



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 08:17 am GMT

PDB ID : 4N5Y
Title : Crystal structure of H5 hemagglutinin mutant (N158D, N224K and Q226L) from the influenza virus A/Viet Nam/1203/2004 (H5N1)
Authors : Zhu, X.; Wilson, I.A.
Deposited on : 2013-10-10
Resolution : 3.16 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

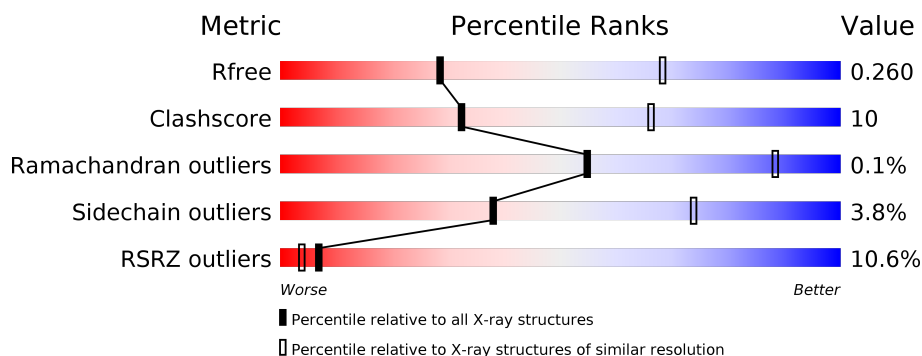
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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}	100719	1259 (3.20-3.12)
Clashscore	112137	1397 (3.20-3.12)
Ramachandran outliers	110173	1368 (3.20-3.12)
Sidechain outliers	110143	1367 (3.20-3.12)
RSRZ outliers	101464	1264 (3.20-3.12)

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>%</div> <div> <div></div> <div>57%</div> <div>36%</div> <div>• •</div> </div> </div>
1	C	334	<div> <div>3%</div> <div> <div></div> <div>60%</div> <div>35%</div> <div>• •</div> </div> </div>
1	E	334	<div> <div>4%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>• •</div> </div> </div>
1	G	334	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>30%</div> <div>• •</div> </div> </div>
1	I	334	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>• •</div> </div> </div>
1	K	334	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>29%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
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 crite-

ria:

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

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 60964 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
			2573	1628	442	488	15			
1	C	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	E	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	G	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	I	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	K	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	M	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	O	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	Q	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	S	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	U	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	W	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	Y	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	a	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			
1	c	324	Total	C	N	O	S	0	1	0
			2573	1628	442	488	15			

There are 105 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
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
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
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
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
K	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33
K	8	ASP	-	EXPRESSION TAG	UNP Q6DQ33
K	9	PRO	-	EXPRESSION TAG	UNP Q6DQ33
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
M	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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
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
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
U	224	LYS	ASN	ENGINEERED MUTATION	UNP Q6DQ33
U	226	LEU	GLN	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
Y	7	ALA	-	EXPRESSION TAG	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

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			
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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	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).

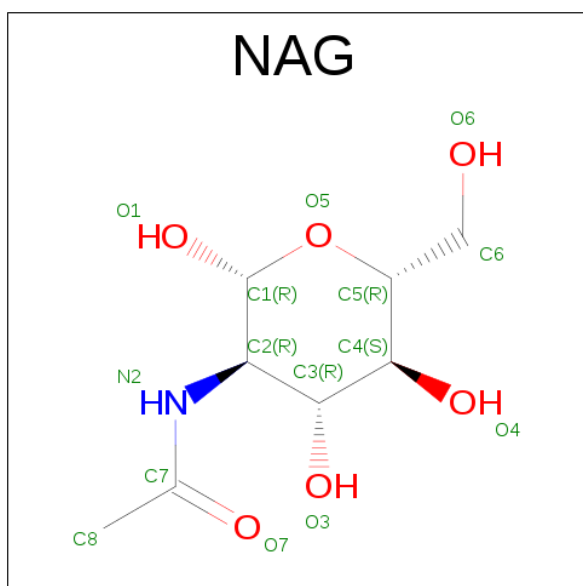
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	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		

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

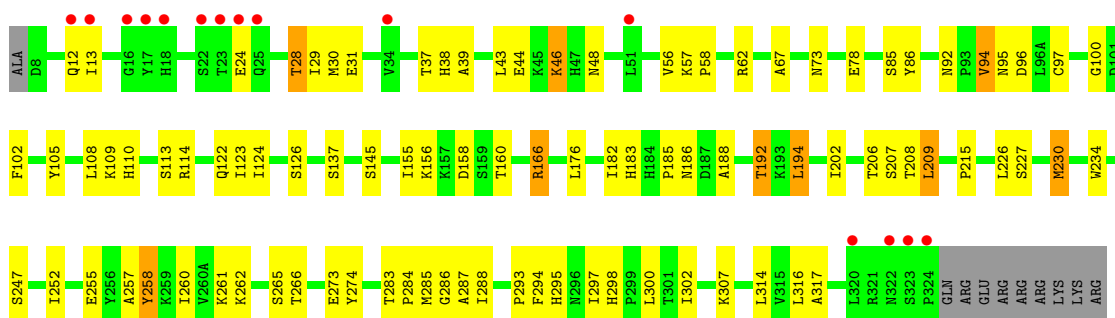
- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



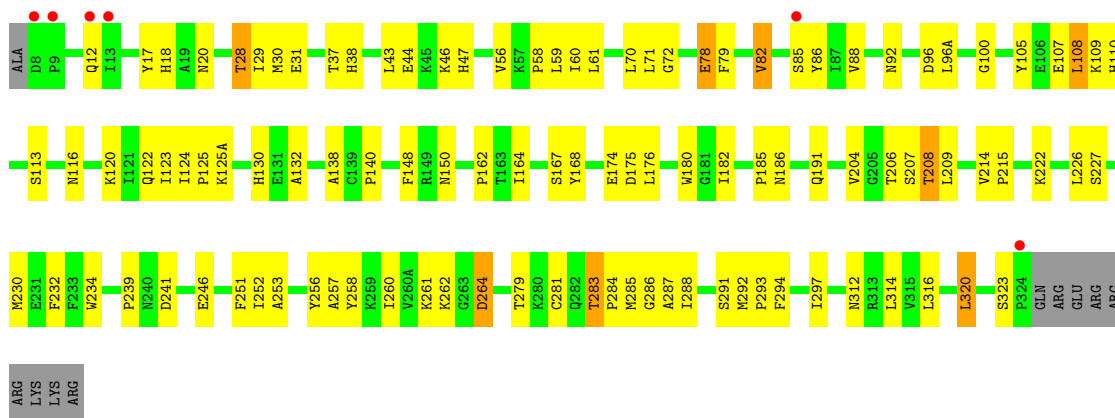
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	O	1	Total	C	N	O	0	0
			14	8	1	5		
5	Y	1	Total	C	N	O	0	0
			14	8	1	5		
5	c	1	Total	C	N	O	0	0
			14	8	1	5		
5	c	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

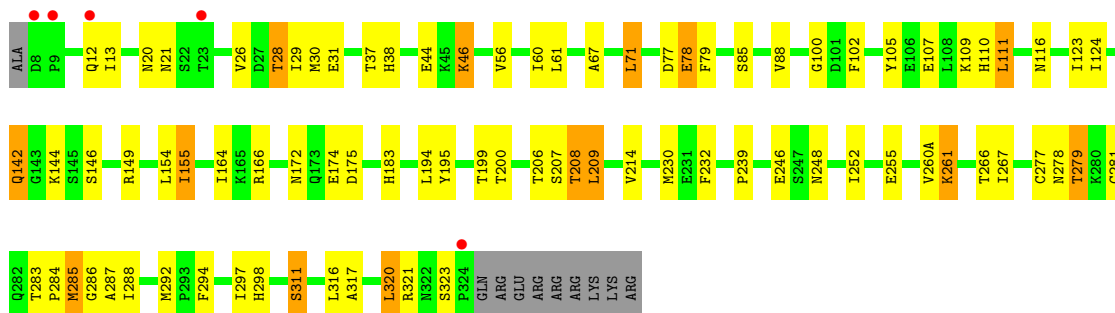
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	Q	4	Total	C	N	O	0	0
			50	28	2	20		



