE:HD2	2:T:78:GLU:HG3	1.82	0.43
1:E:73:ASN:HD21	1:E:97:CYS:HB3	1.83	0.43
1:C:67:ALA:HB2	1:C:105:TYR:CE1	2.54	0.43
1:Y:136:SER:O	1:Y:145:SER:HB2	2.17	0.43
2:P:134:GLY:HA2	2:R:124:LEU:HD22	2.01	0.43
1:O:28:THR:HG22	1:O:31:GLU:H	1.83	0.43
1:O:206:THR:HB	1:O:209:LEU:CB	2.49	0.43
1:A:15:ILE:HG23	2:B:118:LEU:HD23	2.77	0.43
2:B:58:LYS:NZ	2:J:97:GLU:OE1	2.46	0.43
2:X:57:ASP:O	2:X:60:ASN:HB2	2.18	0.43
2:X:58:LYS:HD3	2:X:58:LYS:HA	1.78	0.43
1:G:283:THR:HG22	1:G:285:MET:N	2.11	0.43
1:A:188:ALA:O	1:A:192:THR:HG22	2.41	0.43
2:D:158:ASP:OD1	2:D:160:PRO:HD2	2.23	0.43
1:C:102:PHE:O	1:C:105:TYR:HB2	2.18	0.43
2:H:133:LEU:HD11	2:H:139:GLU:HB2	2.00	0.43
2:D:77:ILE:HA	2:D:80:LEU:HB3	1.99	0.43
2:P:151:SER:O	2:P:156:THR:N	2.52	0.43
2:X:133:LEU:HD12	2:X:137:CYS:HB2	1.99	0.43
2:X:151:SER:O	2:X:156:THR:N	2.52	0.43
1:O:48:ASN:ND2	1:O:287:ALA:HB3	2.34	0.43
1:U:206:THR:CG2	1:U:207:SER:N	2.82	0.43
1:W:126:SER:HB2	1:W:166:ARG:NH2	2.31	0.43
2:D:123:ARG:HB2	2:D:138:PHE:CZ	2.80	0.43
2:H:55:ILE:HG12	2:H:99:LEU:HD21	2.01	0.43
1:A:14:CYS:HB2	2:B:25:HIS:HB3	2.36	0.43
1:U:320:LEU:HB3	2:V:111:HIS:CG	2.54	0.43
1:Y:198:PRO:HD2	1:Y:199:THR:H	1.84	0.43
2:J:24:TYR:CD2	2:J:153:ARG:HG2	2.54	0.43
2:H:94:TYR:CD1	2:H:94:TYR:C	2.92	0.43
1:I:295:HIS:HE2	1:I:301:THR:HG21	1.83	0.43
1:K:29:ILE:HG13	1:K:29:ILE:H	1.67	0.43
1:M:156:LYS:HD2	1:M:196:GLN:HB2	2.01	0.43
1:M:73:ASN:HD21	1:M:97:CYS:HB3	1.83	0.43
2:B:74:GLU:O	2:B:77:ILE:HG13	3.04	0.43
1:U:137:SER:HA	1:U:145:SER:HB2	2.00	0.43
2:N:25:HIS:HA	2:N:33:GLY:O	2.18	0.43
2:Z:74:GLU:O	2:Z:77:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:115:ILE:HD13	1:G:260:ILE:HG12	2.01	0.43
1:M:138:ALA:O	1:M:140:PRO:HD3	2.19	0.43
1:O:202:ILE:HD11	1:O:251:PHE:HA	2.01	0.42
1:O:48:ASN:HD21	1:O:287:ALA:HB3	1.84	0.42
1:E:197:ASN:HA	1:E:198:PRO:HD3	1.91	0.42
1:Y:183:HIS:O	1:Y:185:PRO:HD3	2.19	0.42
1:A:294:PHE:HZ	2:B:59:MET:HG3	1.85	0.42
1:Y:112:LEU:HA	1:Y:112:LEU:HD23	1.87	0.42
1:W:206:THR:CG2	1:W:207:SER:N	2.82	0.42
1:G:288:ILE:HD11	1:G:297:ILE:CG1	2.47	0.42
1:C:279:THR:OG1	1:C:287:ALA:HB1	2.20	0.42
1:M:201:TYR:O	1:M:247:SER:HB2	2.19	0.42
2:H:72:ASN:OD1	2:H:75:ARG:NH2	2.52	0.42
1:K:159:SER:O	1:K:196:GLN:NE2	2.52	0.42
1:M:82:VAL:HA	1:M:83:PRO:HD3	1.73	0.42
1:M:62:ARG:NH2	1:M:78:GLU:OE1	2.53	0.42
1:A:67:ALA:HB2	1:A:105:TYR:CE1	2.54	0.42
1:S:316:LEU:HA	1:S:316:LEU:HD23	1.86	0.42
1:U:112:LEU:HA	1:U:112:LEU:HD23	1.77	0.42
1:I:279:THR:HB	1:I:281:CYS:N	2.28	0.42
1:I:295:HIS:HE1	1:I:298:HIS:O	2.03	0.42
1:C:62:ARG:O	1:C:90:LYS:HD2	2.20	0.42
1:O:164:ILE:O	1:O:246:GLU:HA	2.20	0.42
1:O:173:GLN:HB2	1:O:174:GLU:OE1	2.19	0.42
2:N:118:LEU:HD12	2:N:121:LYS:HD3	2.01	0.42
2:B:116:LYS:HG2	2:B:116:LYS:O	2.19	0.42
1:C:269:LYS:O	1:C:284:PRO:HB3	2.67	0.42
2:N:55:ILE:O	2:N:59:MET:HG2	2.19	0.42
1:Q:206:THR:HG22	1:Q:207:SER:N	2.33	0.42
2:T:84:MET:CE	2:T:85:GLU:HG2	2.49	0.42
1:A:186:ASN:OD1	1:A:227:SER:HB3	2.19	0.42
1:E:175:ASP:OD1	1:E:239:PRO:HD3	2.19	0.42
1:I:318:ILE:HG23	2:J:48:VAL:HG11	2.01	0.42
1:Y:240:ASN:OD1	5:Y:2001:NAG:H5	2.19	0.42
1:Y:295:HIS:CE1	1:Y:308:TYR:HD1	2.37	0.42
2:H:151:SER:HA	2:H:156:THR:HB	2.02	0.42
2:J:167:ARG:NH1	2:J:171:GLU:OE2	2.52	0.42
1:A:20:ASN:ND2	1:A:37:THR:HG23	2.34	0.42
2:D:28:ASN:HB3	2:D:149:MET:CE	3.15	0.42
1:G:14:CYS:O	2:H:24:TYR:HA	2.19	0.42
2:J:58:LYS:HD2	2:J:58:LYS:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:22:SER:O	1:Y:322:ASN:ND2	2.53	0.42
1:A:267:ILE:HD13	1:A:267:ILE:HG21	1.76	0.42
2:V:158:ASP:OD1	2:V:160:PRO:HD2	2.18	0.42
1:C:135:VAL:HG23	1:C:146:SER:HA	3.60	0.42
1:Q:185:PRO:HG3	1:Q:191:GLN:OE1	2.20	0.42
1:Q:11:ASP:OD2	2:R:144:CYS:N	2.50	0.42
1:C:44:GLU:OE1	1:C:46:LYS:HG3	2.20	0.42
1:Q:121:ILE:HD13	1:Q:121:ILE:HG21	1.71	0.42
1:Q:30:MET:HG2	2:N:47:GLY:O	2.19	0.42
2:R:158:ASP:OD1	2:R:160:PRO:HD2	2.20	0.42
1:Q:298:HIS:HA	1:Q:299:PRO:HD3	1.83	0.42
1:E:183:HIS:O	1:E:185:PRO:HD3	2.20	0.42
1:I:123:ILE:HG13	1:I:124:ILE:HG13	2.01	0.42
2:R:51:LYS:HD3	2:R:103:GLU:HB3	2.02	0.42
2:R:68:ARG:NH1	2:R:81:ASN:OD1	2.53	0.42
1:S:83(A):GLU:OE1	1:S:261:LYS:NZ	2.52	0.42
2:R:148:CYS:O	2:R:151:SER:OG	2.24	0.42
1:E:29:ILE:HD11	2:F:102:MET:HG2	2.02	0.42
1:C:183:HIS:ND1	1:C:195:TYR:OH	2.50	0.42
1:G:52:CYS:HB3	1:G:278:ASN:HA	2.01	0.42
1:A:209:LEU:HD12	1:A:209:LEU:HA	2.43	0.42
1:A:29:ILE:HG13	1:A:29:ILE:H	1.72	0.42
2:D:84:MET:CE	2:D:85:GLU:HG2	2.46	0.42
1:S:307:LYS:NZ	2:T:60:ASN:O	2.53	0.42
2:H:116:LYS:HZ1	2:J:116:LYS:NZ	2.17	0.42
1:Q:164:ILE:O	1:Q:246:GLU:HA	2.20	0.42
1:K:293:PRO:HB3	2:L:56:ILE:HG12	2.01	0.42
2:Z:59:MET:HB3	2:Z:62:GLN:OE1	2.19	0.42
1:C:12:GLN:OE1	2:D:139:GLU:HG3	5.83	0.42
2:P:158:ASP:OD1	2:P:160:PRO:HD2	2.18	0.42
1:S:75:MET:HE1	1:S:140:PRO:HG2	2.01	0.42
1:W:181:GLY:O	1:W:252:ILE:HB	2.20	0.42
1:S:44:GLU:OE1	1:S:46:LYS:HE2	2.20	0.42
2:Z:39:GLU:O	2:Z:43:LYS:HG3	2.19	0.42
1:S:73:ASN:HB3	1:S:76:CYS:SG	2.59	0.42
2:P:75:ARG:HA	2:P:75:ARG:HD3	1.90	0.42
1:K:226:LEU:HA	1:K:226:LEU:HD23	1.67	0.42
1:C:133(A):LEU:HA	1:C:133(A):LEU:HD23	2.62	0.41
1:I:18:HIS:N	2:J:21:TRP:O	2.47	0.41
1:A:170:ASN:ND2	1:A:239:PRO:HA	2.75	0.41
1:Q:126:SER:OG	1:Q:166:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ASP:OD1	1:C:149:ARG:NE	2.51	0.41
1:A:179:LEU:CD2	1:A:234:TRP:HB3	3.03	0.41
2:D:3:PHE:HB3	2:D:116:LYS:HD3	3.87	0.41
1:U:29:ILE:HD11	2:V:102:MET:HA	2.01	0.41
1:G:17:TYR:HB2	1:G:320:LEU:HD11	2.02	0.41
1:S:320:LEU:HB3	2:T:111:HIS:CD2	2.55	0.41
1:K:28:THR:HG23	1:K:30:MET:H	1.84	0.41
2:H:58:LYS:HA	2:H:58:LYS:HD3	1.70	0.41
1:M:138:ALA:C	1:M:140:PRO:HD3	2.40	0.41
1:G:267:ILE:HG21	1:G:267:ILE:HD13	1.77	0.41
1:A:283:THR:HG23	1:A:298:HIS:HB3	2.06	0.41
1:I:206:THR:CG2	1:I:207:SER:N	2.82	0.41
1:U:230:MET:SD	1:U:252:ILE:HD11	2.60	0.41
2:B:98:LEU:HD21	2:H:99:LEU:HD13	2.02	0.41
2:P:148:CYS:O	2:P:152:VAL:HG23	2.19	0.41
1:U:20:ASN:HB2	1:U:21[A]:ASN:H	1.70	0.41
1:C:112:LEU:HA	1:C:112:LEU:HD23	1.81	0.41
1:E:121:ILE:HD13	1:E:121:ILE:HG21	1.82	0.41
2:N:106:ARG:HH12	2:R:105:GLU:HB3	1.85	0.41
1:W:141:TYR:CD2	1:W:142:GLN:HG2	2.56	0.41
1:Y:184:HIS:HA	1:Y:185:PRO:HD3	1.85	0.41
1:U:313:ARG:NH2	1:U:315:VAL:HG21	2.35	0.41
1:I:308:TYR:HD2	2:J:89:LEU:HD22	1.86	0.41
1:K:307:LYS:HB3	2:L:62:GLN:NE2	2.36	0.41
1:G:105:TYR:CE2	1:G:109:LYS:HE3	2.55	0.41
1:K:192:THR:H	1:K:192:THR:HG22	1.65	0.41
1:K:12:GLN:N	2:L:27:SER:O	2.49	0.41
1:C:72:GLY:O	1:C:149:ARG:HG3	2.21	0.41
1:A:279:THR:HG21	1:A:287:ALA:HB1	2.05	0.41
1:G:48:ASN:HD21	1:G:287:ALA:HB3	1.85	0.41
2:F:125:GLN:OE1	2:F:155:GLY:HA2	2.20	0.41
1:M:181:GLY:O	1:M:252:ILE:HB	2.21	0.41
1:Q:72:GLY:O	1:Q:148:PHE:HA	2.19	0.41
1:I:194:LEU:N	1:I:194:LEU:HD23	2.36	0.41
1:A:216:ARG:HD3	1:A:216:ARG:HH11	1.73	0.41
1:U:314:LEU:HA	1:U:314:LEU:HD23	1.88	0.41
1:K:98:TYR:CE2	1:K:230:MET:HE1	2.56	0.41
2:V:62:GLN:HG3	2:V:92:TRP:CG	2.55	0.41
1:A:123:ILE:HG13	1:A:124:ILE:HG13	2.02	0.41
1:C:135:VAL:HG22	1:C:146:SER:O	2.21	0.41
1:E:88:VAL:HG22	1:E:268:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:206:THR:HB	1:S:209:LEU:N	2.27	0.41
1:E:200:THR:HG22	1:E:248:ASN:OD1	2.20	0.41
1:S:307:LYS:HB3	2:T:62:GLN:NE2	2.36	0.41
1:O:37:THR:HG22	1:O:38:HIS:ND1	2.36	0.41
2:B:77:ILE:HA	2:B:80:LEU:HB3	2.22	0.41
1:U:176:LEU:HA	1:U:176:LEU:HD23	1.85	0.41
1:G:172:ASN:HB3	1:G:174:GLU:OE2	2.21	0.41
1:E:169:ASN:O	1:E:171:THR:HG23	2.20	0.41
1:G:15:ILE:HD11	2:H:122:VAL:HG21	2.03	0.41
1:I:164:ILE:O	1:I:246:GLU:HA	2.21	0.41
2:N:2:LEU:HD13	2:N:109:ASP:OD2	2.20	0.41
1:I:216:ARG:HH11	1:I:216:ARG:HD3	1.68	0.41
2:N:77:ILE:O	2:N:80:LEU:HB3	2.21	0.41
1:I:206:THR:HG22	1:I:207:SER:N	2.36	0.41
1:S:206:THR:CG2	1:S:207:SER:N	2.84	0.41
1:S:26:VAL:HG12	1:S:315:VAL:HG12	2.03	0.41
1:C:314:LEU:HA	1:C:314:LEU:HD23	1.83	0.41
2:L:77:ILE:O	2:L:80:LEU:HB3	2.20	0.41
1:A:316:LEU:HD21	2:B:100:VAL:HG22	2.03	0.41
1:A:20:ASN:HB2	1:A:21[B]:ASN:H	1.72	0.41
1:I:320:LEU:HD13	2:J:6:ILE:HD13	2.02	0.41
1:S:265:SER:OG	1:S:266:THR:N	2.53	0.41
1:K:317:ALA:O	2:L:107:THR:HG21	2.21	0.41
1:E:135:VAL:HG22	1:E:146:SER:HA	2.01	0.41
1:M:121:ILE:HD13	1:M:121:ILE:HG21	1.75	0.41
1:W:217:ILE:H	1:W:217:ILE:HD12	1.86	0.41
1:W:20:ASN:HB2	1:W:21[A]:ASN:H	1.71	0.41
1:A:206:THR:HB	1:A:209:LEU:CB	2.52	0.41
1:M:283:THR:HG23	1:M:298:HIS:HB3	2.03	0.41
1:C:28:THR:O	1:C:32:LYS:NZ	3.08	0.41
1:I:37:THR:HG22	1:I:38:HIS:CG	2.56	0.41
2:V:106:ARG:HG2	2:X:106:ARG:HH22	1.85	0.41
1:C:58:PRO:HB3	1:C:86:TYR:CZ	2.56	0.41
1:M:206:THR:HB	1:M:209:LEU:H	1.86	0.41
2:R:151:SER:O	2:R:157:TYR:N	2.52	0.41
1:S:76:CYS:O	1:S:78:GLU:N	2.54	0.41
1:I:18:HIS:HB2	2:J:21:TRP:HA	2.03	0.41
1:C:107:GLU:O	1:C:111:LEU:HD13	2.21	0.41
1:S:156:LYS:NZ	1:S:193:LYS:O	2.44	0.41
1:K:160:THR:OG1	1:U:165:LYS:NZ	2.46	0.41
2:L:125:GLN:OE1	2:L:155:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:4:GLY:O	2:N:8:GLY:HA3	2.21	0.41
2:L:19:ASP:N	2:L:19:ASP:OD1	2.54	0.41
1:Y:124:ILE:HD12	1:Y:254:PRO:HG2	2.03	0.41
2:P:44:ALA:HA	2:P:110:PHE:HE2	1.85	0.41
1:S:242:ALA:N	3:S:2001:NAG:H82	2.36	0.41
1:O:138:ALA:O	1:O:140:PRO:HD3	2.21	0.41
1:A:52:CYS:HB3	1:A:278:ASN:HA	2.02	0.41
2:B:101:LEU:HD23	2:B:101:LEU:HA	1.81	0.41
1:W:169:ASN:O	1:W:171:THR:HG23	2.21	0.41
1:I:204:VAL:HG12	1:I:209:LEU:HD23	2.03	0.41
1:S:209:LEU:HA	1:S:209:LEU:HD12	1.76	0.41
1:U:61:LEU:HG	1:U:61:LEU:H	1.72	0.41
1:A:279:THR:HB	1:A:280:LYS:H	1.66	0.41
1:C:206:THR:HG22	1:C:208:THR:H	1.86	0.41
1:O:206:THR:CG2	1:O:207:SER:N	2.84	0.41
2:B:150:GLU:OE2	2:B:153:ARG:HD2	2.20	0.41
1:A:20:ASN:HB2	1:A:21[A]:ASN:H	1.69	0.41
1:E:86:TYR:OH	1:E:282:GLN:HG2	2.21	0.41
2:N:151:SER:O	2:N:156:THR:N	2.53	0.41
1:A:115:ILE:HD13	1:A:260:ILE:HG12	2.17	0.41
1:Q:167:SER:HB2	1:Q:244:ASN:OD1	2.20	0.41
1:Q:212:ARG:HH11	1:Q:212:ARG:HD2	1.72	0.41
1:Q:119:GLU:HB2	1:Q:260(A):VAL:HG21	2.03	0.41
2:N:70:PHE:HD1	2:R:76:ARG:HH11	1.67	0.40
1:A:59:LEU:HD23	1:A:87:ILE:HG12	2.03	0.40
1:U:200:THR:HA	1:U:248:ASN:OD1	2.21	0.40
1:W:11:ASP:HB2	2:X:140:PHE:HB2	2.04	0.40
1:A:74:PRO:HG3	1:A:147:PHE:O	2.21	0.40
1:W:58:PRO:HB3	1:W:86:TYR:CE1	2.56	0.40
2:D:5:ALA:HA	2:D:9:PHE:CE1	2.56	0.40
1:C:56:VAL:HB	1:C:85:SER:HB3	2.02	0.40
1:Y:179:LEU:HD23	1:Y:234:TRP:HB3	2.03	0.40
2:J:123:ARG:HD2	2:J:132:GLU:OE2	2.21	0.40
2:B:9:PHE:CE1	2:B:10:ILE:HG13	2.56	0.40
1:E:317:ALA:O	2:F:107:THR:HG21	2.21	0.40
1:C:192:THR:HG21	1:M:196:GLN:OE1	101.15	0.40
2:F:123:ARG:HH21	2:F:124:LEU:HD21	1.85	0.40
1:S:230:MET:SD	1:S:252:ILE:CD1	3.07	0.40
1:G:82:VAL:H	1:G:82:VAL:HG23	1.67	0.40
1:I:316:LEU:HD21	2:J:100:VAL:HG22	2.03	0.40
1:C:18:HIS:HD2	2:D:20:GLY:O	5.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:174:SER:O	2:J:171:GLU:OE2	2.38	0.40
2:D:24:TYR:CE2	2:D:153:ARG:HG2	2.56	0.40
1:Q:174:GLU:HG3	1:Q:259:LYS:HB3	2.03	0.40
1:W:86:TYR:OH	1:W:282:GLN:HG2	2.21	0.40
2:D:22:TYR:OH	2:D:111:HIS:HB3	3.89	0.40
1:C:136:SER:O	1:C:145:SER:HB2	2.50	0.40
1:W:320:LEU:HB3	2:X:111:HIS:CG	2.55	0.40
1:M:226:LEU:HA	1:M:226:LEU:HD23	1.84	0.40
1:G:220:ARG:HD2	1:G:227:SER:O	2.21	0.40
1:G:282:GLN:HG3	1:G:283:THR:N	2.37	0.40
1:C:29:ILE:HG22	2:F:51:LYS:HG3	2.02	0.40
1:S:83(A):GLU:HA	1:S:117:HIS:CD2	2.57	0.40
2:B:97:GLU:OE1	2:H:58:LYS:NZ	2.49	0.40
1:U:20:ASN:HB2	1:U:21[B]:ASN:H	1.71	0.40
1:I:122:GLN:NE2	1:I:125:PRO:HA	2.36	0.40
1:Y:114:ARG:HH21	1:Y:263:GLY:C	2.24	0.40
1:M:203:SER:OG	1:M:246:GLU:HB3	2.21	0.40
1:M:314:LEU:HA	1:M:314:LEU:HD23	1.74	0.40
1:K:168:TYR:HE2	1:K:176:LEU:CD1	2.33	0.40
2:X:24:TYR:CD2	2:X:153:ARG:HG2	2.57	0.40
2:B:119:TYR:CE1	2:B:136:GLY:HA2	2.56	0.40
1:M:125(A):LYS:HB2	1:M:255:GLU:OE1	2.21	0.40
1:O:220:ARG:HD2	1:O:227:SER:O	2.22	0.40
1:I:15:ILE:HD11	2:J:122:VAL:HG21	2.03	0.40
2:X:77:ILE:HA	2:X:80:LEU:HB3	2.03	0.40
1:G:202:ILE:HD11	1:G:251:PHE:HA	2.03	0.40
2:P:58:LYS:HD3	2:P:58:LYS:HA	1.60	0.40
1:W:112:LEU:HD23	1:W:112:LEU:HA	1.77	0.40
2:R:71:ASN:OD1	2:R:71:ASN:C	2.60	0.40
1:C:293:PRO:HG2	1:C:294:PHE:HD2	3.42	0.40
1:K:283:THR:HG23	1:K:284:PRO:HD2	2.03	0.40
1:Q:314:LEU:HA	1:Q:314:LEU:HD23	1.88	0.40
1:I:102:PHE:O	1:I:105:TYR:HB2	2.21	0.40
1:A:11:ASP:OD2	2:B:144:CYS:N	2.39	0.40
1:Q:122:GLN:NE2	1:Q:125:PRO:HA	2.36	0.40
1:M:47:HIS:HD2	1:M:297:ILE:HD12	1.87	0.40
2:R:58:LYS:HD3	2:R:58:LYS:HA	1.75	0.40
1:Q:133(A):LEU:HA	1:Q:133(A):LEU:HD23	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	323/334 (97%)	301 (93%)	22 (7%)	0	100	100
1	C	323/334 (97%)	305 (94%)	18 (6%)	0	100	100
1	E	323/334 (97%)	302 (94%)	21 (6%)	0	100	100
1	G	323/334 (97%)	304 (94%)	19 (6%)	0	100	100
1	I	323/334 (97%)	301 (93%)	22 (7%)	0	100	100
1	K	323/334 (97%)	304 (94%)	19 (6%)	0	100	100
1	M	323/334 (97%)	301 (93%)	22 (7%)	0	100	100
1	O	323/334 (97%)	303 (94%)	19 (6%)	1 (0%)	46	81
1	Q	323/334 (97%)	300 (93%)	22 (7%)	1 (0%)	46	81
1	S	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	U	323/334 (97%)	305 (94%)	16 (5%)	2 (1%)	30	70
1	W	323/334 (97%)	304 (94%)	19 (6%)	0	100	100
1	Y	323/334 (97%)	303 (94%)	20 (6%)	0	100	100
1	a	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	c	323/334 (97%)	301 (93%)	21 (6%)	1 (0%)	46	81
2	B	175/181 (97%)	166 (95%)	8 (5%)	1 (1%)	30	70
2	D	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	F	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	H	175/181 (97%)	166 (95%)	9 (5%)	0	100	100
2	J	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	L	175/181 (97%)	164 (94%)	10 (6%)	1 (1%)	30	70
2	N	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	P	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	R	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	T	175/181 (97%)	166 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	V	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	X	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	Z	175/181 (97%)	164 (94%)	10 (6%)	1 (1%)	30	70
2	b	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	d	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
All	All	7470/7725 (97%)	7003 (94%)	459 (6%)	8 (0%)	56	89