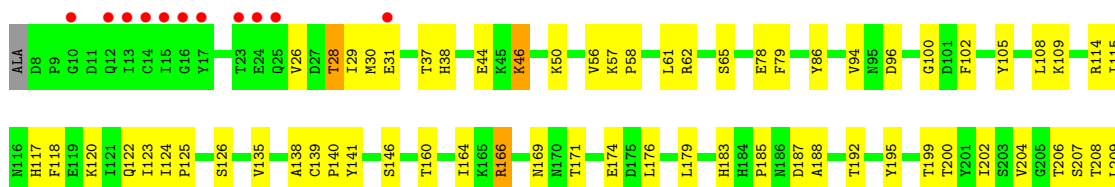
• Molecule 1: Hemagglutinin HA1 chain

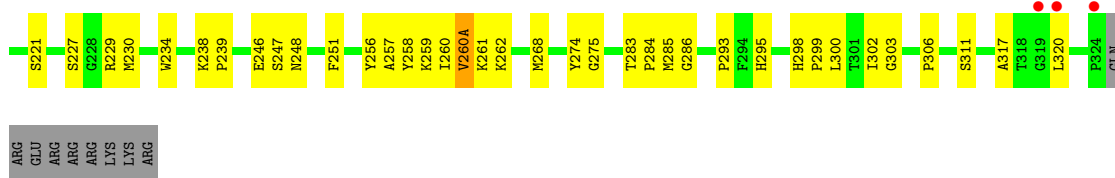


• Molecule 1: Hemagglutinin HA1 chain

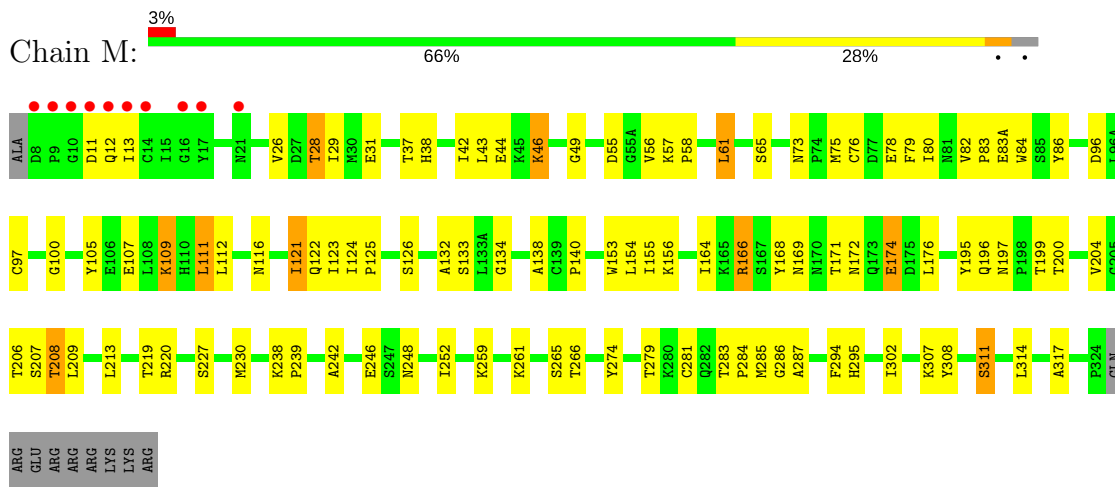


• Molecule 1: Hemagglutinin HA1 chain

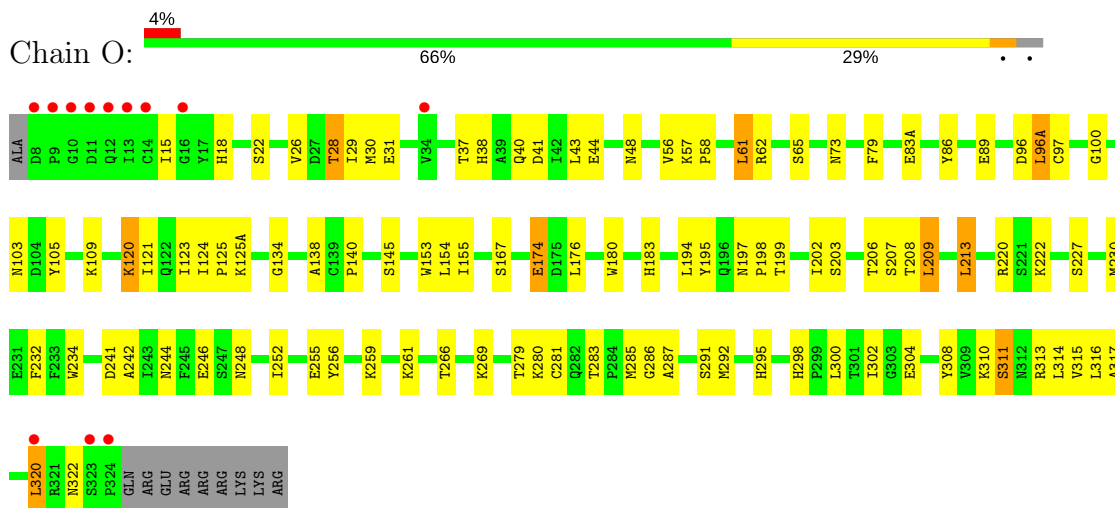




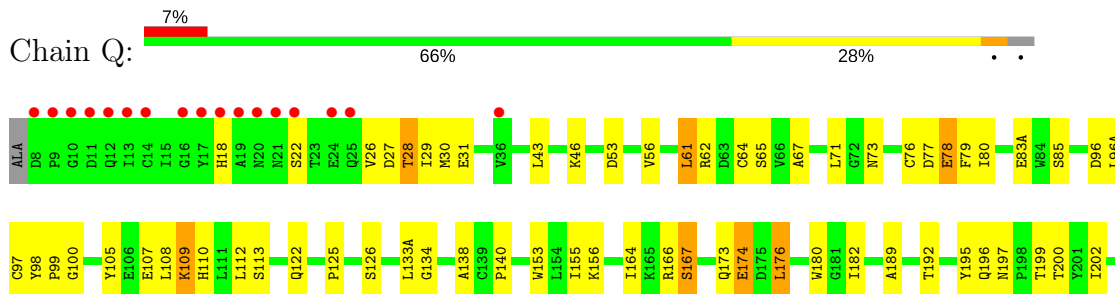
• Molecule 1: Hemagglutinin HA1 chain



• Molecule 1: Hemagglutinin HA1 chain

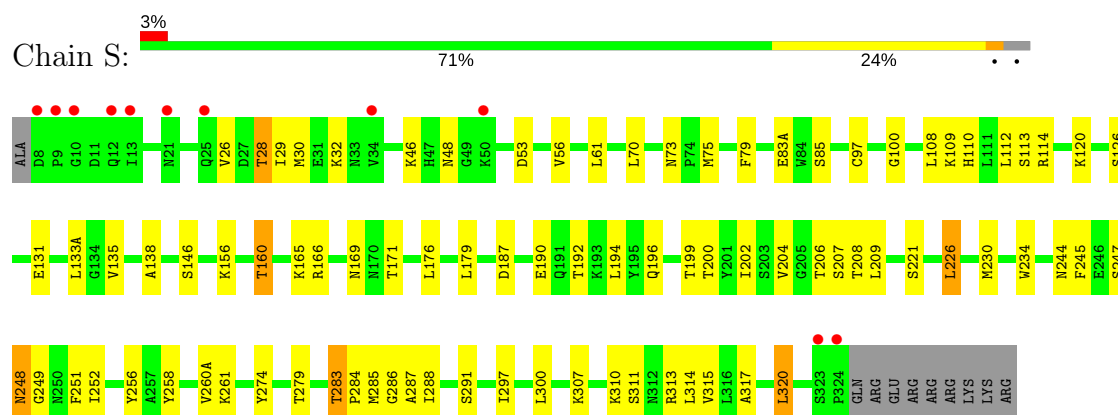


• Molecule 1: Hemagglutinin HA1 chain

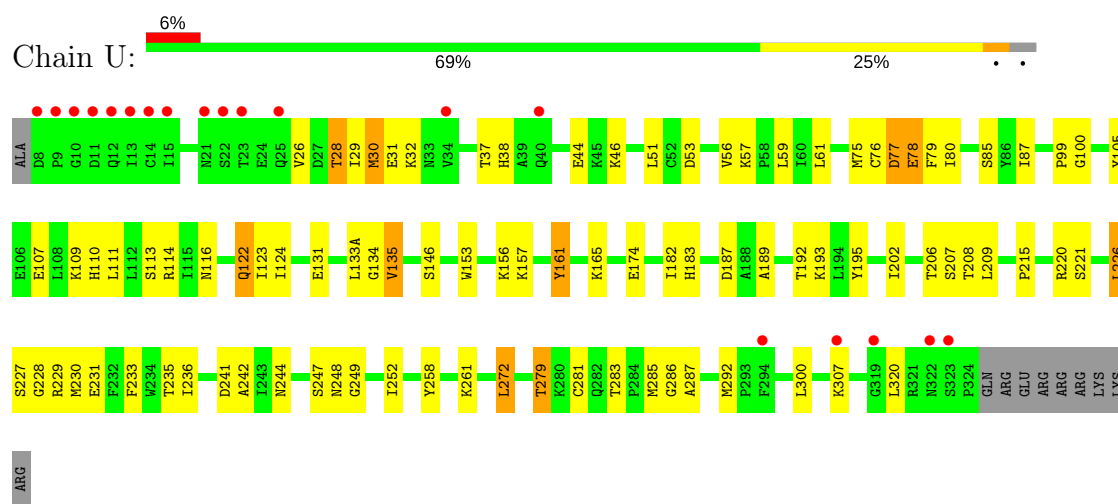




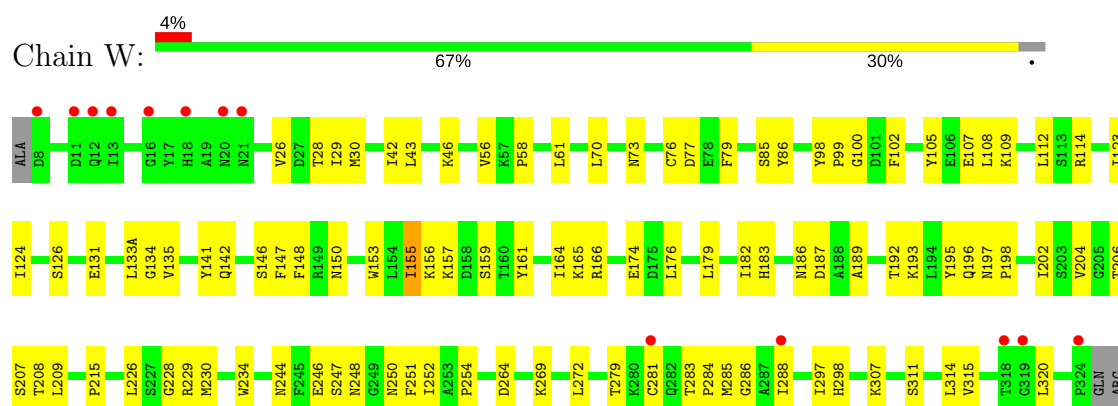
• Molecule 1: Hemagglutinin HA1 chain



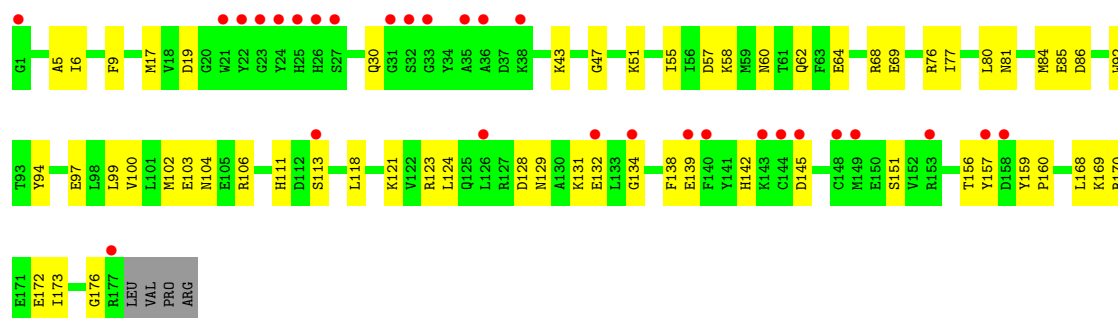
• Molecule 1: Hemagglutinin HA1 chain



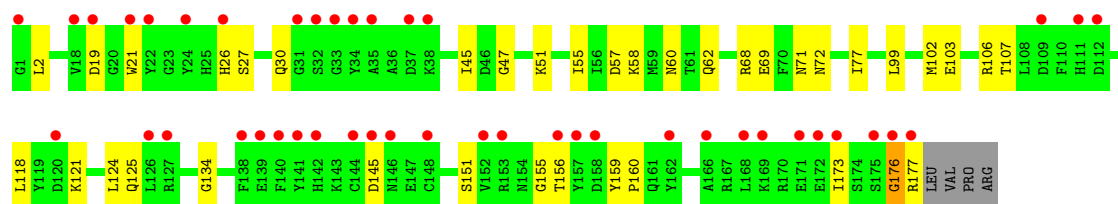
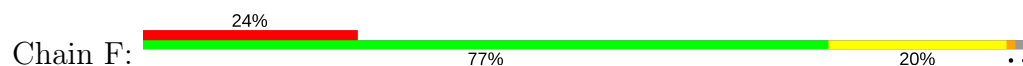
• Molecule 1: Hemagglutinin HA1 chain



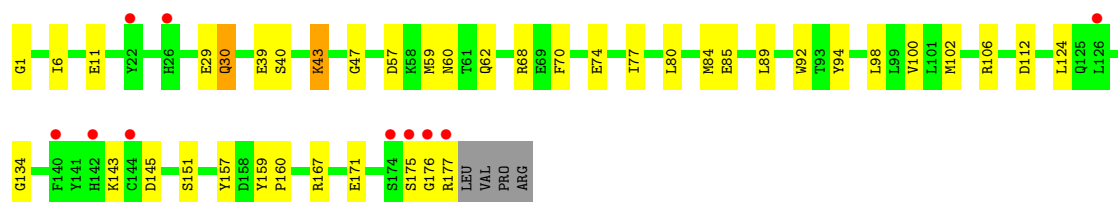
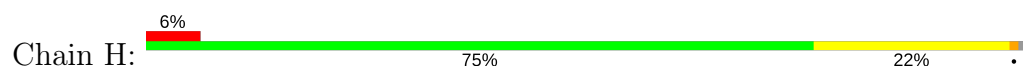
Chain D:  16% 65% 33%



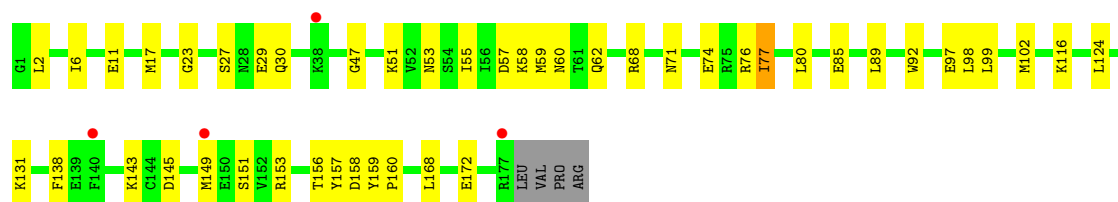
• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain

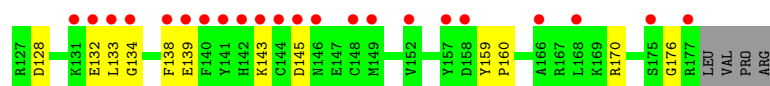


• Molecule 2: Hemagglutinin HA2 chain

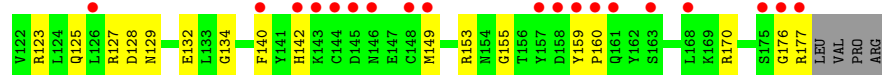
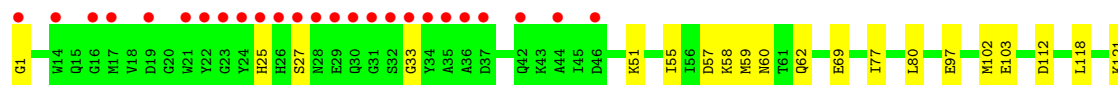
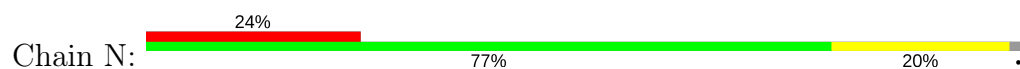


• Molecule 2: Hemagglutinin HA2 chain

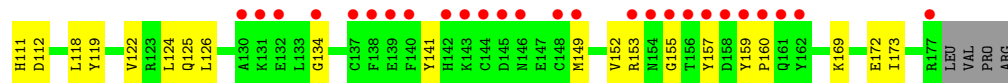
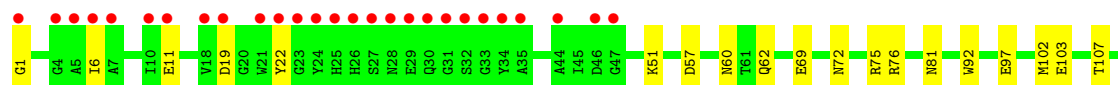
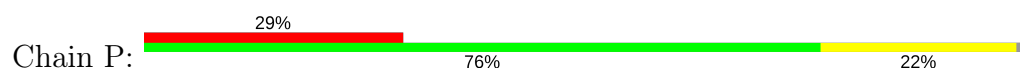




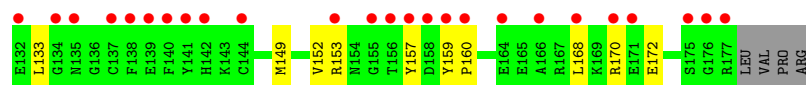
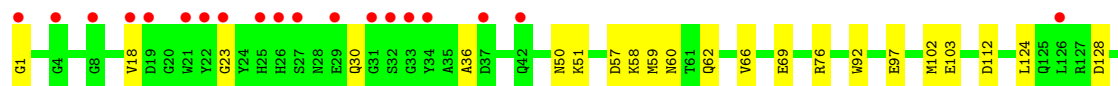
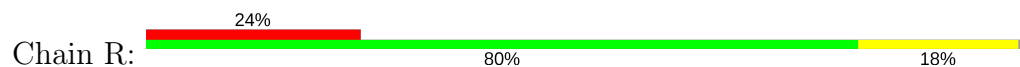
• Molecule 2: Hemagglutinin HA2 chain



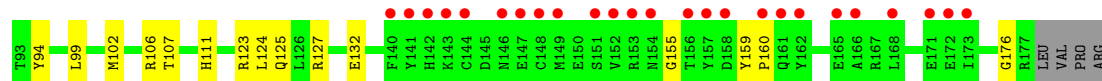
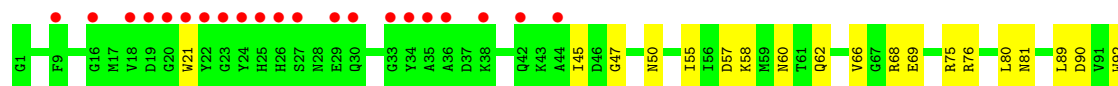
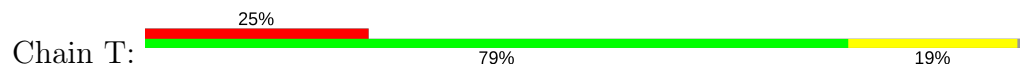
• Molecule 2: Hemagglutinin HA2 chain



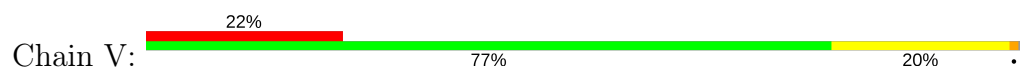
• Molecule 2: Hemagglutinin HA2 chain

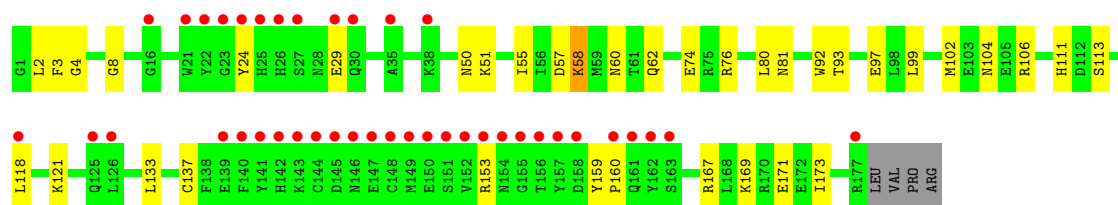


• Molecule 2: Hemagglutinin HA2 chain

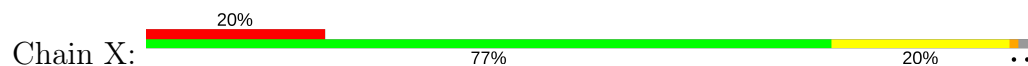


• Molecule 2: Hemagglutinin HA2 chain

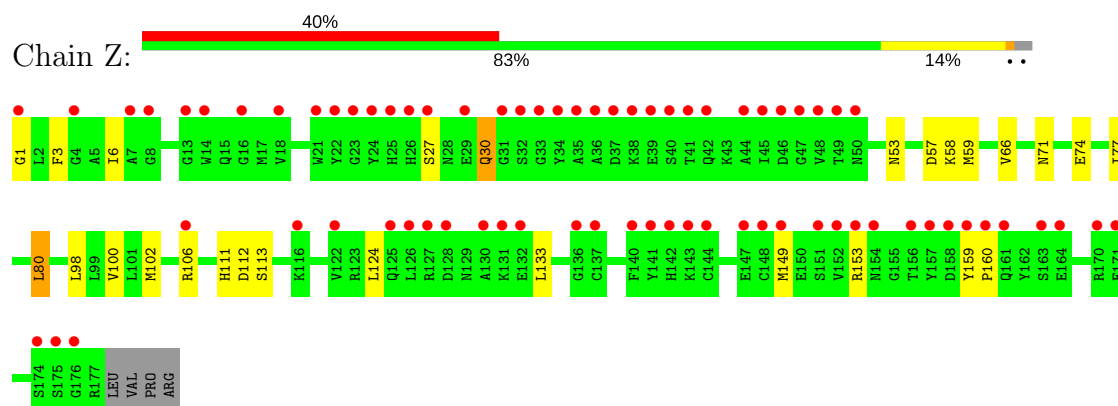




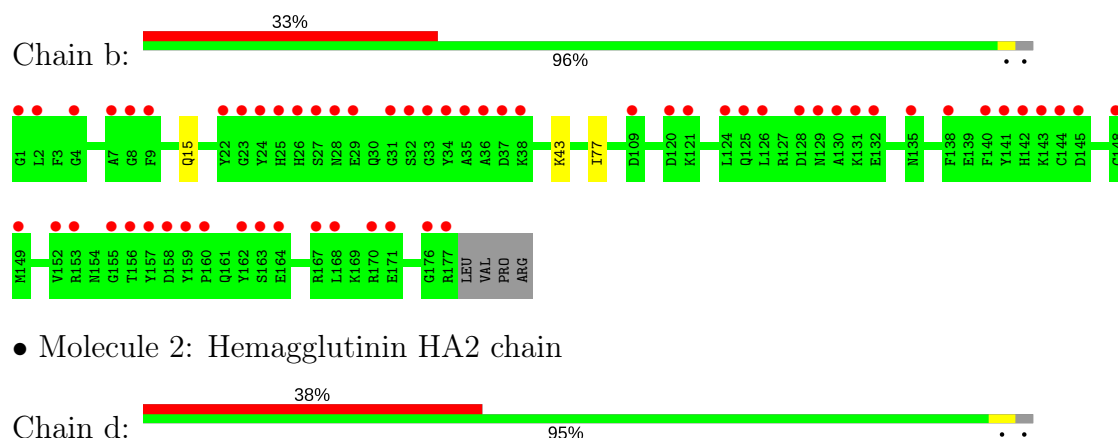
• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain

G134	•	G139	•	G148	•	R177	•
N135	•	F140	•	M149	•	LEU	•
G136	•	Y141	•	E150	•	VAL	•
		H142	•	S151	•	PRO	•
		K143	•	V152	•	ARG	•
		C144	•	R153	•		
				N154	•		
				Q155	•		
				T156	•		
				Y157	•		
				D158	•		
				Y159	•		
				P160	•		
				Q161	•		
				Y162	•		
				S163	•		
				E164	•		
				E165	•		
				A166	•		
				R167	•		
				L168	•		
				K169	•		
				R170	•		
				E171	•		
				E172	•		
				I173	•		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	117.92Å 118.11Å 273.80Å 91.50° 90.18° 119.87°	Depositor
Resolution (Å)	45.28 – 3.16 45.28 – 3.16	Depositor EDS
% Data completeness (in resolution range)	91.1 (45.28-3.16) 91.0 (45.28-3.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.213 , 0.262 0.211 , 0.260	Depositor DCC
R_{free} test set	9975 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	62.8	Xtriage
Anisotropy	0.750	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 67.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.004 for h+k,-h,l 0.004 for -k,h+k,l 0.057 for k,-h-k,l 0.057 for -h-k,h,l 0.024 for h,-h-k,-l 0.011 for -h-k,k,-l 0.000 for -h,-k,l 0.004 for k,h,-l 0.001 for -k,-h,-l 0.000 for -h,h+k,-l 0.000 for h+k,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	60964	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.71	0/2639	0.93	4/3584 (0.1%)
1	C	0.62	0/2639	0.82	2/3584 (0.1%)
1	E	0.61	0/2639	0.81	2/3584 (0.1%)
1	G	0.73	0/2639	0.91	1/3584 (0.0%)
1	I	0.72	0/2639	0.91	2/3584 (0.1%)
1	K	0.62	0/2639	0.81	1/3584 (0.0%)
1	M	0.70	0/2639	0.88	3/3584 (0.1%)
1	O	0.68	0/2639	0.87	7/3584 (0.2%)
1	Q	0.69	1/2639 (0.0%)	0.86	4/3584 (0.1%)
1	S	0.55	0/2639	0.77	0/3584
1	U	0.58	1/2639 (0.0%)	0.76	0/3584
1	W	0.59	0/2639	0.77	1/3584 (0.0%)
1	Y	0.43	0/2639	0.67	0/3584
1	a	0.44	0/2639	0.66	0/3584
1	c	0.43	0/2639	0.67	0/3584
2	B	0.47	0/1460	0.67	1/1961 (0.1%)
2	D	0.40	0/1460	0.58	0/1961
2	F	0.40	0/1460	0.59	1/1961 (0.1%)
2	H	0.50	0/1460	0.68	0/1961
2	J	0.50	0/1460	0.68	0/1961
2	L	0.43	0/1460	0.57	0/1961
2	N	0.44	0/1460	0.61	0/1961
2	P	0.44	0/1460	0.60	0/1961
2	R	0.45	0/1460	0.63	0/1961
2	T	0.37	0/1460	0.59	0/1961
2	V	0.38	0/1460	0.56	0/1961
2	X	0.37	0/1460	0.58	0/1961
2	Z	0.32	0/1460	0.56	1/1961 (0.1%)
2	b	0.33	0/1460	0.55	0/1961
2	d	0.33	0/1460	0.53	0/1961
All	All	0.55	2/61485 (0.0%)	0.74	30/83175 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	U	135	VAL	CB-CG2	-5.77	1.40	1.52
1	Q	180	TRP	CB-CG	5.20	1.59	1.50

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	213	LEU	CA-CB-CG	8.43	134.69	115.30
1	M	213	LEU	CA-CB-CG	8.43	134.69	115.30
1	E	209	LEU	CA-CB-CG	7.10	131.62	115.30
1	A	212	ARG	NE-CZ-NH1	6.38	123.49	120.30
2	Z	80	LEU	CA-CB-CG	6.29	129.76	115.30
1	A	213	LEU	CA-CB-CG	6.23	129.62	115.30
1	O	57	LYS	CD-CE-NZ	5.82	125.08	111.70
1	O	96(A)	LEU	CA-CB-CG	5.78	128.59	115.30
1	A	209	LEU	CA-CB-CG	5.76	128.55	115.30
1	Q	216	ARG	NE-CZ-NH2	5.53	123.06	120.30
1	Q	71	LEU	CA-CB-CG	5.52	128.00	115.30
1	Q	96(A)	LEU	CA-CB-CG	5.52	128.00	115.30
1	K	179	LEU	CB-CG-CD1	-5.46	101.72	111.00
1	E	194	LEU	CB-CG-CD2	-5.43	101.77	111.00
1	Q	209	LEU	CA-CB-CG	5.35	127.61	115.30
1	C	226	LEU	CB-CG-CD2	-5.32	101.95	111.00
1	O	213	LEU	CB-CG-CD2	5.31	120.03	111.00
1	O	241	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	W	155	ILE	CG1-CB-CG2	-5.23	99.89	111.40
1	G	108	LEU	CB-CG-CD2	-5.21	102.14	111.00
2	F	68	ARG	NE-CZ-NH1	-5.21	117.70	120.30
1	C	229	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	I	267	ILE	CG1-CB-CG2	-5.11	100.15	111.40
1	A	161	TYR	CA-CB-CG	5.11	123.11	113.40
1	I	209	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	O	194	LEU	CB-CG-CD2	-5.09	102.34	111.00
2	B	73	LEU	CA-CB-CG	5.09	127.00	115.30
1	O	241	ASP	CB-CG-OD1	5.07	122.86	118.30
1	M	80	ILE	CG1-CB-CG2	-5.05	100.28	111.40
1	M	105	TYR	CB-CG-CD2	-5.04	117.98	121.00

There are no chirality outliers.

There are no planarity outliers.

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	2573	0	2521	105	0
1	C	2573	0	2522	105	0
1	E	2573	0	2521	66	0
1	G	2573	0	2521	75	0
1	I	2573	0	2521	61	0
1	K	2573	0	2521	75	0
1	M	2573	0	2521	71	0
1	O	2573	0	2520	71	0
1	Q	2573	0	2521	67	0
1	S	2573	0	2521	61	0
1	U	2573	0	2521	64	0
1	W	2573	0	2521	70	0
1	Y	2573	0	2521	50	0
1	a	2573	0	2522	0	0
1	c	2573	0	2521	0	0
2	B	1433	0	1340	56	0
2	D	1433	0	1340	50	0
2	F	1433	0	1340	28	0
2	H	1433	0	1340	28	0
2	J	1433	0	1340	37	0
2	L	1433	0	1340	26	0
2	N	1433	0	1340	27	0
2	P	1433	0	1340	27	0
2	R	1433	0	1340	21	0
2	T	1433	0	1340	33	0
2	V	1433	0	1340	36	0
2	X	1433	0	1340	36	0
2	Z	1433	0	1340	21	0
2	b	1433	0	1340	0	0
2	d	1433	0	1340	0	0
3	A	39	0	34	3	0
3	C	39	0	34	2	0
3	E	39	0	34	0	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	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	39	0	34	2	0
3	U	39	0	34	2	0
3	W	39	0	34	0	0
4	A	28	0	25	2	0
4	E	28	0	25	0	0
4	G	28	0	25	0	0
4	I	28	0	25	1	0
4	M	28	0	25	0	0
4	O	28	0	25	1	0
4	Q	28	0	25	0	0
4	S	56	0	50	0	0
4	U	28	0	25	0	0
4	W	28	0	25	1	0
4	Y	28	0	25	1	0
4	a	28	0	25	0	0
5	K	14	0	13	0	0
5	O	14	0	13	0	0
5	Y	14	0	13	1	0
5	c	28	0	26	0	0
6	Q	50	0	43	5	0
All	All	60964	0	58689	1190	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 10.