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	77	ASP
1	O	248	ASN
1	Q	248	ASN
1	c	248	ASN
2	B	60	ASN
2	Z	176	GLY
1	U	248	ASN
2	L	176	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	292/300 (97%)	282 (97%)	10 (3%)	44	79
1	C	292/300 (97%)	285 (98%)	7 (2%)	57	86
1	E	292/300 (97%)	284 (97%)	8 (3%)	52	84
1	G	292/300 (97%)	285 (98%)	7 (2%)	57	86
1	I	292/300 (97%)	277 (95%)	15 (5%)	29	67
1	K	292/300 (97%)	284 (97%)	8 (3%)	52	84
1	M	292/300 (97%)	284 (97%)	8 (3%)	52	84
1	O	292/300 (97%)	284 (97%)	8 (3%)	52	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	292/300 (97%)	282 (97%)	10 (3%)	44	79
1	S	292/300 (97%)	285 (98%)	7 (2%)	57	86
1	U	292/300 (97%)	287 (98%)	5 (2%)	68	90
1	W	292/300 (97%)	284 (97%)	8 (3%)	52	84
1	Y	292/300 (97%)	286 (98%)	6 (2%)	61	88
1	a	292/300 (97%)	285 (98%)	7 (2%)	57	86
1	c	292/300 (97%)	288 (99%)	4 (1%)	74	92
2	B	151/155 (97%)	150 (99%)	1 (1%)	88	96
2	D	151/155 (97%)	150 (99%)	1 (1%)	88	96
2	F	151/155 (97%)	151 (100%)	0	100	100
2	H	151/155 (97%)	148 (98%)	3 (2%)	63	88
2	J	151/155 (97%)	150 (99%)	1 (1%)	88	96
2	L	151/155 (97%)	151 (100%)	0	100	100
2	N	151/155 (97%)	151 (100%)	0	100	100
2	P	151/155 (97%)	150 (99%)	1 (1%)	88	96
2	R	151/155 (97%)	149 (99%)	2 (1%)	76	92
2	T	151/155 (97%)	151 (100%)	0	100	100
2	V	151/155 (97%)	148 (98%)	3 (2%)	63	88
2	X	151/155 (97%)	149 (99%)	2 (1%)	76	92
2	Z	151/155 (97%)	146 (97%)	5 (3%)	45	80
2	b	151/155 (97%)	149 (99%)	2 (1%)	76	92
2	d	151/155 (97%)	148 (98%)	3 (2%)	63	88
All	All	6645/6825 (97%)	6503 (98%)	142 (2%)	61	88