All (1190) 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	1.28	1.14
6:Q:2003:BMA:H2	6:Q:2004:MAN:H5	1.11	1.09
1:I:283:THR:HG22	1:I:285:MET:H	1.24	1.03
1:O:283:THR:HG22	1:O:285:MET:H	1.27	0.98
1:A:283:THR:HG22	1:A:285:MET:H	1.27	0.98
1:C:192:THR:HG21	1:W:192:THR:HG21	1.46	0.97
6:Q:2003:BMA:C2	6:Q:2004:MAN:H5	1.94	0.97
1:Q:283:THR:HG22	1:Q:285:MET:H	1.29	0.97
1:I:206:THR:HG22	1:I:208:THR:H	1.30	0.96
1:C:283:THR:HG22	1:C:285:MET:H	1.29	0.95
2:N:51:LYS:HD3	2:N:103:GLU:HB3	1.45	0.94
1:S:206:THR:HG22	1:S:208:THR:H	1.35	0.92
1:U:283:THR:HG22	1:U:285:MET:H	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:283:THR:HG22	1:K:285:MET:H	1.35	0.90
1:M:283:THR:HG22	1:M:285:MET:H	1.36	0.88
1:G:283:THR:HG22	1:G:285:MET:H	1.35	0.88
2:R:51:LYS:HD3	2:R:103:GLU:HB3	1.54	0.88
6:Q:2003:BMA:H2	6:Q:2004:MAN:C5	2.01	0.87
1:W:283:THR:HG22	1:W:285:MET:H	1.38	0.85
1:S:283:THR:HG22	1:S:285:MET:H	1.40	0.85
1:A:29:ILE:HD11	2:B:102:MET:HG2	1.91	0.84
1:W:206:THR:HB	1:W:209:LEU:H	1.39	0.84
1:G:107:GLU:HG2	2:B:76:ARG:HH21	1.43	0.83
1:U:206:THR:HB	1:U:209:LEU:H	1.44	0.83
1:Y:283:THR:HG22	1:Y:285:MET:H	1.44	0.82
1:E:283:THR:HG22	1:E:285:MET:H	1.44	0.82
1:W:206:THR:HG22	1:W:208:THR:H	1.43	0.82
1:G:206:THR:HB	1:G:209:LEU:H	1.46	0.81
2:T:81:ASN:HD22	2:X:80:LEU:HD13	1.45	0.80
1:K:166:ARG:HG3	1:K:166:ARG:HH11	1.47	0.79
2:B:134:GLY:HA2	2:D:124:LEU:HD22	198.29	0.79
1:Y:29:ILE:HD11	2:Z:102:MET:HG2	1.63	0.79
1:U:29:ILE:HD11	2:V:102:MET:HG2	1.63	0.79
1:G:29:ILE:HD11	2:H:102:MET:HG2	1.66	0.78
1:Q:28:THR:HG22	1:Q:31:GLU:H	1.47	0.78
1:W:131:GLU:HB3	1:W:133(A):LEU:HD23	1.64	0.78
1:E:160:THR:HG21	1:W:165:LYS:HE3	1.63	0.78
2:P:51:LYS:HD3	2:P:103:GLU:HB3	1.64	0.77
1:U:123:ILE:HG13	1:U:124:ILE:HG13	1.66	0.77
1:C:206:THR:HB	1:C:209:LEU:H	1.50	0.76
1:U:131:GLU:HB3	1:U:133(A):LEU:HD23	1.67	0.76
1:U:206:THR:HG22	1:U:208:THR:H	1.51	0.76
1:I:116:ASN:HB2	1:I:261:LYS:HG3	1.69	0.75
1:I:61:LEU:HA	1:I:79:PHE:CZ	2.22	0.74
2:V:80:LEU:HD13	2:X:81:ASN:HD22	1.52	0.74
1:C:192:THR:CG2	1:W:192:THR:HG21	2.18	0.74
2:D:134:GLY:HA2	2:Z:124:LEU:HD22	255.33	0.74
1:E:12:GLN:HB2	2:F:27:SER:HB3	1.70	0.74
1:S:28:THR:HG23	1:S:30:MET:H	1.53	0.73
1:I:206:THR:HB	1:I:209:LEU:H	1.54	0.73
1:C:123:ILE:HG13	1:C:124:ILE:HG13	1.70	0.73
2:H:29:GLU:OE1	2:H:143:LYS:NZ	2.20	0.73
2:V:80:LEU:HD13	2:X:81:ASN:ND2	2.03	0.73
1:U:32:LYS:NZ	2:X:54:SER:OG	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:28:THR:HG22	1:M:31:GLU:H	1.52	0.72
1:U:76:CYS:O	1:U:78:GLU:N	2.21	0.72
2:D:131:LYS:HB3	2:D:139:GLU:HB3	1.72	0.71
1:K:160:THR:HG21	1:U:165:LYS:HE3	1.72	0.71
2:J:57:ASP:O	2:J:60:ASN:HB2	1.90	0.71
1:A:241:ASP:HA	3:A:2001:NAG:H82	1.73	0.71
1:O:320:LEU:HD23	2:P:111:HIS:HB3	1.73	0.71
1:A:28:THR:HG22	1:A:31:GLU:H	1.73	0.70
2:D:51:LYS:HD3	2:D:103:GLU:HB3	1.98	0.70
1:W:70:LEU:O	1:W:150:ASN:ND2	2.24	0.70
1:Q:167:SER:HB2	1:Q:244:ASN:HB3	1.74	0.69
1:G:283:THR:HB	1:G:286:GLY:O	1.93	0.69
1:S:73:ASN:HD21	1:S:97:CYS:HB3	1.55	0.69
1:C:230:MET:SD	1:C:252:ILE:HD11	2.31	0.69
1:Q:283:THR:HB	1:Q:286:GLY:O	1.92	0.69
1:G:206:THR:HG22	1:G:208:THR:H	1.58	0.69
1:O:28:THR:HG22	1:O:31:GLU:H	1.58	0.69
1:S:206:THR:HB	1:S:209:LEU:H	1.57	0.69
1:Q:62:ARG:NH2	1:Q:78:GLU:OE2	2.25	0.69
2:D:106:ARG:HG2	2:F:106:ARG:HH22	1.58	0.68
1:K:283:THR:HB	1:K:286:GLY:O	1.93	0.68
1:M:100:GLY:HA3	1:M:230:MET:O	1.93	0.68
1:C:29:ILE:HD11	2:D:102:MET:HG2	1.75	0.68
1:G:283:THR:HG23	1:G:284:PRO:HD2	1.76	0.68
1:W:135:VAL:HG22	1:W:146:SER:HA	1.76	0.68
1:E:192:THR:HG21	1:U:192:THR:HG21	1.74	0.68
1:Y:61:LEU:HA	1:Y:79:PHE:CZ	2.29	0.68
4:A:2004:NAG:H4	4:A:2005:NAG:H4	1.76	0.68
1:S:29:ILE:HD11	2:T:102:MET:HG2	1.74	0.68
1:K:192:THR:CG2	1:S:192:THR:HG21	2.17	0.67
2:F:57:ASP:O	2:F:60:ASN:HB2	1.94	0.67
2:B:57:ASP:O	2:B:60:ASN:HB2	1.95	0.67
1:O:61:LEU:HA	1:O:79:PHE:CZ	2.30	0.67
1:W:123:ILE:HG13	1:W:124:ILE:HG13	1.75	0.67
1:A:206:THR:HB	1:A:209:LEU:H	1.58	0.67
1:E:73:ASN:HD21	1:E:97:CYS:HB3	1.59	0.67
1:G:175:ASP:OD1	1:G:239:PRO:HD3	1.95	0.67
1:I:279:THR:HB	1:I:281:CYS:H	1.58	0.67
1:K:28:THR:HG22	1:K:31:GLU:H	1.59	0.67
1:W:183:HIS:ND1	1:W:195:TYR:OH	2.25	0.67
1:Y:134:GLY:HA3	1:Y:153:TRP:HB3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:230:MET:SD	1:O:252:ILE:HD11	2.35	0.66
2:T:81:ASN:ND2	2:X:80:LEU:HD13	2.10	0.66
1:A:206:THR:HG22	1:A:208:THR:H	1.60	0.66
1:A:116:ASN:HB2	1:A:261:LYS:HG3	1.75	0.66
2:D:97:GLU:OE1	2:Z:58:LYS:NZ	185.86	0.66
1:O:283:THR:HB	1:O:286:GLY:O	1.94	0.66
1:A:183:HIS:ND1	1:A:195:TYR:OH	2.25	0.66
1:C:183:HIS:ND1	1:C:195:TYR:OH	2.28	0.66
2:P:134:GLY:HA2	2:R:124:LEU:HD22	1.78	0.66
2:T:68:ARG:NH1	2:T:81:ASN:HD21	1.92	0.66
1:M:311:SER:HB3	2:N:97:GLU:OE2	1.96	0.66
2:D:134:GLY:HA2	2:F:124:LEU:HD22	1.77	0.65
1:W:28:THR:HG23	1:W:30:MET:H	1.61	0.65
2:B:106:ARG:HH22	2:Z:106:ARG:HG2	89.82	0.65
1:E:192:THR:CG2	1:U:192:THR:HG21	2.26	0.65
2:B:99:LEU:HD13	2:J:98:LEU:HD21	1.78	0.65
1:M:238:LYS:HD3	1:M:239:PRO:HD2	1.77	0.65
1:Q:22:SER:O	1:Q:322:ASN:ND2	2.30	0.65
2:X:68:ARG:NH1	2:X:81:ASN:HD21	1.93	0.65
1:A:283:THR:HB	1:A:286:GLY:O	1.96	0.65
1:A:26:VAL:HG21	1:A:317:ALA:HB2	1.79	0.65
1:A:28:THR:HG23	1:A:30:MET:H	1.61	0.65
1:A:61:LEU:HA	1:A:79:PHE:CZ	2.38	0.65
1:C:288:ILE:HD11	1:C:297:ILE:HG13	1.78	0.65
1:Y:62:ARG:NH1	1:Y:78:GLU:OE2	2.30	0.65
2:D:19:ASP:N	2:D:19:ASP:OD1	2.87	0.64
1:K:58:PRO:HB3	1:K:86:TYR:CE1	2.32	0.64
1:A:294:PHE:HZ	2:B:59:MET:HG3	1.63	0.64
1:U:135:VAL:HG23	1:U:146:SER:HA	1.77	0.64
2:L:57:ASP:O	2:L:60:ASN:HB2	1.98	0.64
1:Q:100:GLY:HA3	1:Q:230:MET:O	1.98	0.64
1:U:28:THR:HG23	1:U:30:MET:H	1.61	0.64
2:B:106:ARG:HH11	2:H:106:ARG:HH12	1.45	0.64
1:M:283:THR:HB	1:M:286:GLY:O	1.97	0.64
1:Y:200:THR:HA	1:Y:248:ASN:OD1	1.98	0.64
1:A:159:SER:O	1:A:196:GLN:NE2	2.32	0.63
1:C:28:THR:HG22	1:C:31:GLU:H	1.62	0.63
2:D:57:ASP:O	2:D:60:ASN:HB2	1.98	0.63
1:E:260:ILE:HG21	1:E:262:LYS:HE3	1.81	0.63
1:U:283:THR:HB	1:U:286:GLY:O	1.99	0.63
1:I:26:VAL:HG11	1:I:317:ALA:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:THR:HG22	1:E:208:THR:H	1.63	0.63
1:I:183:HIS:ND1	1:I:195:TYR:OH	2.29	0.63
1:O:183:HIS:ND1	1:O:195:TYR:OH	2.26	0.63
1:S:61:LEU:HA	1:S:79:PHE:CZ	2.34	0.63
1:C:61:LEU:HA	1:C:79:PHE:CZ	2.35	0.63
1:C:28:THR:HG22	1:C:30:MET:H	1.77	0.63
1:M:43:LEU:HB2	1:M:314:LEU:HB2	1.81	0.62
1:W:247:SER:OG	1:W:248:ASN:N	2.31	0.62
2:D:169:LYS:HE3	2:D:173:ILE:HD11	1.81	0.62
1:E:29:ILE:HD11	2:F:102:MET:HG2	1.81	0.62
1:Q:73:ASN:HD21	1:Q:97:CYS:HB3	1.64	0.62
1:W:61:LEU:HA	1:W:79:PHE:CZ	2.34	0.62
1:A:100:GLY:HA3	1:A:230:MET:O	2.00	0.62
1:C:206:THR:HG22	1:C:208:THR:H	1.81	0.62
1:K:311:SER:HB3	2:L:97:GLU:OE2	2.00	0.62
2:D:55:ILE:HG12	2:D:99:LEU:HD21	1.99	0.62
2:R:57:ASP:O	2:R:60:ASN:HB2	1.98	0.62
2:L:128:ASP:O	2:L:170:ARG:NH1	2.33	0.62
1:M:61:LEU:HA	1:M:79:PHE:CZ	2.34	0.62
1:C:298:HIS:HE1	1:C:300:LEU:HD12	1.64	0.62
1:K:61:LEU:HA	1:K:79:PHE:CZ	2.35	0.62
1:Q:174:GLU:HG3	1:Q:259:LYS:HB3	1.82	0.62
1:K:62:ARG:NH1	1:K:78:GLU:OE2	2.31	0.62
1:M:200:THR:HA	1:M:248:ASN:OD1	1.99	0.62
1:Y:22:SER:O	1:Y:322:ASN:ND2	2.32	0.62
1:A:78:GLU:O	1:A:78:GLU:HG3	1.96	0.62
1:Q:43:LEU:HB2	1:Q:314:LEU:HB2	1.81	0.62
1:S:179:LEU:HD23	1:S:234:TRP:HB3	1.82	0.62
2:T:76:ARG:NH1	2:V:74:GLU:OE1	2.30	0.62
1:A:283:THR:HG22	1:A:285:MET:N	2.09	0.62
1:C:283:THR:HB	1:C:286:GLY:O	2.00	0.62
1:I:37:THR:HG22	1:I:38:HIS:CD2	2.35	0.62
1:Y:83(A):GLU:OE2	1:Y:261:LYS:NZ	2.32	0.62
1:E:29:ILE:HD11	2:F:102:MET:HA	1.82	0.61
2:T:57:ASP:O	2:T:60:ASN:HB2	1.99	0.61
2:D:43:LYS:HE2	2:D:43:LYS:HA	1.82	0.61
2:B:80:LEU:HD23	2:D:81:ASN:HD22	94.48	0.61
1:M:126:SER:HB2	1:M:166:ARG:NH2	2.15	0.61
1:A:62:ARG:NH1	1:A:78:GLU:OE2	2.68	0.61
1:G:279:THR:HB	1:G:281:CYS:H	1.64	0.61
1:G:283:THR:HG22	1:G:285:MET:N	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:100:GLY:HA3	1:I:230:MET:O	2.01	0.61
1:S:83(A):GLU:OE1	1:S:261:LYS:NZ	2.34	0.61
1:C:43:LEU:HB2	1:C:314:LEU:HB2	1.82	0.61
1:K:206:THR:HG22	1:K:208:THR:H	1.64	0.61
1:O:109:LYS:NZ	2:P:69:GLU:OE2	2.30	0.61
2:B:5:ALA:HB2	2:B:116:LYS:HB2	1.83	0.60
1:Q:134:GLY:HA3	1:Q:153:TRP:HB3	1.83	0.60
1:C:29:ILE:HD11	2:D:102:MET:HA	1.83	0.60
1:E:56:VAL:HB	1:E:85:SER:HB3	1.83	0.60
1:A:26:VAL:HG12	1:A:315:VAL:HG12	2.63	0.60
2:J:29:GLU:OE1	2:J:143:LYS:NZ	2.27	0.60
1:Y:48:ASN:ND2	1:Y:287:ALA:HB3	2.17	0.60
1:O:123:ILE:HG13	1:O:124:ILE:HD12	1.81	0.60
1:I:283:THR:HB	1:I:286:GLY:O	2.00	0.60
1:O:43:LEU:HB2	1:O:314:LEU:HB2	1.84	0.60
1:U:307:LYS:NZ	2:V:60:ASN:O	2.35	0.60
1:I:44:GLU:OE1	1:I:46:LYS:HG3	2.01	0.60
2:F:118:LEU:HD12	2:F:121:LYS:HD3	1.84	0.60
1:O:174:GLU:HG3	1:O:259:LYS:HB3	1.82	0.60
1:E:266:THR:HG22	1:E:302:ILE:HD12	1.84	0.60
1:K:183:HIS:ND1	1:K:195:TYR:OH	2.31	0.60
1:M:174:GLU:HG3	1:M:259:LYS:HB3	1.84	0.60
1:A:126:SER:HB2	1:A:166:ARG:HH22	2.69	0.59
1:G:241:ASP:HA	3:G:2001:NAG:H82	1.84	0.59
2:J:62:GLN:HG3	2:J:92:TRP:CG	2.37	0.59
1:Q:56:VAL:HB	1:Q:85:SER:HB3	1.83	0.59
1:O:73:ASN:HD21	1:O:97:CYS:HB3	1.67	0.59
1:Q:133(A):LEU:HB2	1:Q:155:ILE:HD13	1.85	0.59
1:C:200:THR:HA	1:C:248:ASN:OD1	2.26	0.59
2:H:176:GLY:O	2:H:177:ARG:HG3	2.03	0.59
1:Y:283:THR:HB	1:Y:286:GLY:O	2.02	0.59
1:G:122:GLN:NE2	1:G:125:PRO:HA	2.17	0.59
2:J:151:SER:O	2:J:157:TYR:N	2.35	0.59
1:E:122:GLN:NE2	1:E:255:GLU:OE2	2.36	0.59
1:Q:206:THR:HG22	1:Q:207:SER:N	2.18	0.59
1:O:206:THR:HB	1:O:209:LEU:H	1.68	0.59
1:Q:61:LEU:HA	1:Q:79:PHE:CZ	2.38	0.59
2:X:62:GLN:HG3	2:X:92:TRP:CG	2.38	0.59
1:Y:294:PHE:HZ	2:Z:59:MET:HG3	1.66	0.59
1:A:29:ILE:HD11	2:B:102:MET:HA	1.84	0.59
1:Q:29:ILE:HD11	2:R:102:MET:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:230:MET:SD	1:W:252:ILE:HD11	2.43	0.59
1:A:212:ARG:HG2	1:A:212:ARG:HH11	1.68	0.59
2:D:62:GLN:HG3	2:D:92:TRP:CG	2.37	0.59
1:S:110:HIS:O	1:S:113:SER:OG	2.21	0.59
1:S:307:LYS:NZ	2:T:60:ASN:O	2.36	0.59
1:S:29:ILE:HG22	2:V:51:LYS:HG3	1.85	0.59
1:W:29:ILE:HD11	2:X:102:MET:HG2	1.84	0.59
1:G:206:THR:HB	1:G:209:LEU:N	2.18	0.58
1:E:28:THR:HG23	1:E:30:MET:H	1.67	0.58
2:V:62:GLN:HG3	2:V:92:TRP:CD2	2.38	0.58
1:C:62:ARG:NH1	1:C:78:GLU:OE2	2.33	0.58
2:H:134:GLY:HA2	2:J:124:LEU:HD22	1.84	0.58
2:D:128:ASP:O	2:D:170:ARG:NH1	2.35	0.58
1:M:206:THR:HG22	1:M:208:THR:H	1.68	0.58
1:O:22:SER:O	1:O:322:ASN:ND2	2.37	0.58
1:Q:266:THR:HG22	1:Q:302:ILE:HD12	1.85	0.58
1:E:62:ARG:NH1	1:E:78:GLU:OE2	2.33	0.58
1:S:135:VAL:HG22	1:S:146:SER:HA	1.84	0.58
1:O:266:THR:HG22	1:O:302:ILE:HD12	1.84	0.58
1:K:202:ILE:HG12	1:K:247:SER:OG	2.03	0.58
1:C:48:ASN:HD21	1:C:287:ALA:HB3	1.95	0.58
1:G:116:ASN:HB2	1:G:261:LYS:HG3	1.86	0.58
1:A:108:LEU:HB2	1:A:234:TRP:CZ2	2.39	0.58
1:K:206:THR:HB	1:K:209:LEU:H	1.68	0.58
1:O:100:GLY:HA3	1:O:230:MET:O	2.03	0.58
2:B:169:LYS:HE3	2:B:173:ILE:HD11	1.84	0.58
1:K:166:ARG:CG	1:K:166:ARG:HH11	2.16	0.58
1:Q:28:THR:HG22	1:Q:31:GLU:N	2.19	0.58
1:S:73:ASN:ND2	1:S:97:CYS:HB3	2.19	0.58
2:J:71:ASN:OD1	2:J:74:GLU:HG3	2.04	0.57
1:W:269:LYS:HE3	2:X:69:GLU:OE1	2.03	0.57
1:E:73:ASN:ND2	1:E:97:CYS:HB3	2.18	0.57
1:S:100:GLY:HA3	1:S:230:MET:O	2.03	0.57
1:C:116:ASN:HB2	1:C:261:LYS:HG3	1.86	0.57
1:I:28:THR:HG22	1:I:31:GLU:H	1.70	0.57
1:K:44:GLU:OE1	1:K:46:LYS:HG3	2.04	0.57
2:B:97:GLU:OE1	2:D:58:LYS:NZ	126.87	0.57
1:C:283:THR:HG22	1:C:285:MET:N	2.11	0.57
1:G:283:THR:CG2	1:G:285:MET:H	2.15	0.57
1:Q:138:ALA:O	1:Q:140:PRO:HD3	2.04	0.57
1:W:29:ILE:HD11	2:X:102:MET:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:40:SER:HA	2:H:43:LYS:HB2	1.86	0.57
1:M:116:ASN:HB2	1:M:261:LYS:HG3	1.87	0.57
1:G:204:VAL:HG12	1:G:209:LEU:HD23	1.87	0.57
1:G:59:LEU:HD22	1:G:82:VAL:HG11	1.86	0.57
1:O:73:ASN:ND2	1:O:97:CYS:HB3	2.20	0.57
1:Y:43:LEU:HD23	1:Y:45:LYS:HE3	1.86	0.57
1:G:28:THR:HG22	1:G:31:GLU:H	1.70	0.56
1:C:18:HIS:ND1	2:D:17:MET:O	3.09	0.56
1:G:316:LEU:HD23	2:H:100:VAL:HG13	1.86	0.56
1:A:141:TYR:OH	1:U:261:LYS:HD2	62.67	0.56
1:K:284:PRO:HG2	1:K:298:HIS:CE1	2.40	0.56
1:A:58:PRO:HB3	1:A:86:TYR:CE1	2.39	0.56
1:C:120:LYS:HD3	1:C:256:TYR:CD2	2.39	0.56
1:M:307:LYS:HB3	2:N:62:GLN:OE1	2.04	0.56
1:S:221:SER:HB2	1:U:207:SER:HA	1.87	0.56
1:Q:156:LYS:HD2	1:Q:196:GLN:HB2	1.88	0.56
1:Y:26:VAL:HG21	1:Y:317:ALA:HB2	1.87	0.56
1:A:55:ASP:O	1:A:278:ASN:ND2	3.14	0.56
2:F:51:LYS:HD3	2:F:103:GLU:HB3	1.88	0.56
2:V:55:ILE:HG12	2:V:99:LEU:HD21	1.88	0.56
1:I:279:THR:HG21	1:I:287:ALA:HB1	1.88	0.56
1:A:193:LYS:HG2	1:A:194:LEU:HD23	1.87	0.56
1:E:283:THR:HB	1:E:286:GLY:O	2.06	0.56
2:X:62:GLN:HG3	2:X:92:TRP:CD2	2.41	0.56
1:E:202:ILE:HG12	1:E:247:SER:OG	2.05	0.56
2:X:132:GLU:HG3	2:X:138:PHE:CE1	2.41	0.56
1:K:29:ILE:HD11	2:L:102:MET:HG2	1.89	0.56
1:U:206:THR:HG22	1:U:207:SER:N	2.20	0.55
1:W:114:ARG:NH2	1:W:264:ASP:OD1	2.39	0.55
1:G:78:GLU:O	1:G:78:GLU:HG3	2.05	0.55
2:J:77:ILE:HA	2:J:80:LEU:HB3	1.88	0.55
1:S:288:ILE:HD11	1:S:297:ILE:HG13	1.88	0.55
2:X:6:ILE:HG13	2:X:112:ASP:HA	1.87	0.55
1:M:206:THR:HG22	1:M:207:SER:N	2.20	0.55
1:I:283:THR:HG23	1:I:284:PRO:HD2	1.88	0.55
1:K:320:LEU:HB3	2:L:111:HIS:CG	2.40	0.55
1:M:156:LYS:HD2	1:M:196:GLN:HB2	1.88	0.55
1:S:310:LYS:NZ	2:T:90:ASP:OD1	2.39	0.55
1:U:183:HIS:ND1	1:U:195:TYR:OH	2.38	0.55
1:U:221:SER:HB2	1:W:207:SER:HA	1.89	0.55
1:S:131:GLU:HB3	1:S:133(A):LEU:HD23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:O	1:A:150:ASN:ND2	2.79	0.55
2:D:76:ARG:NH1	2:Z:74:GLU:OE1	117.96	0.55
1:O:44:GLU:HB2	1:O:292:MET:HG3	1.89	0.55
1:G:180:TRP:NE1	1:G:204:VAL:HG21	2.21	0.55
2:P:149:MET:O	2:P:153:ARG:HG3	2.07	0.55
1:I:60:ILE:HG12	1:I:88:VAL:HB	1.89	0.55
1:K:57:LYS:HE2	1:K:274:TYR:HE2	1.72	0.55
1:M:83(A):GLU:OE1	1:M:261:LYS:NZ	2.40	0.55
1:Q:167:SER:HB2	1:Q:244:ASN:CB	2.37	0.55
1:M:29:ILE:HD11	2:N:102:MET:HA	1.88	0.54
1:S:61:LEU:HA	1:S:79:PHE:HZ	1.72	0.54
1:A:44:GLU:HB2	1:A:292:MET:HG3	1.88	0.54
1:C:269:LYS:HE3	2:D:69:GLU:OE2	3.30	0.54
1:E:307:LYS:HB3	2:F:62:GLN:NE2	2.23	0.54
2:D:113:SER:OG	2:L:2:LEU:O	2.24	0.54
1:M:58:PRO:HB3	1:M:86:TYR:CE1	2.41	0.54
1:K:183:HIS:O	1:K:185:PRO:HD3	2.08	0.54
1:O:18:HIS:HD2	1:O:37:THR:HG21	1.72	0.54
1:Q:67:ALA:HB3	1:Q:96:ASP:OD1	2.07	0.54
1:M:279:THR:HG21	1:M:287:ALA:HB1	1.88	0.54
1:Q:107:GLU:HG2	2:P:76:ARG:HH21	1.73	0.54
1:I:288:ILE:HD11	1:I:297:ILE:HG13	1.90	0.54
2:L:118:LEU:HD12	2:L:121:LYS:HD3	1.90	0.54
2:B:58:LYS:NZ	2:J:97:GLU:OE1	2.36	0.54
1:Q:283:THR:HG23	1:Q:284:PRO:HD2	1.88	0.54
1:Q:182:ILE:HD11	1:Q:215:PRO:HD3	1.90	0.54
1:S:247:SER:OG	1:S:248:ASN:N	2.37	0.54
1:E:43:LEU:HB2	1:E:314:LEU:HB2	1.90	0.54
1:G:264:ASP:OD1	1:G:264:ASP:N	2.41	0.54
2:B:80:LEU:HD23	2:D:81:ASN:ND2	94.56	0.54
1:Q:206:THR:HB	1:Q:209:LEU:H	1.72	0.53
1:Q:295:HIS:CE1	1:Q:308:TYR:HD1	2.26	0.53
1:W:126:SER:HB2	1:W:166:ARG:HH22	1.72	0.53
1:G:20:ASN:ND2	1:G:37:THR:HG23	2.24	0.53
1:I:232:PHE:HE1	1:I:252:ILE:HG21	1.72	0.53
1:W:206:THR:HG22	1:W:207:SER:N	2.23	0.53
2:X:133:LEU:HD12	2:X:137:CYS:HB2	1.89	0.53
1:A:43:LEU:HD23	1:A:45:LYS:HE3	2.66	0.53
1:G:279:THR:HG21	1:G:287:ALA:HB1	1.89	0.53
1:G:56:VAL:HB	1:G:85:SER:HB3	1.89	0.53
1:G:30:MET:HG2	2:J:47:GLY:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:311:SER:HB3	2:J:97:GLU:OE2	2.08	0.53
1:K:29:ILE:HD11	2:L:102:MET:HA	1.91	0.53
1:M:37:THR:HG22	1:M:38:HIS:CD2	2.43	0.53
1:Q:126:SER:HB2	1:Q:166:ARG:NH2	2.24	0.53
1:M:138:ALA:O	1:M:140:PRO:HD3	2.09	0.53
1:O:40:GLN:NE2	1:O:41:ASP:O	2.42	0.53
1:Q:195:TYR:O	1:Q:197:ASN:N	2.37	0.53
1:U:44:GLU:HB2	1:U:292:MET:HG3	1.90	0.53
1:C:206:THR:HG22	1:C:207:SER:N	2.27	0.53
1:C:314:LEU:HD22	2:D:100:VAL:HG21	1.97	0.53
1:E:28:THR:HG22	1:E:31:GLU:H	1.74	0.53
1:G:44:GLU:HB2	1:G:292:MET:HG3	1.90	0.53
1:G:61:LEU:HA	1:G:79:PHE:CZ	2.43	0.53
1:M:73:ASN:HD21	1:M:97:CYS:HB3	1.74	0.53
1:O:37:THR:HG22	1:O:38:HIS:CD2	2.44	0.53
1:W:42:ILE:HG13	1:W:314:LEU:HB3	1.90	0.53
2:B:74:GLU:HB3	2:B:77:ILE:HD12	5.32	0.53
1:I:78:GLU:HG3	1:I:78:GLU:O	2.05	0.53
1:K:123:ILE:HG13	1:K:124:ILE:HG13	1.90	0.53
1:K:200:THR:HA	1:K:248:ASN:OD1	2.08	0.53
1:M:26:VAL:HG11	1:M:317:ALA:HB2	1.89	0.53
2:B:159:TYR:HB3	2:B:160:PRO:HD3	1.91	0.53
1:O:206:THR:HG22	1:O:207:SER:N	2.24	0.53
1:U:231:GLU:HG2	1:U:233:PHE:CE2	2.43	0.53
1:W:26:VAL:HG12	1:W:315:VAL:HG12	1.90	0.53
2:B:1:GLY:HA3	2:B:112:ASP:OD2	2.09	0.53
1:G:164:ILE:O	1:G:246:GLU:HA	2.09	0.53
1:G:206:THR:HB	1:G:209:LEU:HB2	1.91	0.53
1:U:28:THR:HG22	1:U:31:GLU:H	1.73	0.53
2:T:68:ARG:HH22	2:X:83:LYS:HZ2	1.55	0.53
1:I:67:ALA:O	1:I:71:LEU:HD12	2.09	0.52
1:K:260:ILE:HG21	1:K:262:LYS:HE3	1.90	0.52
1:S:56:VAL:HB	1:S:85:SER:HB3	1.91	0.52
1:A:242:ALA:N	3:A:2001:NAG:H82	3.06	0.52
1:A:48:ASN:HD21	1:A:287:ALA:HB3	2.45	0.52
1:A:65:SER:OG	1:A:96:ASP:OD1	2.29	0.52
2:D:68:ARG:NH1	2:D:81:ASN:HD21	2.89	0.52
4:I:2004:NAG:H4	4:I:2005:NAG:H4	1.90	0.52
1:M:279:THR:HB	1:M:281:CYS:H	1.73	0.52
1:S:187:ASP:OD1	1:S:190:GLU:N	2.25	0.52
2:V:2:LEU:HD21	2:X:110:PHE:HD1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:LEU:O	1:G:150:ASN:ND2	2.41	0.52
1:M:123:ILE:O	1:M:124:ILE:HG13	2.10	0.52
1:M:220:ARG:HD2	1:M:227:SER:O	2.09	0.52
1:Q:73:ASN:ND2	1:Q:97:CYS:HB3	2.24	0.52
1:O:28:THR:HG23	1:O:30:MET:H	1.74	0.52
1:U:100:GLY:HA3	1:U:230:MET:O	2.08	0.52
1:A:222:LYS:HD3	1:A:225:GLY:HA2	1.92	0.52
1:E:182:ILE:HD11	1:E:215:PRO:HD3	1.91	0.52
1:K:122:GLN:NE2	1:K:125:PRO:HA	2.24	0.52
1:S:176:LEU:HD23	1:S:258:TYR:O	2.10	0.52
1:C:108:LEU:HB2	1:C:234:TRP:CZ2	2.45	0.52
2:N:128:ASP:O	2:N:170:ARG:NH1	2.42	0.52
1:Q:311:SER:HB3	2:R:97:GLU:OE2	2.09	0.52
1:A:48:ASN:ND2	1:A:287:ALA:HB3	2.78	0.52
2:B:127:ARG:HD2	2:J:131:LYS:NZ	2.25	0.52
2:L:159:TYR:HB3	2:L:160:PRO:HD3	1.92	0.52
1:Y:266:THR:HG22	1:Y:302:ILE:HD12	1.92	0.52
1:A:15:ILE:HD13	2:B:119:TYR:CD1	2.45	0.52
2:D:30:GLN:HE22	2:D:145:ASP:HA	1.75	0.52
2:L:84:MET:HE1	2:L:85:GLU:HG2	1.92	0.52
2:V:159:TYR:HB3	2:V:160:PRO:HD3	1.92	0.52
1:W:206:THR:HB	1:W:209:LEU:HB2	1.92	0.52
1:A:37:THR:HG22	1:A:38:HIS:CD2	2.45	0.51
2:X:57:ASP:O	2:X:60:ASN:HB2	2.11	0.51
1:A:288:ILE:HD11	1:A:297:ILE:HG13	2.25	0.51
1:A:13:ILE:HG22	2:B:138:PHE:HB2	2.44	0.51
1:I:71:LEU:HD11	1:I:102:PHE:CE2	2.45	0.51
1:M:266:THR:HG22	1:M:302:ILE:HD12	1.92	0.51
1:S:317:ALA:O	2:T:107:THR:HG21	2.11	0.51
1:Y:28:THR:HG22	1:Y:31:GLU:H	1.75	0.51
1:C:314:LEU:HD21	2:D:97:GLU:HA	2.43	0.51