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	112	LEU
1	A	174	GLU
1	A	219	THR
1	A	261	LYS
1	A	264	ASP
1	A	283	THR

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Mol	Chain	Res	Type
1	A	300	LEU
1	A	310	LYS
1	A	313	ARG
1	C	28	THR
1	C	46	LYS
1	C	120	LYS
1	C	135	VAL
1	C	174	GLU
1	C	261	LYS
1	C	310	LYS
1	E	46	LYS
1	E	114	ARG
1	E	166	ARG
1	E	174	GLU
1	E	199	THR
1	E	230	MET
1	E	261	LYS
1	E	273	GLU
1	G	28	THR
1	G	112	LEU
1	G	167	SER
1	G	208	THR
1	G	252	ILE
1	G	261	LYS
1	G	313	ARG
1	I	28	THR
1	I	65	SER
1	I	75	MET
1	I	80	ILE
1	I	111	LEU
1	I	137	SER
1	I	142	GLN
1	I	166	ARG
1	I	167	SER
1	I	194	LEU
1	I	208	THR
1	I	261	LYS
1	I	264	ASP
1	I	279	THR
1	I	313	ARG
1	K	46	LYS
1	K	56	VAL

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Mol	Chain	Res	Type
1	K	155	ILE
1	K	160	THR
1	K	187	ASP
1	K	261	LYS
1	K	273	GLU
1	K	313	ARG
1	M	28	THR
1	M	56	VAL
1	M	133	SER
1	M	219	THR
1	M	261	LYS
1	M	310	LYS
1	M	311	SER
1	M	313	ARG
1	O	56	VAL
1	O	176	LEU
1	O	208	THR
1	O	248	ASN
1	O	256	TYR
1	O	261	LYS
1	O	310	LYS
1	O	320	LEU
1	Q	28	THR
1	Q	94	VAL
1	Q	135	VAL
1	Q	166	ARG
1	Q	167	SER
1	Q	174	GLU
1	Q	176	LEU
1	Q	261	LYS
1	Q	313	ARG
1	Q	320	LEU
1	S	75	MET
1	S	174	GLU
1	S	208	THR
1	S	261	LYS
1	S	300	LEU
1	S	311	SER
1	S	313	ARG
1	U	28	THR
1	U	111	LEU
1	U	261	LYS

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Mol	Chain	Res	Type
1	U	272	LEU
1	U	313	ARG
1	W	28	THR
1	W	75	MET
1	W	155	ILE
1	W	264	ASP
1	W	272	LEU
1	W	311	SER
1	W	313	ARG
1	W	320	LEU
1	Y	28	THR
1	Y	114	ARG
1	Y	174	GLU
1	Y	261	LYS
1	Y	264	ASP
1	Y	309	VAL
1	a	65	SER
1	a	81	ASN
1	a	87	ILE
1	a	114	ARG
1	a	199	THR
1	a	261	LYS
1	a	291	SER
1	c	28	THR
1	c	114	ARG
1	c	261	LYS
1	c	312	ASN
2	B	43	LYS
2	D	113	SER
2	H	30	GLN
2	H	57	ASP
2	H	94	TYR
2	J	11	GLU
2	P	116	LYS
2	R	50	ASN
2	R	94	TYR
2	V	17	MET
2	V	29	GLU
2	V	94	TYR
2	X	86	ASP
2	X	94	TYR
2	Z	30	GLN

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Mol	Chain	Res	Type
2	Z	57	ASP
2	Z	66	VAL
2	Z	77	ILE
2	Z	80	LEU
2	b	43	LYS
2	b	80	LEU
2	d	19	ASP
2	d	30	GLN
2	d	86	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	HIS
1	C	122	GLN
1	E	110	HIS
1	E	197	ASN
1	G	117	HIS
1	G	210	ASN
1	I	122	GLN
1	I	150	ASN
1	K	196	GLN
1	K	197	ASN
1	M	12	GLN
1	M	197	ASN
1	M	322	ASN
1	O	150	ASN
1	Q	117	HIS
1	Q	196	GLN
1	S	110	HIS
1	S	122	GLN
1	U	122	GLN
1	W	150	ASN
1	Y	38	HIS
1	Y	197	ASN
1	c	18	HIS
2	L	62	GLN
2	P	142	HIS
2	V	117	ASN
2	b	142	HIS
2	d	30	GLN