1:C:48:ASN:ND2	1:C:287:ALA:HB3	2.30	0.51
2:D:159:TYR:HB3	2:D:160:PRO:HD3	1.94	0.51
2:F:30:GLN:HE22	2:F:145:ASP:HA	1.75	0.51
1:K:206:THR:HG22	1:K:207:SER:N	2.25	0.51
2:L:62:GLN:HG3	2:L:92:TRP:CG	2.45	0.51
1:O:83(A):GLU:OE2	1:O:261:LYS:NZ	2.41	0.51
2:B:51:LYS:HD3	2:B:103:GLU:HB3	2.32	0.51
1:E:100:GLY:HA3	1:E:230:MET:O	2.10	0.51
1:E:283:THR:HG23	1:E:284:PRO:HD2	1.92	0.51
2:T:21:TRP:CZ3	2:T:45:ILE:HG13	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:GLY:HA2	2:H:124:LEU:HD22	1.93	0.51
1:C:206:THR:HB	1:C:209:LEU:HB2	2.22	0.51
1:C:43:LEU:HD21	1:C:296:ASN:ND2	3.58	0.51
2:N:134:GLY:HA2	2:P:124:LEU:HD22	1.93	0.51
1:U:220:ARG:HD2	1:U:227:SER:O	2.10	0.51
1:Y:206:THR:HG22	1:Y:207:SER:N	2.26	0.51
1:Y:206:THR:HB	1:Y:209:LEU:H	1.75	0.51
1:E:102:PHE:O	1:E:105:TYR:HB2	2.10	0.51
1:K:141:TYR:HE2	1:O:62:ARG:HH21	1.57	0.51
1:K:176:LEU:HD22	1:K:257:ALA:HB1	1.93	0.51
1:K:283:THR:HG22	1:K:285:MET:N	2.17	0.51
2:T:106:ARG:HG3	2:V:106:ARG:HH22	1.76	0.51
1:C:154:LEU:O	1:C:155:ILE:HG13	2.10	0.51
1:O:154:LEU:O	1:O:155:ILE:HG13	2.10	0.51
1:I:175:ASP:OD1	1:I:239:PRO:HD3	2.11	0.51
1:I:29:ILE:HD11	2:J:102:MET:HA	1.93	0.51
1:M:12:GLN:HB2	2:N:27:SER:HB3	1.92	0.51
1:O:203:SER:OG	1:O:246:GLU:HB3	2.11	0.51
1:Q:26:VAL:HG11	1:Q:317:ALA:HB2	1.93	0.51
1:U:110:HIS:O	1:U:113:SER:OG	2.28	0.51
1:A:279:THR:HB	1:A:281:CYS:H	1.75	0.51
1:C:320:LEU:HB3	2:D:111:HIS:CG	2.46	0.51
2:P:159:TYR:HB3	2:P:160:PRO:HD3	1.93	0.51
1:C:182:ILE:HD11	1:C:215:PRO:HD3	1.91	0.50
1:K:37:THR:HG22	1:K:38:HIS:CD2	2.46	0.50
1:M:109:LYS:NZ	2:N:69:GLU:OE2	2.44	0.50
2:X:62:GLN:NE2	2:X:92:TRP:HB3	2.26	0.50
1:Q:206:THR:HG22	1:Q:207:SER:H	1.74	0.50
1:Q:230:MET:SD	1:Q:252:ILE:HD11	2.51	0.50
1:A:14:CYS:O	2:B:24:TYR:HA	2.11	0.50
1:A:97:CYS:HA	1:A:224:LYS:NZ	2.92	0.50
1:C:77:ASP:O	1:C:80:ILE:HG13	2.26	0.50
1:G:37:THR:HG22	1:G:38:HIS:CD2	2.46	0.50
1:K:299:PRO:HG2	1:K:300:LEU:HD12	1.94	0.50
2:T:106:ARG:CG	2:V:106:ARG:HH22	2.24	0.50
2:X:159:TYR:HB3	2:X:160:PRO:HD3	1.93	0.50
1:Y:33:ASN:ND2	5:Y:2003:NAG:O7	2.44	0.50
2:D:84:MET:HE2	2:D:85:GLU:HG2	1.93	0.50
1:U:37:THR:HG22	1:U:38:HIS:CD2	2.46	0.50
2:X:55:ILE:HG12	2:X:99:LEU:HD21	1.92	0.50
1:E:160:THR:HG21	1:W:165:LYS:CE	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:295:HIS:CD2	1:K:306:PRO:HG2	2.47	0.50
2:P:57:ASP:O	2:P:60:ASN:HB2	2.12	0.50
1:I:206:THR:HB	1:I:209:LEU:HB2	1.94	0.50
1:U:134:GLY:HA3	1:U:153:TRP:HB3	1.94	0.50
1:W:288:ILE:HD11	1:W:297:ILE:HG13	1.94	0.50
1:Y:50:LYS:HD3	1:Y:275:GLY:HA3	1.94	0.50
1:C:58:PRO:HB3	1:C:86:TYR:CE1	2.46	0.50
4:O:2004:NAG:O3	4:O:2005:NAG:H2	2.12	0.50
1:A:156:LYS:NZ	1:A:192:THR:O	2.64	0.50
1:E:108:LEU:HB2	1:E:234:TRP:CE2	2.47	0.50
1:K:141:TYR:HE2	1:O:62:ARG:NH2	2.10	0.50
2:N:58:LYS:NZ	2:R:97:GLU:OE1	2.45	0.50
2:R:23:GLY:HA3	2:R:36:ALA:HA	1.93	0.50
1:S:156:LYS:HD2	1:S:196:GLN:HB2	1.94	0.50
2:B:106:ARG:HH22	2:Z:106:ARG:CG	89.41	0.49
1:E:12:GLN:N	2:F:27:SER:O	2.41	0.49
1:A:73:ASN:ND2	1:A:97:CYS:HB3	2.26	0.49
1:E:206:THR:HG22	1:E:207:SER:N	2.27	0.49
1:E:48:ASN:ND2	1:E:287:ALA:HB3	2.27	0.49
1:I:164:ILE:O	1:I:246:GLU:HA	2.12	0.49
2:T:94:TYR:CE2	2:V:58:LYS:HB3	2.47	0.49
1:C:164:ILE:O	1:C:246:GLU:HA	2.34	0.49
1:C:30:MET:HG2	2:F:47:GLY:O	2.12	0.49
1:K:204:VAL:HG12	1:K:209:LEU:HD23	1.94	0.49
1:M:206:THR:HB	1:M:209:LEU:H	1.77	0.49
1:U:182:ILE:HD11	1:U:215:PRO:HD3	1.94	0.49
2:X:132:GLU:HG3	2:X:138:PHE:HE1	1.77	0.49
1:Y:48:ASN:HD21	1:Y:287:ALA:HB3	1.77	0.49
1:A:134:GLY:HA3	1:A:153:TRP:HB3	2.11	0.49
1:C:260:ILE:HG21	1:C:262:LYS:HE3	1.95	0.49
2:D:131:LYS:N	2:D:139:GLU:O	2.38	0.49
1:E:298:HIS:HE1	1:E:300:LEU:HD12	1.76	0.49
2:J:159:TYR:HB3	2:J:160:PRO:HD3	1.94	0.49
1:O:103:ASN:HB2	1:O:232:PHE:O	2.12	0.49
1:S:48:ASN:HD21	1:S:287:ALA:HB3	1.76	0.49
1:G:206:THR:HG22	1:G:207:SER:N	2.27	0.49
1:U:241:ASP:OD1	1:U:242:ALA:N	2.45	0.49
1:U:320:LEU:HB3	2:V:111:HIS:CG	2.47	0.49
1:W:131:GLU:OE2	1:W:157:LYS:HG3	2.12	0.49
1:W:284:PRO:HG2	1:W:298:HIS:CE1	2.47	0.49
1:S:204:VAL:HG22	1:S:245:PHE:HD1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:320:LEU:HB3	2:V:111:HIS:CD2	2.48	0.49
1:Y:100:GLY:HA3	1:Y:230:MET:O	2.13	0.49
1:Y:73:ASN:HB3	1:Y:76:CYS:SG	2.52	0.49
1:C:57:LYS:HE2	1:C:274:TYR:CE2	2.48	0.49
1:I:30:MET:HG2	2:B:47:GLY:O	2.12	0.49
1:K:100:GLY:HA3	1:K:230:MET:O	2.13	0.49
1:M:116:ASN:HB2	1:M:261:LYS:CG	2.43	0.49
1:U:122:GLN:HB2	1:U:122:GLN:HE21	1.39	0.49
1:E:137:SER:HA	1:E:145:SER:CB	2.42	0.49
2:J:51:LYS:O	2:J:55:ILE:HD12	2.12	0.49
1:G:58:PRO:HB3	1:G:86:TYR:CE1	2.47	0.49
2:P:72:ASN:OD1	2:P:75:ARG:NH2	2.45	0.49
2:V:167:ARG:O	2:V:171:GLU:HG2	2.13	0.49
2:V:62:GLN:HG3	2:V:92:TRP:CG	2.48	0.49
1:A:182:ILE:HD12	1:A:202:ILE:HD12	1.95	0.49
2:B:133:LEU:HD12	2:B:137:CYS:HB2	2.47	0.49
1:C:134:GLY:HA3	1:C:153:TRP:HB3	2.33	0.49
1:Q:189:ALA:HA	1:Q:192:THR:HG22	1.95	0.49
1:U:206:THR:HB	1:U:209:LEU:N	2.22	0.49
1:W:43:LEU:HB2	1:W:314:LEU:HB2	1.95	0.49
1:I:123:ILE:HG13	1:I:124:ILE:HG13	1.95	0.48
1:K:58:PRO:HB3	1:K:86:TYR:CZ	2.48	0.48
2:L:132:GLU:HG3	2:L:138:PHE:HE1	1.78	0.48
1:M:134:GLY:HA3	1:M:153:TRP:HB3	1.95	0.48
2:N:159:TYR:HB3	2:N:160:PRO:HD3	1.94	0.48
2:V:4:GLY:O	2:V:8:GLY:HA3	2.12	0.48
1:Y:50:LYS:HD3	1:Y:275:GLY:CA	2.42	0.48
1:A:278:ASN:C	1:A:278:ASN:OD1	2.87	0.48
2:B:168:LEU:O	2:B:172:GLU:HG3	2.14	0.48
1:C:160:THR:HG21	1:S:165:LYS:HE3	1.96	0.48
1:E:29:ILE:HG22	2:L:51:LYS:HG3	1.96	0.48
1:Q:78:GLU:HG3	1:Q:78:GLU:O	2.10	0.48
1:M:107:GLU:HG2	2:R:76:ARG:HH21	1.78	0.48
1:S:120:LYS:HD3	1:S:256:TYR:CD2	2.48	0.48
4:W:2004:NAG:H3	4:W:2005:NAG:O7	2.14	0.48
1:E:109:LYS:NZ	2:F:69:GLU:OE2	2.45	0.48
1:G:138:ALA:HB2	1:G:226:LEU:HD12	1.95	0.48
1:G:72:GLY:O	1:G:148:PHE:HA	2.14	0.48
1:I:56:VAL:HB	1:I:85:SER:HB3	1.94	0.48
2:L:84:MET:CE	2:L:85:GLU:HG2	2.43	0.48
2:N:57:ASP:O	2:N:60:ASN:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:164:ILE:O	1:Q:246:GLU:HA	2.13	0.48
2:V:169:LYS:HE3	2:V:173:ILE:HD11	1.94	0.48
1:W:98:TYR:CD1	1:W:99:PRO:HD2	2.48	0.48
1:C:100:GLY:HA3	1:C:230:MET:O	2.13	0.48
1:C:108:LEU:HB2	1:C:234:TRP:CE2	2.48	0.48
1:C:43:LEU:HD21	1:C:296:ASN:HD22	3.47	0.48
1:I:78:GLU:HG2	1:I:79:PHE:CE2	2.48	0.48
1:Y:195:TYR:O	1:Y:197:ASN:N	2.43	0.48
1:A:167:SER:HB2	1:A:244:ASN:OD1	2.13	0.48
2:D:151:SER:O	2:D:156:THR:N	2.47	0.48
1:E:126:SER:HB2	1:E:166:ARG:NH2	2.27	0.48
1:O:48:ASN:ND2	1:O:287:ALA:HB3	2.28	0.48
1:W:206:THR:HB	1:W:209:LEU:N	2.17	0.48
1:W:307:LYS:NZ	2:X:60:ASN:O	2.44	0.48
1:C:283:THR:HG21	1:C:297:ILE:HG22	1.95	0.48
2:B:127:ARG:HD2	2:J:131:LYS:HZ3	1.78	0.48
2:B:113:SER:OG	2:J:2:LEU:O	2.21	0.48
2:L:28:ASN:HD22	2:L:145:ASP:HA	1.79	0.48
1:U:61:LEU:HA	1:U:79:PHE:CZ	2.49	0.48
2:B:116:LYS:HG2	2:B:116:LYS:O	2.13	0.48
2:R:159:TYR:HB3	2:R:160:PRO:HD3	1.95	0.48
2:V:118:LEU:HD12	2:V:121:LYS:HD3	1.95	0.48
1:A:164:ILE:O	1:A:246:GLU:HA	2.14	0.48
1:A:293:PRO:HG2	1:A:294:PHE:HD1	5.00	0.48
1:I:320:LEU:HD12	1:I:321:ARG:N	2.28	0.48
1:M:58:PRO:HB3	1:M:86:TYR:CZ	2.49	0.48
1:C:188:ALA:O	1:C:192:THR:HG22	2.14	0.48
1:C:284:PRO:HG2	1:C:298:HIS:CE1	2.49	0.48
2:H:159:TYR:HB3	2:H:160:PRO:HD3	1.95	0.48
1:I:13:ILE:HG22	2:J:138:PHE:HB2	1.96	0.48
1:Q:176:LEU:HD22	1:Q:258:TYR:O	2.14	0.48
1:C:288:ILE:HD11	1:C:297:ILE:CG1	2.44	0.48
1:I:320:LEU:HD13	2:J:6:ILE:HD13	1.95	0.48
1:A:182:ILE:HG13	1:A:183:HIS:N	2.29	0.47
1:A:206:THR:HG22	1:A:207:SER:N	2.29	0.47
1:C:28:THR:CG2	1:C:30:MET:H	2.27	0.47
2:J:151:SER:O	2:J:156:THR:N	2.47	0.47
1:Q:126:SER:HB2	1:Q:166:ARG:HH22	1.78	0.47
1:Q:65:SER:OG	1:Q:96:ASP:HA	2.14	0.47
2:T:159:TYR:HB3	2:T:160:PRO:HD3	1.96	0.47
1:A:242:ALA:H	3:A:2001:NAG:H82	2.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:VAL:HG12	1:C:209:LEU:HD23	1.96	0.47
1:E:58:PRO:HB3	1:E:86:TYR:CE1	2.49	0.47
1:M:123:ILE:C	1:M:124:ILE:HG13	2.34	0.47
2:N:1:GLY:HA3	2:N:112:ASP:OD2	2.14	0.47
1:O:120:LYS:HD3	1:O:256:TYR:CD2	2.49	0.47
2:Z:159:TYR:HB3	2:Z:160:PRO:HD3	1.96	0.47
1:A:185:PRO:HD3	1:A:250:ASN:HD22	1.79	0.47
1:C:105:TYR:CE2	1:C:109:LYS:HE3	2.49	0.47
2:F:134:GLY:HA2	2:L:124:LEU:HD22	1.95	0.47
1:S:138:ALA:HB2	1:S:226:LEU:HD11	1.95	0.47
1:W:283:THR:HG23	1:W:284:PRO:HD2	1.94	0.47
1:K:274:TYR:HD1	1:K:275:GLY:N	2.12	0.47
1:K:26:VAL:HG11	1:K:317:ALA:HB2	1.97	0.47
1:Q:110:HIS:O	1:Q:113:SER:OG	2.30	0.47
1:Q:18:HIS:CE1	2:R:18:VAL:HA	2.48	0.47
6:Q:2003:BMA:O2	6:Q:2004:MAN:H3	2.15	0.47
1:Q:293:PRO:HG2	1:Q:294:PHE:CD2	2.49	0.47
2:V:106:ARG:HH11	2:X:106:ARG:HH12	1.62	0.47
1:M:295:HIS:CE1	1:M:308:TYR:HD2	2.32	0.47
2:R:168:LEU:O	2:R:172:GLU:HG3	2.14	0.47
1:W:100:GLY:HA3	1:W:230:MET:O	2.14	0.47
1:A:200:THR:HA	1:A:248:ASN:OD1	2.27	0.47
1:Q:98:TYR:CD1	1:Q:99:PRO:HD2	2.49	0.47
1:Y:179:LEU:HD23	1:Y:234:TRP:HB3	1.96	0.47
1:A:116:ASN:HB2	1:A:261:LYS:CG	2.45	0.47
1:C:147:PHE:CG	1:C:148:PHE:N	2.83	0.47
1:O:123:ILE:O	1:O:124:ILE:HG13	2.15	0.47
2:J:17:MET:SD	2:J:23:GLY:HA3	2.55	0.47
2:R:128:ASP:O	2:R:170:ARG:NH1	2.47	0.47
1:I:29:ILE:HD11	2:J:102:MET:HG2	1.97	0.47
1:K:28:THR:HG23	1:K:30:MET:H	1.78	0.47
1:O:48:ASN:HD21	1:O:287:ALA:HB3	1.80	0.47
1:Q:294:PHE:HZ	2:R:59:MET:HG3	1.79	0.47
1:Q:78:GLU:HG2	1:Q:79:PHE:CE2	2.50	0.47
1:A:182:ILE:HD12	1:A:202:ILE:CD1	2.44	0.47
2:N:25:HIS:HA	2:N:33:GLY:O	2.15	0.47
1:O:58:PRO:HB3	1:O:86:TYR:CE1	2.50	0.47
1:U:59:LEU:HD23	1:U:87:ILE:HG12	1.97	0.47
1:A:47:HIS:ND1	1:A:286:GLY:HA3	2.30	0.47
1:C:312:ASN:OD1	1:C:312:ASN:N	3.22	0.47
2:D:168:LEU:O	2:D:172:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:317:ALA:O	2:F:107:THR:HG21	2.15	0.47
1:E:57:LYS:HE2	1:E:274:TYR:CE2	2.50	0.47
1:I:77:ASP:OD2	1:I:149:ARG:NH2	2.39	0.47
1:U:133(A):LEU:O	1:U:135:VAL:HG12	2.15	0.47
1:C:97:CYS:HA	1:C:224:LYS:NZ	3.02	0.46
1:K:120:LYS:HG2	1:K:256:TYR:HB3	1.97	0.46
2:L:68:ARG:HD2	2:L:81:ASN:OD1	2.15	0.46
1:M:206:THR:CG2	1:M:207:SER:N	2.78	0.46
1:M:73:ASN:HB3	1:M:76:CYS:SG	2.55	0.46
1:Y:98:TYR:CZ	1:Y:226:LEU:HD13	2.50	0.46
2:B:127:ARG:NH1	2:Z:133:LEU:O	85.44	0.46
1:C:26:VAL:HG21	1:C:317:ALA:HB2	2.14	0.46
2:B:106:ARG:HG2	2:D:106:ARG:HH12	149.26	0.46
1:G:214:VAL:HG13	1:G:215:PRO:HD2	1.96	0.46
1:K:188:ALA:O	1:K:192:THR:HG22	2.15	0.46
1:M:172:ASN:HB3	1:M:174:GLU:OE2	2.15	0.46
1:Q:26:VAL:HG21	1:Q:317:ALA:HB2	1.97	0.46
2:T:125:GLN:OE1	2:T:155:GLY:HA2	2.15	0.46
1:C:197:ASN:HA	1:C:198:PRO:HD3	1.83	0.46
1:G:123:ILE:HG13	1:G:124:ILE:HG13	1.97	0.46
1:G:28:THR:CG2	1:G:30:MET:H	2.29	0.46
1:O:140:PRO:HA	1:O:145:SER:HA	1.98	0.46
1:W:58:PRO:HB3	1:W:86:TYR:CE1	2.50	0.46
1:C:56:VAL:HB	1:C:85:SER:HB3	2.22	0.46
1:C:70:LEU:O	1:C:150:ASN:ND2	2.47	0.46
1:E:24:GLU:OE1	1:E:39:ALA:HB3	2.16	0.46
2:F:21:TRP:HZ3	2:F:45:ILE:HG13	1.80	0.46
2:H:167:ARG:O	2:H:171:GLU:HG3	2.16	0.46
2:J:158:ASP:OD1	2:J:160:PRO:HD2	2.15	0.46
1:K:293:PRO:HB3	2:L:56:ILE:HG12	1.96	0.46
2:P:1:GLY:HA3	2:P:112:ASP:OD2	2.15	0.46
2:R:58:LYS:HD3	2:R:58:LYS:HA	1.76	0.46
1:U:56:VAL:HB	1:U:85:SER:HB3	1.97	0.46
1:Y:57:LYS:HE2	1:Y:274:TYR:CE2	2.50	0.46
2:B:77:ILE:HD12	2:J:77:ILE:HG21	1.98	0.46
1:C:183:HIS:O	1:C:185:PRO:HD3	2.15	0.46
1:E:123:ILE:HG13	1:E:124:ILE:HG13	1.97	0.46
1:K:135:VAL:HG22	1:K:146:SER:O	2.16	0.46
1:K:247:SER:OG	1:K:248:ASN:N	2.46	0.46
1:O:89:GLU:OE1	1:O:269:LYS:HE2	2.15	0.46
1:C:17:TYR:CE2	2:D:6:ILE:HA	3.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:GLU:OE1	1:E:46:LYS:HG3	2.15	0.46
1:G:108:LEU:HB2	1:G:234:TRP:CE2	2.50	0.46
1:K:139:CYS:O	1:K:146:SER:HB3	2.16	0.46
1:M:230:MET:SD	1:M:252:ILE:HD11	2.56	0.46
1:M:84:TRP:O	1:M:116:ASN:ND2	2.43	0.46
1:O:206:THR:HG22	1:O:207:SER:H	1.81	0.46
1:O:167:SER:HB2	1:O:244:ASN:OD1	2.15	0.46
1:W:134:GLY:HA3	1:W:153:TRP:HB3	1.98	0.46
1:W:186:ASN:HD21	1:W:228:GLY:N	2.14	0.46
1:A:175:ASP:OD1	1:A:238:LYS:HE2	2.16	0.46
2:H:30:GLN:HE22	2:H:145:ASP:HA	1.80	0.46
1:I:28:THR:CG2	1:I:30:MET:H	2.28	0.46
1:K:105:TYR:CE2	1:K:109:LYS:HE3	2.50	0.46
2:N:149:MET:O	2:N:153:ARG:HG3	2.16	0.46
2:R:1:GLY:HA3	2:R:112:ASP:OD2	2.16	0.46
1:U:242:ALA:N	3:U:2001:NAG:H82	2.31	0.46
1:A:73:ASN:HD21	1:A:97:CYS:HB3	1.81	0.46
1:C:295:HIS:CD2	1:C:306:PRO:HG2	2.51	0.46
1:C:320:LEU:HD13	2:D:6:ILE:HD13	2.88	0.46
1:E:206:THR:HB	1:E:209:LEU:H	1.81	0.46
1:I:316:LEU:HD23	1:I:316:LEU:HA	1.68	0.46
2:J:53:ASN:O	2:J:57:ASP:HB2	2.16	0.46
2:P:62:GLN:HG3	2:P:92:TRP:CG	2.50	0.46
2:R:62:GLN:HG3	2:R:92:TRP:CG	2.51	0.46
1:S:313:ARG:CZ	1:S:315:VAL:HG21	2.45	0.46
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.66	0.46
1:Q:283:THR:HG22	1:Q:285:MET:N	2.12	0.46
1:S:179:LEU:HD23	1:S:234:TRP:CB	2.45	0.46
1:Y:58:PRO:HB3	1:Y:86:TYR:CE1	2.51	0.46
2:B:118:LEU:HD12	2:B:121:LYS:HD3	2.74	0.46
1:C:307:LYS:HE2	2:D:64:GLU:OE2	3.19	0.46
1:G:260:ILE:HG21	1:G:262:LYS:HE3	1.98	0.46
1:M:112:LEU:HA	1:M:112:LEU:HD23	1.56	0.46
1:O:283:THR:HG23	1:O:298:HIS:HB3	1.98	0.46
1:A:183:HIS:O	1:A:185:PRO:HD3	2.16	0.45
1:C:80:ILE:O	1:C:120:LYS:NZ	2.49	0.45
1:E:37:THR:HG22	1:E:38:HIS:CD2	2.52	0.45
1:W:179:LEU:O	1:W:254:PRO:HG3	2.15	0.45
1:C:98:TYR:CE2	1:C:226:LEU:HD13	2.95	0.45
1:O:125(A):LYS:HB2	1:O:255:GLU:OE1	2.16	0.45
1:W:164:ILE:O	1:W:246:GLU:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:ALA:N	3:C:2001:NAG:H82	2.48	0.45
1:C:176:LEU:HD23	1:C:258:TYR:O	2.56	0.45
1:E:288:ILE:HD11	1:E:297:ILE:HG13	1.97	0.45
1:E:13:ILE:HA	2:F:26:HIS:HA	1.99	0.45
1:G:43:LEU:HB2	1:G:314:LEU:HB2	1.98	0.45
2:H:1:GLY:HA3	2:H:112:ASP:OD2	2.16	0.45
1:I:102:PHE:O	1:I:105:TYR:HB2	2.16	0.45
2:J:85:GLU:O	2:J:89:LEU:HG	2.17	0.45
2:N:118:LEU:HD12	2:N:121:LYS:HD3	1.97	0.45
2:P:125:GLN:OE1	2:P:155:GLY:HA2	2.17	0.45
1:W:56:VAL:HB	1:W:85:SER:HB3	1.98	0.45
1:A:58:PRO:HB3	1:A:86:TYR:CZ	2.51	0.45
1:A:15:ILE:HD13	2:B:119:TYR:HD1	1.81	0.45
1:C:185:PRO:HG3	1:C:191:GLN:OE1	2.17	0.45
2:F:125:GLN:OE1	2:F:155:GLY:HA2	2.16	0.45
1:G:176:LEU:HD23	1:G:258:TYR:O	2.15	0.45
1:S:176:LEU:HA	1:S:176:LEU:HD23	1.75	0.45
1:U:279:THR:HB	1:U:281:CYS:H	1.82	0.45
1:U:279:THR:HG21	1:U:287:ALA:HB1	1.98	0.45
2:T:127:ARG:NH1	2:X:131:LYS:HE2	2.31	0.45
1:A:141:TYR:CE1	1:A:149:ARG:NH2	3.73	0.45
1:E:12:GLN:O	2:F:27:SER:N	2.41	0.45
1:G:47:HIS:ND1	1:G:286:GLY:HA3	2.31	0.45
1:M:13:ILE:HD12	2:N:149:MET:SD	2.56	0.45
1:U:107:GLU:HG2	2:T:76:ARG:HH21	1.82	0.45
1:A:230:MET:SD	1:A:252:ILE:HD11	2.82	0.45
1:A:108:LEU:HB2	1:A:234:TRP:CE2	2.52	0.45
2:F:58:LYS:HD3	2:F:58:LYS:HA	1.80	0.45
1:G:232:PHE:HE1	1:G:252:ILE:HG21	1.81	0.45
1:I:142:GLN:C	1:I:144:LYS:H	2.19	0.45
1:I:260(A):VAL:O	1:I:260(A):VAL:HG13	2.16	0.45
1:O:242:ALA:N	3:O:2001:NAG:H82	2.32	0.45
1:O:220:ARG:HD2	1:O:227:SER:O	2.16	0.45
1:O:242:ALA:H	3:O:2001:NAG:H82	1.80	0.45
1:Y:123:ILE:HG13	1:Y:124:ILE:HG13	1.98	0.45
1:A:28:THR:HG22	1:A:31:GLU:N	2.31	0.45
2:H:77:ILE:HA	2:H:80:LEU:HB3	1.98	0.45
1:M:283:THR:HG23	1:M:284:PRO:HD2	1.98	0.45
2:B:151:SER:O	2:B:156:THR:N	2.50	0.45
2:B:53:ASN:O	2:B:57:ASP:HB2	2.17	0.45
2:F:173:ILE:HG23	2:F:177:ARG:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:293:PRO:HG2	1:G:294:PHE:CD2	2.52	0.45
1:I:294:PHE:HZ	2:J:59:MET:HG3	1.81	0.45
1:O:134:GLY:HA3	1:O:153:TRP:HB3	1.98	0.45
1:O:29:ILE:HD11	2:P:102:MET:HA	1.98	0.45
1:Q:73:ASN:HB3	1:Q:76:CYS:SG	2.57	0.45
1:W:105:TYR:CE2	1:W:109:LYS:HE3	2.51	0.45
1:I:206:THR:HG22	1:I:207:SER:N	2.32	0.45
1:K:169:ASN:O	1:K:171:THR:HG23	2.16	0.45
2:L:29:GLU:OE1	2:L:143:LYS:NZ	2.43	0.45
1:M:169:ASN:O	1:M:171:THR:HG23	2.17	0.45
1:M:49:GLY:HA2	1:M:285:MET:O	2.17	0.45
1:S:108:LEU:HB2	1:S:234:TRP:CZ2	2.52	0.45
1:U:53:ASP:OD1	1:U:57:LYS:HA	2.17	0.45
1:W:206:THR:CG2	1:W:207:SER:N	2.80	0.45
2:X:65:ALA:HB1	2:X:85:GLU:OE1	2.17	0.45
1:A:105:TYR:CE2	1:A:109:LYS:HE3	2.52	0.45
1:G:110:HIS:O	1:G:113:SER:OG	2.26	0.45
1:I:124:ILE:O	1:I:255:GLU:HG3	2.17	0.45
1:K:160:THR:HG21	1:U:165:LYS:CE	2.43	0.45
2:D:124:LEU:HD22	2:L:134:GLY:HA2	1.98	0.45
2:N:129:ASN:HB3	2:N:142:HIS:HE1	1.80	0.45
1:O:29:ILE:HD11	2:P:102:MET:HG2	1.98	0.45
2:T:62:GLN:HG3	2:T:92:TRP:CD2	2.52	0.45
1:G:180:TRP:HE1	1:G:204:VAL:HG21	1.81	0.44
1:I:288:ILE:HD11	1:I:297:ILE:CG1	2.46	0.44
1:O:311:SER:HB3	2:P:97:GLU:OE2	2.17	0.44
1:S:202:ILE:HD11	1:S:251:PHE:HA	1.99	0.44
1:U:247:SER:OG	1:U:248:ASN:N	2.43	0.44
2:V:97:GLU:HB3	2:X:58:LYS:NZ	2.32	0.44
1:Y:12:GLN:HB2	2:Z:27:SER:HB3	1.99	0.44
1:I:105:TYR:CE2	1:I:109:LYS:HE3	2.53	0.44
1:K:102:PHE:O	1:K:105:TYR:HB2	2.17	0.44
1:S:206:THR:HG22	1:S:207:SER:N	2.32	0.44
1:U:51:LEU:HG	1:U:272:LEU:HD12	1.99	0.44
2:X:103:GLU:OE2	2:X:106:ARG:HD3	2.16	0.44
1:A:141:TYR:CZ	1:A:149:ARG:NH2	3.65	0.44
2:D:84:MET:CE	2:D:85:GLU:HG2	2.46	0.44
1:K:317:ALA:O	2:L:107:THR:HG21	2.17	0.44
1:M:42:ILE:HG13	1:M:314:LEU:HB3	1.99	0.44
1:O:280:LYS:O	1:O:304:GLU:N	2.51	0.44
1:Q:206:THR:CG2	1:Q:207:SER:N	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:127:ARG:NH1	2:R:133:LEU:HA	2.33	0.44
1:S:194:LEU:HD23	1:S:194:LEU:HA	1.77	0.44
1:A:120:LYS:HG2	1:A:256:TYR:HB3	2.00	0.44
1:C:141:TYR:HB2	1:C:146:SER:HB2	2.45	0.44
1:C:214:VAL:HA	1:C:215:PRO:HD2	2.00	0.44
1:E:110:HIS:O	1:E:113:SER:OG	2.28	0.44
1:K:174:GLU:HG3	1:K:259:LYS:HB3	1.99	0.44
1:U:206:THR:CG2	1:U:207:SER:N	2.80	0.44
1:W:107:GLU:HG2	2:V:76:ARG:HH21	1.82	0.44
1:W:283:THR:HB	1:W:286:GLY:O	2.17	0.44
1:A:43:LEU:HB2	1:A:314:LEU:HB2	1.98	0.44
1:G:107:GLU:O	1:G:110:HIS:HB3	2.17	0.44
1:K:86:TYR:HE2	1:K:268:MET:HE2	1.82	0.44
1:M:65:SER:OG	1:M:96:ASP:HA	2.17	0.44
2:T:58:LYS:HA	2:T:58:LYS:HD3	1.80	0.44
1:A:257:ALA:C	1:A:258:TYR:HD1	2.21	0.44
2:F:2:LEU:O	2:L:113:SER:OG	2.27	0.44
1:O:316:LEU:HD23	1:O:316:LEU:HA	1.84	0.44
1:Q:269:LYS:HE3	2:R:69:GLU:OE1	2.18	0.44
1:Q:316:LEU:HD23	1:Q:316:LEU:HA	1.87	0.44
1:Q:53:ASP:OD1	1:Q:274:TYR:OH	2.23	0.44
1:U:161:TYR:CE2	1:U:249:GLY:HA2	2.53	0.44
1:A:147:PHE:HE2	1:A:151:VAL:HG23	1.82	0.44
1:A:56:VAL:HB	1:A:85:SER:HB3	2.22	0.44
1:A:98:TYR:CD1	1:A:99:PRO:HD2	2.88	0.44
2:B:58:LYS:HG3	2:J:98:LEU:CD1	2.48	0.44
2:B:72:ASN:O	2:B:75:ARG:HG2	2.18	0.44
1:C:226:LEU:HD23	1:C:226:LEU:HA	1.70	0.44
1:E:108:LEU:HB2	1:E:234:TRP:CZ2	2.52	0.44
1:G:186:ASN:OD1	1:G:227:SER:HB3	2.18	0.44
1:G:288:ILE:HD11	1:G:297:ILE:HG13	2.00	0.44
1:A:107:GLU:HG2	2:J:76:ARG:HH21	1.83	0.44
1:K:138:ALA:O	1:K:140:PRO:HD3	2.18	0.44
2:P:152:VAL:HG22	2:P:157:TYR:CD1	2.53	0.44