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 ⓘ

58 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	A	2001	1,3	14,14,15	1.06	1 (7%)	15,19,21	1.00	1 (6%)
3	NAG	A	2002	3	14,14,15	0.30	0	15,19,21	0.47	0
3	BMA	A	2003	3	11,11,12	1.65	3 (27%)	14,15,17	1.37	3 (21%)
4	NAG	A	2004	1,4	14,14,15	0.99	1 (7%)	15,19,21	1.22	2 (13%)
4	NAG	A	2005	4	14,14,15	1.44	2 (14%)	15,19,21	1.27	1 (6%)
3	NAG	C	2001	1,3	14,14,15	0.34	0	15,19,21	0.52	0
3	NAG	C	2002	3	14,14,15	0.58	0	15,19,21	0.58	0
3	BMA	C	2003	3	11,11,12	2.11	4 (36%)	14,15,17	1.63	4 (28%)
3	NAG	E	2001	1,3	14,14,15	0.65	1 (7%)	15,19,21	1.01	1 (6%)
3	NAG	E	2002	3	14,14,15	1.24	1 (7%)	15,19,21	1.27	2 (13%)
3	BMA	E	2003	3	11,11,12	1.55	1 (9%)	14,15,17	1.79	3 (21%)
4	NAG	E	2004	1,4	14,14,15	1.19	1 (7%)	15,19,21	1.42	3 (20%)
4	NAG	E	2005	4	14,14,15	0.67	1 (7%)	15,19,21	0.33	0
3	NAG	G	2001	1,3	14,14,15	1.62	1 (7%)	15,19,21	1.31	2 (13%)
3	NAG	G	2002	3	14,14,15	0.86	1 (7%)	15,19,21	0.68	0
3	BMA	G	2003	3	11,11,12	1.97	4 (36%)	14,15,17	1.22	1 (7%)
4	NAG	G	2004	1,4	14,14,15	1.25	1 (7%)	15,19,21	1.41	2 (13%)
4	NAG	G	2005	4	14,14,15	0.63	0	15,19,21	0.32	0
3	NAG	I	2001	1,3	14,14,15	1.39	1 (7%)	15,19,21	1.26	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	I	2002	3	14,14,15	1.00	1 (7%)	15,19,21	0.83	1 (6%)
3	BMA	I	2003	3	11,11,12	2.37	5 (45%)	14,15,17	1.74	3 (21%)
4	NAG	I	2004	1,4	14,14,15	0.77	1 (7%)	15,19,21	1.14	2 (13%)
4	NAG	I	2005	4	14,14,15	1.60	2 (14%)	15,19,21	0.94	1 (6%)
3	NAG	K	2001	1,3	14,14,15	0.63	1 (7%)	15,19,21	0.70	1 (6%)
3	NAG	K	2002	3	14,14,15	0.43	0	15,19,21	0.75	0
3	BMA	K	2003	3	11,11,12	2.18	4 (36%)	14,15,17	1.71	3 (21%)
3	NAG	M	2001	1,3	14,14,15	0.59	0	15,19,21	0.54	0
3	NAG	M	2002	3	14,14,15	0.92	1 (7%)	15,19,21	0.84	1 (6%)
3	BMA	M	2003	3	11,11,12	1.95	3 (27%)	14,15,17	1.60	3 (21%)
3	NAG	O	2001	1,3	14,14,15	0.35	0	15,19,21	0.94	1 (6%)
3	NAG	O	2002	3	14,14,15	0.64	1 (7%)	15,19,21	0.30	0
3	BMA	O	2003	3	11,11,12	1.60	3 (27%)	14,15,17	1.41	3 (21%)
4	NAG	O	2004	1,4	14,14,15	1.16	1 (7%)	15,19,21	1.09	2 (13%)
4	NAG	O	2005	4	14,14,15	0.43	0	15,19,21	0.70	1 (6%)
3	NAG	Q	2001	1,3	14,14,15	0.61	1 (7%)	15,19,21	0.74	1 (6%)
3	NAG	Q	2002	3	14,14,15	0.21	0	15,19,21	0.48	0
3	BMA	Q	2003	3	11,11,12	0.70	0	14,15,17	2.03	4 (28%)
4	NAG	Q	2004	1,4	14,14,15	1.12	1 (7%)	15,19,21	0.99	0
4	NAG	Q	2005	4	14,14,15	0.48	0	15,19,21	0.46	0
3	NAG	S	2001	1,3	14,14,15	0.29	0	15,19,21	0.72	1 (6%)
3	NAG	S	2002	3	14,14,15	0.48	0	15,19,21	0.73	0
3	BMA	S	2003	3	11,11,12	1.98	2 (18%)	14,15,17	2.03	5 (35%)
4	NAG	S	2004	1,4	14,14,15	0.53	0	15,19,21	0.68	0
4	NAG	S	2005	4	14,14,15	1.52	2 (14%)	15,19,21	1.13	1 (6%)
3	NAG	U	2001	1,3	14,14,15	0.42	0	15,19,21	0.51	0
3	NAG	U	2002	3	14,14,15	1.48	2 (14%)	15,19,21	0.91	1 (6%)
3	BMA	U	2003	3	11,11,12	1.14	0	14,15,17	1.86	2 (14%)
4	NAG	U	2004	1,4	14,14,15	0.45	0	15,19,21	0.47	0
4	NAG	U	2005	4	14,14,15	0.39	0	15,19,21	0.30	0
3	NAG	W	2001	1,3	14,14,15	0.59	0	15,19,21	1.06	2 (13%)
3	NAG	W	2002	3	14,14,15	0.57	0	15,19,21	0.88	0
3	BMA	W	2003	3	11,11,12	0.57	0	14,15,17	0.79	0
4	NAG	W	2004	1,4	14,14,15	1.31	1 (7%)	15,19,21	1.44	3 (20%)
4	NAG	W	2005	4	14,14,15	0.69	0	15,19,21	0.63	0
4	NAG	Y	2002	1,4	14,14,15	0.36	0	15,19,21	0.25	0
4	NAG	Y	2003	4	14,14,15	0.33	0	15,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	c	2002	1,4	14,14,15	0.59	0	15,19,21	0.98	1 (6%)
4	NAG	c	2003	4	14,14,15	0.42	0	15,19,21	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	A	2003	3	-	0/2/19/22	0/1/1/1
4	NAG	A	2004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2005	4	-	0/6/23/26	0/1/1/1
3	NAG	C	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	C	2003	3	-	0/2/19/22	0/1/1/1
3	NAG	E	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	E	2003	3	-	0/2/19/22	0/1/1/1
4	NAG	E	2004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	2005	4	-	0/6/23/26	0/1/1/1
3	NAG	G	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	G	2003	3	-	0/2/19/22	0/1/1/1
4	NAG	G	2004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2005	4	-	0/6/23/26	0/1/1/1
3	NAG	I	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	I	2003	3	-	0/2/19/22	0/1/1/1
4	NAG	I	2004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	2005	4	-	0/6/23/26	0/1/1/1
3	NAG	K	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	K	2003	3	-	0/2/19/22	0/1/1/1
3	NAG	M	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	M	2003	3	-	0/2/19/22	0/1/1/1
3	NAG	O	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	O	2003	3	-	0/2/19/22	0/1/1/1
4	NAG	O	2004	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	O	2005	4	-	0/6/23/26	0/1/1/1
3	NAG	Q	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	Q	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	Q	2003	3	-	0/2/19/22	0/1/1/1
4	NAG	Q	2004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2005	4	-	0/6/23/26	0/1/1/1
3	NAG	S	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	S	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	S	2003	3	-	0/2/19/22	0/1/1/1
4	NAG	S	2004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2005	4	-	0/6/23/26	0/1/1/1
3	NAG	U	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	U	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	U	2003	3	-	0/2/19/22	0/1/1/1
4	NAG	U	2004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	U	2005	4	-	0/6/23/26	0/1/1/1
3	NAG	W	2001	1,3	-	0/6/23/26	0/1/1/1
3	NAG	W	2002	3	-	0/6/23/26	0/1/1/1
3	BMA	W	2003	3	-	0/2/19/22	0/1/1/1
4	NAG	W	2004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	W	2005	4	-	0/6/23/26	0/1/1/1
4	NAG	Y	2002	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Y	2003	4	-	0/6/23/26	0/1/1/1
4	NAG	c	2002	1,4	-	0/6/23/26	0/1/1/1
4	NAG	c	2003	4	-	0/6/23/26	0/1/1/1

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2001	NAG	O5-C1	-5.56	1.34	1.43
3	U	2002	NAG	O5-C1	-4.81	1.35	1.43
4	S	2005	NAG	O5-C1	-4.74	1.35	1.43
3	I	2001	NAG	O5-C1	-4.71	1.35	1.43
4	W	2004	NAG	O5-C1	-4.58	1.36	1.43
4	G	2004	NAG	O5-C1	-4.41	1.36	1.43
4	E	2004	NAG	O5-C1	-4.29	1.36	1.43
3	E	2002	NAG	O5-C1	-4.11	1.36	1.43
4	Q	2004	NAG	O5-C1	-3.95	1.37	1.43
4	O	2004	NAG	O5-C1	-3.85	1.37	1.43
3	I	2002	NAG	O5-C1	-3.47	1.37	1.43
4	A	2004	NAG	O5-C1	-3.43	1.38	1.43
3	G	2002	NAG	O5-C1	-3.12	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	2003	BMA	O5-C1	-2.60	1.39	1.43
3	M	2002	NAG	O5-C1	-2.52	1.39	1.43
4	I	2004	NAG	O5-C1	-2.49	1.39	1.43
3	M	2003	BMA	O5-C1	-2.33	1.39	1.43
3	Q	2001	NAG	O5-C1	-2.21	1.40	1.43
3	O	2002	NAG	O5-C1	-2.01	1.40	1.43
3	G	2003	BMA	C1-C2	2.03	1.57	1.52
3	I	2003	BMA	O2-C2	2.04	1.47	1.43
3	I	2003	BMA	C2-C3	2.13	1.55	1.52
3	K	2001	NAG	C1-C2	2.17	1.55	1.52
3	O	2003	BMA	C4-C3	2.18	1.58	1.52
4	S	2005	NAG	C1-C2	2.24	1.55	1.52
3	U	2002	NAG	C1-C2	2.27	1.55	1.52
3	C	2003	BMA	O3-C3	2.32	1.48	1.43
3	E	2001	NAG	O5-C1	2.36	1.47	1.43
4	E	2005	NAG	C1-C2	2.37	1.55	1.52
3	A	2003	BMA	C2-C3	2.44	1.55	1.52
3	I	2003	BMA	C1-C2	2.44	1.58	1.52
3	K	2003	BMA	C6-C5	2.45	1.60	1.51
3	A	2003	BMA	C4-C3	2.49	1.58	1.52
3	K	2003	BMA	O3-C3	2.59	1.49	1.43
3	G	2003	BMA	C2-C3	2.64	1.56	1.52
3	G	2003	BMA	C4-C5	2.93	1.59	1.53
3	C	2003	BMA	C1-C2	3.00	1.59	1.52
3	C	2003	BMA	C4-C3	3.09	1.60	1.52
4	A	2005	NAG	O5-C1	3.15	1.49	1.43
3	M	2003	BMA	C4-C3	3.23	1.60	1.52
3	O	2003	BMA	C4-C5	3.42	1.60	1.53
3	A	2001	NAG	C1-C2	3.44	1.57	1.52
3	E	2003	BMA	C1-C2	3.58	1.60	1.52
3	A	2003	BMA	C1-C2	3.63	1.60	1.52
3	G	2003	BMA	C4-C3	3.78	1.62	1.52
4	I	2005	NAG	C1-C2	3.79	1.57	1.52
3	S	2003	BMA	C1-C2	3.85	1.61	1.52
3	K	2003	BMA	C4-C5	3.88	1.61	1.53
3	K	2003	BMA	C4-C3	4.11	1.63	1.52
4	A	2005	NAG	C1-C2	4.11	1.58	1.52
3	M	2003	BMA	C4-C5	4.19	1.62	1.53
3	I	2003	BMA	C4-C5	4.34	1.62	1.53
3	C	2003	BMA	C4-C5	4.39	1.62	1.53
4	I	2005	NAG	O5-C1	4.44	1.51	1.43
3	I	2003	BMA	C4-C3	4.53	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	2003	BMA	C2-C3	4.67	1.58	1.52

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	2003	BMA	O5-C1-C2	-3.37	105.39	110.86
3	Q	2003	BMA	O3-C3-C4	-3.36	102.78	110.34
3	M	2002	NAG	C1-O5-C5	-2.73	108.78	112.25
3	E	2003	BMA	O2-C2-C3	-2.64	104.80	110.12
4	E	2004	NAG	C1-O5-C5	-2.60	108.94	112.25
4	O	2004	NAG	C1-O5-C5	-2.52	109.04	112.25
3	U	2003	BMA	O2-C2-C3	-2.51	105.06	110.12
3	I	2001	NAG	C1-O5-C5	-2.41	109.19	112.25
3	C	2003	BMA	O2-C2-C3	-2.39	105.32	110.12
3	K	2003	BMA	O2-C2-C3	-2.34	105.40	110.12
3	W	2001	NAG	C3-C2-N2	-2.26	105.14	110.56
3	I	2002	NAG	C1-O5-C5	-2.22	109.42	112.25
3	M	2003	BMA	O2-C2-C3	-2.15	105.79	110.12
4	W	2004	NAG	C1-O5-C5	-2.13	109.54	112.25
3	O	2003	BMA	C1-C2-C3	-2.05	107.11	109.54
3	I	2001	NAG	C3-C4-C5	2.01	113.69	110.20
3	K	2003	BMA	C3-C4-C5	2.03	113.74	110.20
3	K	2001	NAG	C1-O5-C5	2.04	114.84	112.25
3	M	2003	BMA	C1-O5-C5	2.06	114.86	112.25
3	C	2003	BMA	C1-O5-C5	2.07	114.87	112.25
4	I	2004	NAG	C4-C3-C2	2.10	114.50	111.23
4	c	2002	NAG	C4-C3-C2	2.16	114.58	111.23
3	S	2001	NAG	C1-O5-C5	2.17	115.01	112.25
3	G	2003	BMA	C3-C4-C5	2.23	114.08	110.20
4	A	2004	NAG	C4-C3-C2	2.24	114.70	111.23
3	E	2002	NAG	C4-C3-C2	2.24	114.72	111.23
3	U	2002	NAG	C4-C3-C2	2.26	114.74	111.23
3	O	2003	BMA	C3-C4-C5	2.29	114.19	110.20
3	A	2003	BMA	O2-C2-C1	2.30	113.82	109.21
3	W	2001	NAG	C1-O5-C5	2.31	115.19	112.25
3	S	2003	BMA	O2-C2-C1	2.35	113.91	109.21
4	O	2005	NAG	C1-O5-C5	2.40	115.29	112.25
3	C	2003	BMA	C3-C4-C5	2.42	114.41	110.20
3	O	2003	BMA	C1-O5-C5	2.50	115.42	112.25
4	O	2004	NAG	C4-C3-C2	2.51	115.14	111.23
3	C	2003	BMA	O2-C2-C1	2.55	114.32	109.21
3	A	2003	BMA	C1-C2-C3	2.56	112.57	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	2003	BMA	C2-C3-C4	2.59	115.44	111.04
3	A	2003	BMA	O5-C1-C2	2.62	115.11	110.86
3	G	2001	NAG	C3-C4-C5	2.70	114.90	110.20
3	Q	2001	NAG	C1-O5-C5	2.71	115.69	112.25
3	I	2003	BMA	C2-C3-C4	2.71	115.65	111.04
3	A	2001	NAG	C1-O5-C5	2.74	115.73	112.25
3	S	2003	BMA	C1-O5-C5	2.76	115.75	112.25
4	G	2004	NAG	C4-C3-C2	2.81	115.59	111.23
3	I	2003	BMA	O2-C2-C1	2.90	115.03	109.21
3	E	2003	BMA	C1-O5-C5	3.05	116.12	112.25
3	S	2003	BMA	O5-C1-C2	3.09	115.87	110.86
4	E	2004	NAG	C3-C4-C5	3.10	115.60	110.20
3	I	2001	NAG	C4-C3-C2	3.12	116.08	111.23
4	E	2004	NAG	C4-C3-C2	3.21	116.22	111.23
3	O	2001	NAG	C1-O5-C5	3.22	116.34	112.25
4	W	2004	NAG	C4-C3-C2	3.26	116.30	111.23
4	I	2005	NAG	C1-O5-C5	3.37	116.53	112.25
3	Q	2003	BMA	O3-C3-C2	3.43	116.19	110.00
4	S	2005	NAG	C4-C3-C2	3.53	116.71	111.23
4	I	2004	NAG	C3-C4-C5	3.58	116.44	110.20
3	E	2001	NAG	C1-O5-C5	3.59	116.81	112.25
4	A	2004	NAG	C3-C4-C5	3.81	116.83	110.20
3	E	2003	BMA	O2-C2-C1	3.83	116.88	109.21
3	G	2001	NAG	C4-C3-C2	3.87	117.25	111.23
4	W	2004	NAG	C3-C4-C5	3.88	116.97	110.20
3	I	2003	BMA	C3-C4-C5	3.94	117.07	110.20
3	E	2002	NAG	C3-C4-C5	4.06	117.27	110.20
3	M	2003	BMA	C3-C4-C5	4.06	117.28	110.20
3	K	2003	BMA	C1-O5-C5	4.06	117.40	112.25
4	G	2004	NAG	C3-C4-C5	4.17	117.46	110.20
3	Q	2003	BMA	C3-C4-C5	4.35	117.78	110.20
4	A	2005	NAG	C1-O5-C5	4.65	118.15	112.25
3	S	2003	BMA	C1-C2-C3	4.67	115.07	109.54
3	U	2003	BMA	C1-O5-C5	5.13	118.76	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	NAG	1	0
3	C	2002	NAG	1	0
3	E	2001	NAG	1	0
3	E	2002	NAG	1	0
3	G	2001	NAG	1	0
4	G	2004	NAG	1	0
4	G	2005	NAG	1	0
4	I	2004	NAG	1	0
4	I	2005	NAG	1	0
4	Q	2004	NAG	1	0
4	Q	2005	NAG	1	0
3	S	2001	NAG	1	0
4	S	2004	NAG	1	0
4	S	2005	NAG	1	0
4	W	2004	NAG	1	0
4	W	2005	NAG	1	0
4	Y	2002	NAG	1	0
4	Y	2003	NAG	1	0

5.6 Ligand geometry ⓘ

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	C	2004	1	14,14,15	0.86	1 (7%)	15,19,21	0.87	0
5	NAG	K	2004	1	14,14,15	0.63	0	15,19,21	0.46	0
5	NAG	M	2004	1	14,14,15	0.30	0	15,19,21	0.30	0
5	NAG	O	2006	1	14,14,15	0.98	1 (7%)	15,19,21	0.98	2 (13%)
5	NAG	Y	2001	1	14,14,15	0.35	0	15,19,21	1.01	1 (6%)
5	NAG	a	2001	1	14,14,15	0.58	0	15,19,21	0.66	1 (6%)
5	NAG	c	2001	1	14,14,15	0.62	1 (7%)	15,19,21	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	2004	1	-	0/6/23/26	0/1/1/1
5	NAG	K	2004	1	-	0/6/23/26	0/1/1/1
5	NAG	M	2004	1	-	0/6/23/26	0/1/1/1
5	NAG	O	2006	1	-	0/6/23/26	0/1/1/1
5	NAG	Y	2001	1	-	0/6/23/26	0/1/1/1
5	NAG	a	2001	1	-	0/6/23/26	0/1/1/1
5	NAG	c	2001	1	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	2006	NAG	O5-C1	-2.93	1.38	1.43
5	C	2004	NAG	O5-C1	-2.46	1.39	1.43
5	c	2001	NAG	O5-C1	-2.11	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a	2001	NAG	C1-O5-C5	2.29	115.15	112.25
5	O	2006	NAG	C3-C4-C5	2.37	114.34	110.20
5	O	2006	NAG	C4-C3-C2	2.46	115.06	111.23
5	Y	2001	NAG	C1-O5-C5	3.64	116.86	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Y	2001	NAG	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	324/334 (97%)	-0.18	7 (2%) 65 44	32, 52, 87, 162	0
1	C	324/334 (97%)	0.04	10 (3%) 52 33	38, 63, 124, 185	0
1	E	324/334 (97%)	-0.03	6 (1%) 70 50	36, 58, 115, 196	0
1	G	324/334 (97%)	-0.15	5 (1%) 76 57	28, 51, 92, 170	0
1	I	324/334 (97%)	-0.12	4 (1%) 81 63	27, 49, 94, 166	0
1	K	324/334 (97%)	-0.04	8 (2%) 61 39	37, 59, 112, 178	0
1	M	324/334 (97%)	-0.16	12 (3%) 45 27	28, 54, 114, 206	0
1	O	324/334 (97%)	-0.07	9 (2%) 56 36	32, 54, 117, 190	0
1	Q	324/334 (97%)	-0.13	8 (2%) 61 39	34, 53, 117, 181	0
1	S	324/334 (97%)	-0.10	10 (3%) 52 33	37, 63, 128, 177	0
1	U	324/334 (97%)	0.05	13 (4%) 42 25	36, 66, 124, 186	0
1	W	324/334 (97%)	0.12	16 (4%) 33 19	41, 64, 125, 183	0
1	Y	324/334 (97%)	0.58	27 (8%) 14 7	57, 83, 178, 247	0
1	a	324/334 (97%)	0.59	35 (10%) 8 4	59, 86, 197, 263	0
1	c	324/334 (97%)	0.60	40 (12%) 5 2	55, 87, 184, 267	0
2	B	177/181 (97%)	0.27	8 (4%) 37 21	36, 94, 134, 165	0
2	D	177/181 (97%)	0.97	31 (17%) 2 1	42, 124, 175, 199	0
2	F	177/181 (97%)	0.88	31 (17%) 2 1	45, 123, 173, 182	0
2	H	177/181 (97%)	0.24	8 (4%) 37 21	35, 97, 139, 151	0
2	J	177/181 (97%)	0.45	14 (7%) 15 8	36, 95, 136, 152	0
2	L	177/181 (97%)	0.89	28 (15%) 3 1	42, 123, 163, 171	0
2	N	177/181 (97%)	0.94	33 (18%) 2 1	37, 123, 176, 197	0
2	P	177/181 (97%)	0.81	28 (15%) 3 1	31, 120, 174, 185	0
2	R	177/181 (97%)	1.10	39 (22%) 1 1	42, 122, 189, 220	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	T	177/181 (97%)	0.74	30 (16%) 2 1	48, 123, 166, 184	0
2	V	177/181 (97%)	0.76	25 (14%) 4 2	45, 123, 167, 180	0
2	X	177/181 (97%)	0.88	30 (16%) 2 1	47, 123, 171, 182	0
2	Z	177/181 (97%)	2.49	78 (44%) 0 0	68, 193, 265, 299	0
2	b	177/181 (97%)	2.89	85 (48%) 0 0	74, 189, 251, 272	0
2	d	177/181 (97%)	2.57	78 (44%) 0 0	68, 193, 239, 274	0
All	All	7515/7725 (97%)	0.44	756 (10%) 9 5	27, 75, 185, 299	0

All (756) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	16	GLY	35.5
2	b	16	GLY	29.2
2	Z	23	GLY	27.5
1	c	16	GLY	18.1
2	Z	24	TYR	16.1
1	Y	15	ILE	15.6
2	b	141	TYR	15.1
2	b	176	GLY	14.4
2	Z	35	ALA	13.5
2	d	22	TYR	13.4
1	a	16	GLY	13.4
1	a	9	PRO	12.9
2	d	36	ALA	12.5
2	b	152	VAL	12.5
2	d	26	HIS	12.4
2	d	35	ALA	12.1
2	b	153	ARG	11.5
2	d	138	PHE	10.7
2	b	18	VAL	10.5
2	Z	136	GLY	10.5
1	c	15	ILE	10.3
2	Z	141	TYR	10.0
2	N	27	SER	9.9
2	T	140	PHE	9.9
1	a	8	ASP	9.8
1	M	9	PRO	9.6
2	d	130	ALA	9.5
1	a	14	CYS	9.2
2	b	157	TYR	9.2

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Mol	Chain	Res	Type	RSRZ
1	a	21[A]	ASN	9.0
2	b	34	TYR	8.9
1	c	21[A]	ASN	8.9
2	d	16	GLY	8.7
1	O	9	PRO	8.6
2	b	140	PHE	8.5
2	L	140	PHE	8.5
2	d	15	GLN	8.5
1	I	324	PRO	8.5
2	Z	22	TYR	8.5
1	Y	22	SER	8.4
1	W	324	PRO	8.3
1	a	15	ILE	8.3
1	Y	23	THR	8.2
1	E	324	PRO	8.2
2	d	33	GLY	8.0
1	Q	8	ASP	7.9
2	Z	163	SER	7.9
2	Z	16	GLY	7.8
2	d	141	TYR	7.7
2	b	35	ALA	7.6
2	d	111	HIS	7.5
2	d	143	LYS	7.5
2	b	24	TYR	7.5
2	d	24	TYR	7.3
2	b	133	LEU	7.1
2	N	26	HIS	7.1
2	b	33	GLY	7.1
2	d	157	TYR	7.1
2	T	141	TYR	7.0
2	N	22	TYR	7.0
2	b	25	HIS	6.9
1	U	324	PRO	6.8
2	b	168	LEU	6.8
2	R	177	ARG	6.8
2	d	165	GLU	6.8
2	b	169	LYS	6.7
2	b	32	SER	6.7
2	Z	128	ASP	6.7
2	Z	175	SER	6.6
1	c	13	ILE	6.6
1	a	10	GLY	6.6

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Mol	Chain	Res	Type	RSRZ
2	d	34	TYR	6.5
2	Z	138	PHE	6.5
2	N	140	PHE	6.5
2	d	38	LYS	6.5
1	c	14	CYS	6.4
2	Z	134	GLY	6.4
2	L	22	TYR	6.3
2	b	21	TRP	6.3
2	b	44	ALA	6.3
2	d	107	THR	6.3
2	Z	36	ALA	6.3
2	P	31	GLY	6.3
1	Y	319	GLY	6.2
2	d	122	VAL	6.2
2	d	153	ARG	6.2
1	Y	323	SER	6.2
2	Z	152	VAL	6.2
1	K	12	GLN	6.2
2	b	131	LYS	6.1
2	b	143	LYS	6.1
1	c	8	ASP	6.1
2	d	140	PHE	6.1
1	Q	9	PRO	6.0
1	S	8	ASP	6.0
2	d	168	LEU	6.0
1	c	22	SER	6.0
2	b	149	MET	6.0
2	R	158	ASP	5.9
2	Z	10	ILE	5.9
1	Y	324	PRO	5.9
2	Z	148	CYS	5.9
1	I	8	ASP	5.9
1	A	8	ASP	5.9
2	b	125	GLN	5.8
2	d	23	GLY	5.8
2	d	126	LEU	5.8
1	K	13	ILE	5.8
2	b	177	ARG	5.8
2	b	174	SER	5.8
2	P	176	GLY	5.7
2	b	1	GLY	5.7
2	D	21	TRP	5.7

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Mol	Chain	Res	Type	RSRZ
2	X	22	TYR	5.7
1	W	8	ASP	5.7
2	R	126	LEU	5.7
2	d	125	GLN	5.7
1	M	10	GLY	5.6
1	U	9	PRO	5.6
2	Z	143	LYS	5.6
2	R	22	TYR	5.6
1	O	10	GLY	5.6
1	E	12	GLN	5.6
1	M	8	ASP	5.5
1	Q	14	CYS	5.5
2	Z	119	TYR	5.5
2	P	27	SER	5.5
2	R	140	PHE	5.5
2	N	176	GLY	5.4
2	d	137	CYS	5.4
2	b	142	HIS	5.4
2	Z	7	ALA	5.4
2	b	13	GLY	5.4
2	Z	34	TYR	5.4
2	b	26	HIS	5.4
2	Z	5	ALA	5.3
1	E	9	PRO	5.3
2	V	140	PHE	5.3
2	L	138	PHE	5.3
2	P	32	SER	5.3
2	b	48	VAL	5.3
2	b	173	ILE	5.3
1	E	8	ASP	5.3
2	R	176	GLY	5.3
2	R	29	GLU	5.2
1	a	324	PRO	5.2
2	b	175	SER	5.2
2	Z	57	ASP	5.1
2	d	132	GLU	5.1
2	b	22	TYR	5.1
2	V	160	PRO	5.1
2	H	140	PHE	5.1
2	d	128	ASP	5.0
2	b	27	SER	5.0
1	a	23	THR	5.0

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Mol	Chain	Res	Type	RSRZ
2	N	31	GLY	5.0
1	C	12	GLN	5.0
2	b	138	PHE	5.0
2	b	41	THR	5.0
1	a	12	GLN	4.9
2	Z	160	PRO	4.9
2	d	17	MET	4.9
2	b	119	TYR	4.9
2	Z	25	HIS	4.8
2	L	32	SER	4.8
2	b	37	ASP	4.8
2	b	38	LYS	4.8
2	N	131	LYS	4.8
1	a	17	TYR	4.8
2	Z	142	HIS	4.8
1	Y	21[A]	ASN	4.8
2	d	139	GLU	4.8
2	R	36	ALA	4.8
1	Y	20	ASN	4.8
2	b	126	LEU	4.7
1	Y	320	LEU	4.7
2	Z	37	ASP	4.7
1	Y	17	TYR	4.7
2	Z	164	GLU	4.7
2	L	33	GLY	4.6
2	d	133	LEU	4.6
2	D	32	SER	4.6
1	Y	13	ILE	4.6
2	D	22	TYR	4.6
2	d	32	SER	4.6
2	N	32	SER	4.6
2	Z	168	LEU	4.6
2	X	157	TYR	4.6
2	b	17	MET	4.5
1	a	13	ILE	4.5
2	F	177	ARG	4.5
1	c	9	PRO	4.5
2	D	128	ASP	4.5
2	Z	14	TRP	4.5
2	b	154	ASN	4.5
1	U	323	SER	4.5
2	N	46	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	324	PRO	4.5
2	Z	9	PHE	4.5
1	A	323	SER	4.5
2	d	1	GLY	4.5
1	a	323	SER	4.4
1	Y	14	CYS	4.4
2	R	138	PHE	4.4
2	Z	8	GLY	4.4
1	Y	24	GLU	4.4
2	P	1	GLY	4.4
2	Z	6	ILE	4.4
2	R	18	VAL	4.4
2	d	150	GLU	4.4
2	X	24	TYR	4.3
2	D	140	PHE	4.3
2	d	142	HIS	4.3
2	R	32	SER	4.3
2	d	164	GLU	4.3
2	d	14	TRP	4.3
1	K	15	ILE	4.2
1	c	34	VAL	4.2
2	P	170	ARG	4.2
1	c	10	GLY	4.2
2	D	31	GLY	4.2
2	Z	132	GLU	4.2
1	c	23	THR	4.2
1	O	12	GLN	4.2
2	R	35	ALA	4.2
2	b	137	CYS	4.2
2	F	139	GLU	4.2
2	X	140	PHE	4.2
2	d	25	HIS	4.2
2	N	160	PRO	4.2
2	X	139	GLU	4.2
1	W	9	PRO	4.1
2	b	139	GLU	4.1
2	N	138	PHE	4.1
1	c	282	GLN	4.1
2	V	34	TYR	4.1
2	d	115	VAL	4.1
2	X	143	LYS	4.1
1	U	12	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
2	X	23	GLY	4.1
2	N	33	GLY	4.1
1	a	39	ALA	4.1
2	P	156	THR	4.1
2	F	140	PHE	4.1
2	N	164	GLU	4.1
2	d	109	ASP	4.1
2	d	31	GLY	4.0
1	O	8	ASP	4.0
2	d	106	ARG	4.0
2	d	127	ARG	4.0
2	T	22	TYR	4.0
2	b	170	ARG	4.0
2	L	27	SER	4.0
2	d	158	ASP	4.0
2	L	126	LEU	3.9
2	Z	144	CYS	3.9
2	X	38	LYS	3.9
2	Z	149	MET	3.9
2	F	1	GLY	3.9
2	b	23	GLY	3.9
2	F	138	PHE	3.9
2	D	33	GLY	3.9
2	Z	106	ARG	3.9
2	Z	121	LYS	3.9
1	E	10	GLY	3.9
2	L	31	GLY	3.9
2	R	175	SER	3.9
1	G	324	PRO	3.9
2	Z	157	TYR	3.9
2	J	144	CYS	3.8
1	c	12	GLN	3.8
2	b	132	GLU	3.8
1	c	20	ASN	3.8
1	a	35	THR	3.8
2	d	162	TYR	3.8
1	Y	318	ILE	3.8
2	Z	124	LEU	3.8
2	d	3	PHE	3.8
1	C	324	PRO	3.8
2	D	1	GLY	3.8
2	D	24	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
2	L	1	GLY	3.8
1	C	55(A)	GLY	3.8
1	W	12	GLN	3.8
1	U	14	CYS	3.8
1	Y	322	ASN	3.7
2	b	36	ALA	3.7
2	d	21	TRP	3.7
1	Q	12	GLN	3.7
1	c	11	ASP	3.7
2	N	177	ARG	3.7
2	R	27	SER	3.7
2	Z	135	ASN	3.7
1	S	12	GLN	3.7
2	V	167	ARG	3.7
2	P	30	GLN	3.7
2	Z	125	GLN	3.7
2	V	157	TYR	3.7
2	V	162	TYR	3.6
2	Z	126	LEU	3.6
1	c	35	THR	3.6
1	U	13	ILE	3.6
2	Z	127	ARG	3.6
2	X	150	GLU	3.6
2	N	16	GLY	3.6
1	K	8	ASP	3.6
2	Z	177	ARG	3.6
1	W	323	SER	3.6
2	D	26	HIS	3.6
2	D	35	ALA	3.6
2	X	147	GLU	3.6
1	K	14	CYS	3.6
1	a	36	VAL	3.6
1	S	39	ALA	3.6
2	N	25	HIS	3.5
2	X	35	ALA	3.5
2	B	38	LYS	3.5
1	c	324	PRO	3.5
2	b	150	GLU	3.5
2	D	20	GLY	3.5
2	J	1	GLY	3.5
2	P	29	GLU	3.5
2	R	162	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
2	V	24	TYR	3.5
2	Z	21	TRP	3.5
2	R	161	GLN	3.5
2	F	29	GLU	3.5
2	R	133	LEU	3.5
2	d	2	LEU	3.5
2	L	25	HIS	3.5
2	Z	109	ASP	3.5
2	V	141	TYR	3.5
2	b	144	CYS	3.5
2	J	142	HIS	3.5
1	M	13	ILE	3.5
2	F	141	TYR	3.5
1	a	22	SER	3.4
2	b	45	ILE	3.4
2	H	156	THR	3.4
2	N	30	GLN	3.4
2	L	20	GLY	3.4
2	T	25	HIS	3.4
2	B	177	ARG	3.4
2	Z	140	PHE	3.4
2	d	116	LYS	3.4
2	Z	17	MET	3.4
1	O	16	GLY	3.4
2	V	144	CYS	3.4
2	J	143	LYS	3.4
2	L	26	HIS	3.4
2	d	156	THR	3.4
1	Q	10	GLY	3.4
2	b	14	TRP	3.4
2	d	176	GLY	3.4
2	P	173	ILE	3.4
2	b	29	GLU	3.4
2	T	160	PRO	3.4
1	M	12	GLN	3.4
2	D	141	TYR	3.3
1	c	315	VAL	3.3
2	V	166	ALA	3.3
1	c	273	GLU	3.3
2	d	113	SER	3.3
1	C	8	ASP	3.3
2	V	143	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
2	T	157	TYR	3.3
2	J	39	GLU	3.3
1	S	77	ASP	3.3
2	H	27	SER	3.3
2	N	29	GLU	3.3
2	R	1	GLY	3.3
2	b	3	PHE	3.3
1	U	10	GLY	3.3
2	R	144	CYS	3.2
1	W	13	ILE	3.2
2	T	27	SER	3.2
1	a	315	VAL	3.2
2	R	31	GLY	3.2
2	R	26	HIS	3.2
2	N	143	LYS	3.2
2	b	12	GLY	3.2
1	A	12	GLN	3.2
2	D	27	SER	3.2
2	D	177	ARG	3.2
2	b	40	SER	3.2
2	d	177	ARG	3.2
1	A	9	PRO	3.2
2	Z	170	ARG	3.2
1	Y	37	THR	3.2
2	Z	29	GLU	3.2
2	b	172	GLU	3.2
1	W	10	GLY	3.2
1	U	8	ASP	3.2
2	R	25	HIS	3.2
2	P	171	GLU	3.1
1	S	9	PRO	3.1
2	b	5	ALA	3.1
2	R	159	TYR	3.1
2	d	5	ALA	3.1
1	S	13	ILE	3.1
2	L	21	TRP	3.1
2	b	162	TYR	3.1
2	J	38	LYS	3.1
1	M	16	GLY	3.1
2	R	33	GLY	3.1
2	b	7	ALA	3.1
1	S	40	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	a	86	TYR	3.1
2	Z	1	GLY	3.1
2	b	122	VAL	3.1
1	a	322	ASN	3.1
2	N	28	ASN	3.1
2	T	175	SER	3.1
2	F	4	GLY	3.1
2	T	32	SER	3.1
2	d	27	SER	3.1
1	G	12	GLN	3.1
1	G	9	PRO	3.1
2	D	142	HIS	3.1
2	Z	15	GLN	3.1
2	d	108	LEU	3.1
2	d	148	CYS	3.1
2	P	26	HIS	3.1
1	U	320	LEU	3.0
1	a	320	LEU	3.0
2	b	158	ASP	3.0
2	X	20	GLY	3.0
2	b	136	GLY	3.0
2	D	14	TRP	3.0
1	I	9	PRO	3.0
2	V	158	ASP	3.0
2	b	102	MET	3.0
2	F	42	GLN	3.0
2	d	119	TYR	3.0
2	B	140	PHE	3.0
2	b	128	ASP	3.0
1	M	324	PRO	3.0
2	R	160	PRO	3.0
2	d	19	ASP	3.0
1	M	11	ASP	2.9
2	Z	4	GLY	2.9
1	U	16	GLY	2.9
2	D	158	ASP	2.9
2	b	15	GLN	2.9
1	U	322	ASN	2.9
2	N	126	LEU	2.9
1	c	323	SER	2.9
1	W	40	GLN	2.9
1	c	17	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	22	TYR	2.9
1	c	55(A)	GLY	2.9
2	J	176	GLY	2.9
2	T	139	GLU	2.9
2	d	52	VAL	2.9
2	Z	113	SER	2.9
2	D	173	ILE	2.9
2	d	118	LEU	2.9
2	D	139	GLU	2.9
2	V	27	SER	2.9
2	D	34	TYR	2.9
2	d	18	VAL	2.9
2	Z	32	SER	2.9
2	d	20	GLY	2.9
2	b	115	VAL	2.8
1	W	15	ILE	2.8
2	J	31	GLY	2.8
2	Z	114	ASN	2.8
2	D	18	VAL	2.8
2	X	34	TYR	2.8
1	W	14	CYS	2.8
2	T	1	GLY	2.8
2	N	14	TRP	2.8
1	Q	21[A]	ASN	2.8
2	T	143	LYS	2.8
2	F	145	ASP	2.8
2	P	177	ARG	2.8
2	F	127	ARG	2.8
1	S	32	LYS	2.8
2	F	175	SER	2.8
2	P	15	GLN	2.8
2	R	23	GLY	2.8
2	D	157	TYR	2.8
2	L	38	LYS	2.8
2	T	138	PHE	2.8
2	R	139	GLU	2.8
2	b	159	TYR	2.8
2	L	130	ALA	2.8
2	X	27	SER	2.8
1	S	11	ASP	2.8
2	d	136	GLY	2.8
1	a	302	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	X	158	ASP	2.8
2	d	41	THR	2.8
1	a	303	GLY	2.7
2	T	26	HIS	2.7
2	T	168	LEU	2.7
2	D	170	ARG	2.7
2	R	24	TYR	2.7
2	P	25	HIS	2.7
1	c	141	TYR	2.7
1	C	290	SER	2.7
2	D	19	ASP	2.7
2	Z	105	GLU	2.7
2	V	25	HIS	2.7
2	Z	131	LYS	2.7
2	P	140	PHE	2.7
2	X	149	MET	2.7
2	H	125	GLN	2.7
1	Y	9	PRO	2.7
2	d	151	SER	2.6
2	b	31	GLY	2.6
1	a	43	LEU	2.6
2	F	146	ASN	2.6
2	J	35	ALA	2.6
2	P	18	VAL	2.6
2	Z	3	PHE	2.6
2	V	168	LEU	2.6
2	B	149	MET	2.6
2	X	1	GLY	2.6
2	d	160	PRO	2.6
1	I	323	SER	2.6
1	a	25	GLN	2.6
1	c	173	GLN	2.6
2	R	125	GLN	2.6
2	T	111	HIS	2.6
2	Z	27	SER	2.6
2	Z	92	TRP	2.6
2	D	176	GLY	2.6
2	P	135	ASN	2.6
2	T	166	ALA	2.6
2	D	168	LEU	2.6
2	R	30	GLN	2.6
2	b	120	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	320	LEU	2.6
1	O	324	PRO	2.6
2	P	22	TYR	2.6
1	c	64	CYS	2.5
2	D	167	ARG	2.5
2	F	106	ARG	2.5
2	Z	13	GLY	2.5
2	b	146	ASN	2.5
1	W	38	HIS	2.5
2	H	142	HIS	2.5
2	V	142	HIS	2.5
2	b	106	ARG	2.5
2	Z	162	TYR	2.5
2	d	4	GLY	2.5
1	a	317	ALA	2.5
2	T	130	ALA	2.5
2	d	161	GLN	2.5
1	O	11	ASP	2.5
2	D	175	SER	2.5
2	R	117	ASN	2.5
2	T	167	ARG	2.5
2	V	173	ILE	2.5
2	B	27	SER	2.5
2	P	164	GLU	2.5
2	J	140	PHE	2.5
2	d	152	VAL	2.5
2	T	177	ARG	2.5
1	Y	40	GLN	2.5
1	c	32	LYS	2.5
2	T	142	HIS	2.5
2	Z	26	HIS	2.5
2	F	173	ILE	2.5
2	L	139	GLU	2.5
2	P	35	ALA	2.5
1	G	8	ASP	2.5
2	F	114	ASN	2.5
2	F	144	CYS	2.5
2	J	29	GLU	2.5
2	Z	123	ARG	2.5
2	b	118	LEU	2.5
1	c	88	VAL	2.5
2	Z	40	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	c	31	GLU	2.4
2	V	135	ASN	2.4
2	N	23	GLY	2.4
2	Z	153	ARG	2.4
2	J	27	SER	2.4
2	Z	156	THR	2.4
2	Z	171	GLU	2.4
2	F	169	LYS	2.4
2	L	24	TYR	2.4
2	T	24	TYR	2.4
1	c	75	MET	2.4
1	Q	13	ILE	2.4
2	N	146	ASN	2.4
2	F	3	PHE	2.4
2	d	63	PHE	2.4
2	F	174	SER	2.4
2	V	164	GLU	2.4
2	Z	111	HIS	2.4
1	C	9	PRO	2.4
2	N	47	GLY	2.4
2	B	153	ARG	2.4
2	L	158	ASP	2.4
1	c	317	ALA	2.4
1	C	13	ILE	2.4
2	V	134	GLY	2.4
2	X	173	ILE	2.4
2	D	117	ASN	2.4
2	b	113	SER	2.4
1	A	23	THR	2.4
2	P	142	HIS	2.4
2	H	177	ARG	2.3
2	b	4	GLY	2.3
2	b	55	ILE	2.3
2	d	120	ASP	2.3
1	K	320	LEU	2.3
2	Z	107	THR	2.3
2	T	29	GLU	2.3
2	V	171	GLU	2.3
2	X	39	GLU	2.3
1	c	318	ILE	2.3
2	Z	47	GLY	2.3
1	c	96(A)	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	133	LEU	2.3
2	L	141	TYR	2.3
2	L	177	ARG	2.3
2	X	163	SER	2.3
2	P	21	TRP	2.3
2	V	149	MET	2.3
1	a	11	ASP	2.3
1	O	318	ILE	2.3
2	V	120	ASP	2.3
1	M	21[A]	ASN	2.3
1	W	21[A]	ASN	2.3
1	c	83(A)	GLU	2.3
2	T	164	GLU	2.3
2	X	29	GLU	2.3
1	C	18	HIS	2.3
2	b	165	GLU	2.3
1	Y	55(A)	GLY	2.3
2	Z	112	ASP	2.3
2	V	35	ALA	2.3
1	Q	38	HIS	2.3
1	Y	95	ASN	2.3
1	Y	64	CYS	2.3
2	b	147	GLU	2.3
1	C	55	ASP	2.2
2	N	1	GLY	2.3
2	X	126	LEU	2.3
2	Z	110	PHE	2.2
1	Y	36	VAL	2.2
2	L	168	LEU	2.2
2	L	170	ARG	2.2
2	d	56	ILE	2.2
2	H	126	LEU	2.2
2	T	23	GLY	2.2
1	a	41	ASP	2.2
2	L	160	PRO	2.2
2	T	21	TRP	2.2
2	H	38	LYS	2.2
2	X	25	HIS	2.2
2	F	113	SER	2.2
1	Y	316	LEU	2.2
2	F	170	ARG	2.2
2	L	153	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
2	b	19	ASP	2.2
2	X	175	SER	2.2
2	b	135	ASN	2.2
1	K	16	GLY	2.2
2	Z	122	VAL	2.2
2	X	168	LEU	2.2
1	Y	42	ILE	2.2
1	K	56	VAL	2.2
2	F	11	GLU	2.2
2	b	121	LYS	2.2
2	b	130	ALA	2.2
1	M	114	ARG	2.2
1	M	321	ARG	2.2
2	N	45	ILE	2.2
2	Z	161	GLN	2.2
1	c	242	ALA	2.2
2	N	36	ALA	2.2
2	N	153	ARG	2.2
1	a	63	ASP	2.2
2	R	150	GLU	2.2
2	b	59	MET	2.2
2	d	167	ARG	2.2
2	L	129	ASN	2.2
1	G	323	SER	2.1
2	N	155	GLY	2.1
2	X	6	ILE	2.1
2	D	17	MET	2.1
2	N	142	HIS	2.1
1	U	11	ASP	2.1
2	N	165	GLU	2.1
1	S	34	VAL	2.1
1	Y	12	GLN	2.1
2	R	34	TYR	2.1
2	R	132	GLU	2.1
2	X	21	TRP	2.1
2	Z	28	ASN	2.1
2	V	32	SER	2.1
2	B	176	GLY	2.1
2	P	33	GLY	2.1
2	b	134	GLY	2.1
2	d	62	GLN	2.1
2	J	156	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	c	98	TYR	2.1
2	F	38	LYS	2.1
2	R	131	LYS	2.1
1	a	52	CYS	2.1
2	P	167	ARG	2.1
2	L	142	HIS	2.1
1	U	80	ILE	2.1
1	W	42	ILE	2.1
2	B	9	PHE	2.1
2	P	23	GLY	2.1
2	T	20	GLY	2.1
1	A	13	ILE	2.1
1	a	278	ASN	2.1
1	c	54	LEU	2.1
1	c	74	PRO	2.1
2	R	130	ALA	2.1
2	L	127	ARG	2.1
2	L	176	GLY	2.1
1	a	20	ASN	2.1
1	c	46	LYS	2.1
1	a	34	VAL	2.1
2	P	174	SER	2.1
2	P	175	SER	2.1
2	Z	151	SER	2.1
1	W	39	ALA	2.1
1	Y	79	PHE	2.0
2	T	145	ASP	2.0
1	c	37	THR	2.0
2	b	6	ILE	2.0
2	d	114	ASN	2.0
1	C	320	LEU	2.0
2	F	18	VAL	2.0
2	T	153	ARG	2.0
2	d	9	PHE	2.0
1	a	38	HIS	2.0
2	J	26	HIS	2.0
1	W	321	ARG	2.0
2	R	141	TYR	2.0
2	R	134	GLY	2.0
2	F	132	GLU	2.0
2	T	149	MET	2.0
2	d	102	MET	2.0

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Mol	Chain	Res	Type	RSRZ
2	X	142	HIS	2.0
2	X	30	GLN	2.0
2	X	146	ASN	2.0
1	c	30	MET	2.0
2	F	21	TRP	2.0
1	E	13	ILE	2.0
1	O	320	LEU	2.0
1	a	141	TYR	2.0
2	F	24	TYR	2.0
2	R	8	GLY	2.0
1	W	294	PHE	2.0
2	N	139	GLU	2.0
2	F	27	SER	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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	M	2001	14/15	0.94	0.15	3.59	50,58,79,79	0
3	NAG	U	2001	14/15	0.88	0.22	1.79	59,71,87,99	0
3	NAG	E	2001	14/15	0.93	0.24	1.28	74,93,116,124	0
3	NAG	W	2001	14/15	0.85	0.16	0.81	64,71,80,92	0
3	NAG	O	2001	14/15	0.89	0.19	0.38	58,72,90,97	0
3	NAG	C	2001	14/15	0.90	0.23	0.20	70,89,102,112	0
3	NAG	S	2001	14/15	0.94	0.13	-0.07	57,81,97,97	0
3	NAG	G	2001	14/15	0.93	0.16	-0.18	57,65,73,85	0
3	NAG	Q	2001	14/15	0.94	0.14	-0.64	52,67,75,77	0
3	NAG	A	2001	14/15	0.92	0.13	-0.65	49,69,79,82	0
3	NAG	I	2001	14/15	0.93	0.13	-0.99	50,58,78,80	0
4	NAG	I	2004	14/15	0.91	0.17	-	89,94,103,109	0
3	BMA	U	2003	11/12	0.73	0.30	-	114,127,131,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	M	2002	14/15	0.83	0.24	-	76,91,113,128	0
4	NAG	U	2005	14/15	0.83	0.20	-	136,154,160,165	0
3	NAG	S	2002	14/15	0.81	0.18	-	87,110,127,135	0
3	BMA	O	2003	11/12	0.79	0.14	-	119,127,132,132	0
3	NAG	Q	2002	14/15	0.93	0.11	-	67,88,103,115	0
3	BMA	C	2003	11/12	0.82	0.24	-	48,70,90,94	0
4	NAG	A	2005	14/15	0.62	0.18	-	112,122,129,132	0
4	NAG	S	2005	14/15	0.81	0.18	-	150,164,166,166	0
3	NAG	I	2002	14/15	0.95	0.12	-	44,57,67,71	0
4	NAG	Q	2005	14/15	0.76	0.26	-	120,148,158,161	0
3	BMA	W	2003	11/12	0.74	0.17	-	113,124,130,135	0
4	NAG	O	2004	14/15	0.80	0.15	-	123,134,139,143	0
4	NAG	Y	2002	14/15	0.85	0.20	-	155,161,168,175	0
4	NAG	O	2005	14/15	0.68	0.20	-	117,139,146,146	0
3	NAG	U	2002	14/15	0.81	0.19	-	89,104,121,126	0
4	NAG	S	2004	14/15	0.78	0.18	-	128,150,163,163	0
3	NAG	C	2002	14/15	0.86	0.30	-	98,106,110,110	0
3	BMA	M	2003	11/12	0.65	0.22	-	105,121,134,135	0
3	NAG	K	2002	14/15	0.91	0.25	-	81,97,102,102	0
4	NAG	W	2005	14/15	0.83	0.19	-	122,134,141,141	0
3	BMA	A	2003	11/12	0.83	0.17	-	81,83,101,101	0
3	NAG	G	2002	14/15	0.92	0.13	-	49,63,83,84	0
4	NAG	E	2005	14/15	0.81	0.20	-	106,128,134,134	0
4	NAG	U	2004	14/15	0.74	0.17	-	130,142,151,153	0
4	NAG	Q	2004	14/15	0.84	0.14	-	101,118,133,146	0
4	NAG	G	2004	14/15	0.88	0.13	-	102,107,113,114	0
3	BMA	Q	2003	11/12	0.85	0.12	-	116,120,126,127	0
3	NAG	W	2002	14/15	0.80	0.23	-	77,96,107,119	0
3	NAG	K	2001	14/15	0.85	0.20	-	56,78,99,101	0
4	NAG	I	2005	14/15	0.85	0.13	-	111,117,124,133	0
4	NAG	E	2004	14/15	0.90	0.10	-	112,124,125,126	0
3	BMA	I	2003	11/12	0.80	0.20	-	56,83,91,91	0
3	NAG	O	2002	14/15	0.83	0.20	-	83,102,117,123	0
4	NAG	G	2005	14/15	0.85	0.15	-	106,120,127,128	0
3	BMA	G	2003	11/12	0.82	0.16	-	63,85,93,95	0
3	NAG	A	2002	14/15	0.92	0.14	-	59,82,94,97	0
4	NAG	c	2003	14/15	0.69	0.25	-	168,181,188,188	0
3	NAG	E	2002	14/15	0.81	0.33	-	103,121,127,128	0
3	BMA	E	2003	11/12	0.68	0.23	-	74,81,103,103	0
4	NAG	c	2002	14/15	0.87	0.21	-	159,180,187,188	0
4	NAG	W	2004	14/15	0.79	0.19	-	114,128,139,141	0
3	BMA	S	2003	11/12	0.62	0.24	-	110,125,137,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	Y	2003	14/15	0.64	0.23	-	159,180,187,187	0
4	NAG	A	2004	14/15	0.84	0.15	-	93,112,119,119	0
3	BMA	K	2003	11/12	0.77	0.21	-	67,77,85,86	0

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	Y	2001	14/15	0.84	0.20	0.65	75,93,108,120	0
5	NAG	a	2001	14/15	0.82	0.20	-0.09	92,112,119,128	0
5	NAG	c	2001	14/15	0.88	0.22	-0.21	91,102,120,122	0
5	NAG	C	2004	14/15	0.78	0.17	-	125,149,153,153	0
5	NAG	O	2006	14/15	0.88	0.24	-	96,105,117,126	0
5	NAG	K	2004	14/15	0.84	0.11	-	127,135,145,149	0
5	NAG	M	2004	14/15	0.88	0.11	-	119,135,154,161	0

6.5 Other polymers [i](#)

There are no such residues in this entry.