1:Q:200:THR:HG21	1:Q:249:GLY:HA3	1.99	0.44
1:W:30:MET:HG2	2:T:47:GLY:O	2.16	0.44
1:G:18:HIS:HD2	1:G:37:THR:HG21	1.83	0.44
2:J:58:LYS:HA	2:J:58:LYS:HD3	1.57	0.44
1:M:44:GLU:OE1	1:M:46:LYS:HG3	2.17	0.44
1:M:82:VAL:HA	1:M:83:PRO:HD3	1.83	0.44
2:T:124:LEU:HD22	2:X:134:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:MET:HG2	2:H:47:GLY:O	2.18	0.44
1:A:73:ASN:ND2	1:A:96:ASP:O	3.16	0.44
1:C:179:LEU:O	1:C:254:PRO:HB3	2.50	0.44
1:A:78:GLU:HG2	1:A:79:PHE:CE2	2.53	0.43
2:H:98:LEU:HD21	2:J:99:LEU:HD13	2.00	0.43
1:M:57:LYS:HE2	1:M:274:TYR:CE2	2.52	0.43
1:O:283:THR:HG22	1:O:285:MET:N	2.11	0.43
1:S:48:ASN:ND2	1:S:287:ALA:HB3	2.33	0.43
1:U:77:ASP:O	1:U:80:ILE:HG13	2.18	0.43
2:X:58:LYS:HD3	2:X:58:LYS:HA	1.83	0.43
1:Y:84:TRP:NE1	1:Y:115:ILE:O	2.51	0.43
2:Z:3:PHE:CE2	2:Z:113:SER:HB2	2.52	0.43
1:A:18:HIS:ND1	2:B:17:MET:O	4.28	0.43
1:C:26:VAL:HG11	1:C:317:ALA:HB2	2.03	0.43
1:E:176:LEU:HA	1:E:176:LEU:HD23	1.81	0.43
2:F:55:ILE:HG12	2:F:99:LEU:HD21	2.00	0.43
1:M:61:LEU:HG	1:M:61:LEU:H	1.57	0.43
1:S:283:THR:HB	1:S:286:GLY:O	2.17	0.43
2:V:3:PHE:CE1	2:V:113:SER:HB3	2.53	0.43
2:T:94:TYR:HE2	2:V:58:LYS:HB3	1.82	0.43
1:W:108:LEU:HB2	1:W:234:TRP:CZ2	2.53	0.43
2:B:158:ASP:OD1	2:B:160:PRO:HD2	2.44	0.43
1:I:20:ASN:HB2	1:I:21[B]:ASN:H	1.60	0.43
1:M:242:ALA:N	3:M:2001:NAG:H82	2.32	0.43
1:M:28:THR:HG22	1:M:31:GLU:N	2.26	0.43
1:O:138:ALA:O	1:O:140:PRO:HD3	2.18	0.43
1:O:314:LEU:HD23	1:O:314:LEU:HA	1.73	0.43
2:D:129:ASN:HB3	2:D:142:HIS:CE1	4.31	0.43
1:G:120:LYS:HD3	1:G:256:TYR:CD2	2.53	0.43
1:K:202:ILE:HD11	1:K:251:PHE:HA	2.01	0.43
1:K:320:LEU:HB3	2:L:111:HIS:CD2	2.53	0.43
1:S:206:THR:HB	1:S:209:LEU:HB2	2.00	0.43
2:T:123:ARG:HD2	2:T:132:GLU:OE2	2.18	0.43
1:U:230:MET:SD	1:U:252:ILE:HD11	2.59	0.43
1:W:204:VAL:HG12	1:W:209:LEU:HD23	1.99	0.43
1:W:279:THR:HB	1:W:281:CYS:H	1.83	0.43
1:C:114:ARG:HH21	1:C:263:GLY:C	2.21	0.43
1:E:137:SER:HA	1:E:145:SER:HB2	2.01	0.43
2:H:70:PHE:CD1	2:H:70:PHE:N	2.87	0.43
1:M:132:ALA:HA	1:M:154:LEU:HD23	2.01	0.43
1:M:78:GLU:O	1:M:78:GLU:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:55:ILE:O	2:N:59:MET:HG2	2.17	0.43
1:Q:108:LEU:HD13	1:Q:234:TRP:CD2	2.54	0.43
1:S:249:GLY:O	1:S:251:PHE:N	2.51	0.43
1:Y:320:LEU:HB3	2:Z:111:HIS:CD2	2.53	0.43
1:C:13:ILE:HG22	2:D:138:PHE:HB2	2.35	0.43
2:F:19:ASP:N	2:F:19:ASP:OD1	2.50	0.43
1:G:176:LEU:HD22	1:G:257:ALA:HB1	2.00	0.43
1:K:118:PHE:CD1	1:K:258:TYR:HB3	2.54	0.43
1:K:28:THR:CG2	1:K:30:MET:H	2.32	0.43
1:S:283:THR:HG23	1:S:284:PRO:HD2	2.01	0.43
2:T:176:GLY:HA2	2:V:167:ARG:NH2	2.32	0.43
1:W:228:GLY:O	1:W:229:ARG:HD3	2.19	0.43
1:Y:314:LEU:HA	1:Y:314:LEU:HD23	1.80	0.43
1:A:126:SER:HB2	1:A:166:ARG:NH2	2.93	0.43
1:A:214:VAL:HG13	1:A:215:PRO:HD2	2.00	0.43
1:O:28:THR:HG22	1:O:31:GLU:N	2.28	0.43
1:S:32:LYS:HE2	2:V:50:ASN:ND2	2.33	0.43
1:A:257:ALA:C	1:A:258:TYR:CD1	2.91	0.43
2:F:159:TYR:HB3	2:F:160:PRO:HD3	2.00	0.43
1:G:105:TYR:CE2	1:G:109:LYS:HD2	2.54	0.43
1:I:232:PHE:CE1	1:I:252:ILE:HG21	2.52	0.43
1:M:123:ILE:HB	1:M:168:TYR:CD2	2.54	0.43
1:O:28:THR:CG2	1:O:30:MET:H	2.31	0.43
2:P:19:ASP:OD1	2:P:19:ASP:N	2.51	0.43
1:C:112:LEU:HA	1:C:112:LEU:HD23	1.85	0.43
1:E:316:LEU:HD23	1:E:316:LEU:HA	1.90	0.43
1:G:100:GLY:HA3	1:G:230:MET:O	2.19	0.43
2:H:151:SER:O	2:H:157:TYR:N	2.50	0.43
1:Q:206:THR:CG2	1:Q:207:SER:H	2.32	0.43
1:S:279:THR:OG1	1:S:287:ALA:HB1	2.18	0.43
1:U:228:GLY:O	1:U:229:ARG:HD3	2.19	0.43
1:W:202:ILE:HD11	1:W:251:PHE:HA	2.01	0.43
1:Y:197:ASN:HA	1:Y:198:PRO:HD3	1.86	0.43
1:A:181:GLY:O	1:A:252:ILE:HB	2.46	0.43
1:A:264:ASP:OD1	1:A:264:ASP:N	2.51	0.43
2:D:5:ALA:HA	2:D:9:PHE:CE1	2.53	0.43
1:E:155:ILE:HG12	1:E:194:LEU:HD22	2.00	0.43
1:E:252:ILE:HG22	1:E:252:ILE:O	2.19	0.43
1:E:284:PRO:HG2	1:E:298:HIS:CE1	2.54	0.43
2:F:176:GLY:O	2:F:177:ARG:HB2	2.19	0.43
1:G:130:HIS:CE1	1:G:162:PRO:HG2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:204:VAL:HG12	1:M:209:LEU:HD23	2.01	0.43
2:P:122:VAL:O	2:P:126:LEU:HG	2.18	0.43
1:Q:77:ASP:OD1	1:Q:80:ILE:HD11	2.19	0.43
2:V:24:TYR:CD2	2:V:153:ARG:HG2	2.53	0.43
1:W:99:PRO:HD2	1:W:226:LEU:HD12	2.00	0.43
1:E:257:ALA:C	1:E:258:TYR:HD1	2.23	0.42
1:E:293:PRO:HG2	1:E:294:PHE:HD1	1.84	0.42
1:G:222:LYS:HA	1:G:226:LEU:O	2.18	0.42
2:V:57:ASP:O	2:V:60:ASN:HB2	2.19	0.42
1:Y:115:ILE:HD13	1:Y:260:ILE:HG12	2.00	0.42
2:Z:71:ASN:OD1	2:Z:74:GLU:HG3	2.19	0.42
1:A:258:TYR:CD1	1:A:258:TYR:N	2.86	0.42
2:B:106:ARG:HH11	2:H:106:ARG:NH1	2.13	0.42
2:H:62:GLN:HG3	2:H:92:TRP:CG	2.54	0.42
2:B:83:LYS:HG3	2:H:68:ARG:HH21	1.83	0.42
1:I:206:THR:HB	1:I:209:LEU:CB	2.49	0.42
1:I:200:THR:HA	1:I:248:ASN:OD1	2.19	0.42
1:O:313:ARG:NH2	1:O:315:VAL:HG21	2.34	0.42
1:W:159:SER:O	1:W:196:GLN:NE2	2.51	0.42
1:Y:83(A):GLU:CD	1:Y:261:LYS:HZ3	2.21	0.42
1:A:26:VAL:HB	2:B:104:ASN:ND2	2.87	0.42
1:A:283:THR:HG23	1:A:284:PRO:HD2	2.02	0.42
1:E:188:ALA:O	1:E:192:THR:HG22	2.19	0.42
1:I:12:GLN:HB2	2:J:27:SER:HB3	2.00	0.42
2:J:149:MET:O	2:J:153:ARG:HG3	2.19	0.42
1:M:122:GLN:NE2	1:M:125:PRO:HA	2.34	0.42
1:M:283:THR:HG22	1:M:285:MET:N	2.17	0.42
1:O:121:ILE:HD13	1:O:121:ILE:HG21	1.66	0.42
1:O:65:SER:OG	1:O:96:ASP:HA	2.19	0.42
1:S:126:SER:HB2	1:S:166:ARG:HH22	1.84	0.42
1:S:135:VAL:HG22	1:S:146:SER:CA	2.49	0.42
2:V:133:LEU:HD12	2:V:137:CYS:HB2	2.01	0.42
2:X:70:PHE:CE2	2:X:78:GLU:HA	2.55	0.42
1:Y:119:GLU:O	1:Y:121:ILE:HG23	2.20	0.42
1:I:107:GLU:O	1:I:110:HIS:HB3	2.18	0.42
1:I:206:THR:HB	1:I:209:LEU:N	2.29	0.42
2:D:106:ARG:HH22	2:L:106:ARG:CG	2.32	0.42
2:T:68:ARG:HH22	2:X:83:LYS:NZ	2.18	0.42
1:W:197:ASN:HA	1:W:198:PRO:HD3	1.87	0.42
1:W:311:SER:HB3	2:X:97:GLU:OE2	2.19	0.42
1:Y:298:HIS:HE1	1:Y:300:LEU:HD12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ILE:HG13	1:C:124:ILE:N	2.34	0.42
1:C:185:PRO:HD3	1:C:250:ASN:HD22	1.84	0.42
2:D:151:SER:O	2:D:157:TYR:N	2.51	0.42
1:M:164:ILE:O	1:M:246:GLU:HA	2.20	0.42
1:Q:122:GLN:NE2	1:Q:125:PRO:HA	2.34	0.42
1:Q:242:ALA:HB3	6:Q:2001:NAG:H82	2.00	0.42
2:R:152:VAL:HG22	2:R:157:TYR:CD1	2.54	0.42
1:S:314:LEU:HA	1:S:314:LEU:HD23	1.94	0.42
1:Y:314:LEU:HD22	2:Z:100:VAL:HG21	2.01	0.42
1:G:316:LEU:HD23	1:G:316:LEU:HA	1.78	0.42
1:I:154:LEU:O	1:I:155:ILE:HD12	2.19	0.42
2:L:77:ILE:HA	2:L:80:LEU:HB3	2.00	0.42
1:Q:280:LYS:O	1:Q:304:GLU:N	2.52	0.42
2:T:80:LEU:HD13	2:V:81:ASN:OD1	2.20	0.42
1:U:135:VAL:HG23	1:U:146:SER:CA	2.48	0.42
2:V:106:ARG:CG	2:X:106:ARG:HH22	2.33	0.42
1:Y:183:HIS:O	1:Y:185:PRO:HD3	2.20	0.42
1:A:47:HIS:CE1	1:A:285:MET:O	2.72	0.42
2:D:118:LEU:HD12	2:D:121:LYS:HD3	2.01	0.42
1:K:61:LEU:HA	1:K:79:PHE:CE1	2.53	0.42
1:Q:28:THR:HG23	1:Q:30:MET:H	1.84	0.42
1:S:108:LEU:HB2	1:S:234:TRP:CE2	2.55	0.42
2:T:55:ILE:HG12	2:T:99:LEU:HD21	2.01	0.42
1:U:131:GLU:OE2	1:U:157:LYS:HG3	2.20	0.42
1:W:314:LEU:HA	1:W:314:LEU:HD23	1.79	0.42
1:A:278:ASN:OD1	1:A:279:THR:N	2.64	0.42
2:D:123:ARG:HD2	2:D:132:GLU:OE2	2.19	0.42
1:G:28:THR:HG23	1:G:30:MET:H	1.84	0.42
1:K:65:SER:OG	1:K:96:ASP:OD1	2.28	0.42
1:M:154:LEU:O	1:M:155:ILE:HG13	2.19	0.42
1:W:182:ILE:HD11	1:W:215:PRO:HD3	2.02	0.42
2:Z:6:ILE:HD11	2:Z:111:HIS:HB3	2.02	0.42
2:Z:1:GLY:HA3	2:Z:112:ASP:OD2	2.19	0.42
1:A:154:LEU:O	1:A:155:ILE:HG13	2.20	0.42
1:A:195:TYR:O	1:A:196:GLN:HB3	2.19	0.42
2:B:142:HIS:CE1	2:B:162:TYR:CD2	3.08	0.42
2:B:75:ARG:O	2:B:78:GLU:HB3	2.19	0.42
1:C:206:THR:HG22	1:C:207:SER:H	1.84	0.42
1:G:167:SER:OG	1:G:168:TYR:N	2.51	0.42
1:O:180:TRP:CZ3	1:O:234:TRP:HA	2.54	0.42
1:O:30:MET:O	2:R:50:ASN:ND2	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:169:LYS:HD2	2:P:172:GLU:OE1	2.20	0.42
2:P:6:ILE:HG13	2:P:112:ASP:HA	2.02	0.42
2:N:80:LEU:HD13	2:P:81:ASN:OD1	2.20	0.42
1:Q:105:TYR:CE2	1:Q:109:LYS:HE3	2.55	0.42
3:U:2001:NAG:H61	3:U:2002:NAG:HN2	1.85	0.42
2:V:58:LYS:HD3	2:V:58:LYS:HA	1.44	0.42
1:W:102:PHE:O	1:W:105:TYR:HB2	2.20	0.42
1:W:77:ASP:OD2	1:W:141:TYR:HE1	2.03	0.42
1:W:156:LYS:NZ	1:W:193:LYS:O	2.51	0.42
1:A:124:ILE:HA	1:A:125:PRO:HD3	1.73	0.42
1:E:183:HIS:O	1:E:185:PRO:HD3	2.20	0.42
1:E:94:VAL:HG12	1:E:95:ASN:OD1	2.20	0.42
1:E:67:ALA:HB3	1:E:96:ASP:OD1	2.20	0.42
1:C:207:SER:HA	1:K:221:SER:HB2	2.02	0.42
1:O:26:VAL:HG21	1:O:317:ALA:HB2	2.01	0.42
2:T:89:LEU:HD23	2:T:89:LEU:HA	1.91	0.42
1:W:126:SER:HB2	1:W:166:ARG:NH2	2.35	0.42
1:W:182:ILE:HG13	1:W:250:ASN:O	2.19	0.42
1:A:180:TRP:NE1	1:A:204:VAL:HG21	2.34	0.41
1:C:156:LYS:HD2	1:C:196:GLN:HB2	2.15	0.41
1:C:202:ILE:HD11	1:C:251:PHE:HA	2.52	0.41
1:C:283:THR:HG23	1:C:284:PRO:HD2	2.02	0.41
1:I:111:LEU:HD12	1:I:111:LEU:HA	1.92	0.41
1:K:302:ILE:HG13	1:K:303:GLY:N	2.35	0.41
2:N:125:GLN:OE1	2:N:155:GLY:HA2	2.20	0.41
1:O:320:LEU:HD12	1:O:320:LEU:H	1.85	0.41
1:U:252:ILE:HG22	1:U:252:ILE:O	2.19	0.41
1:Y:236:ILE:HA	1:Y:236:ILE:HD13	1.86	0.41
2:Z:30:GLN:HE21	2:Z:30:GLN:N	2.17	0.41
1:C:209:LEU:HA	1:C:209:LEU:HD12	2.02	0.41
1:C:62:ARG:O	1:C:90:LYS:HD2	2.21	0.41
1:G:60:ILE:HG12	1:G:88:VAL:HB	2.03	0.41
1:K:108:LEU:HB2	1:K:234:TRP:CZ2	2.55	0.41
1:K:50:LYS:HB3	1:K:275:GLY:HA3	2.03	0.41
1:O:197:ASN:HA	1:O:198:PRO:HD3	1.88	0.41
2:T:75:ARG:HA	2:T:75:ARG:HD3	1.88	0.41
1:U:77:ASP:O	1:U:79:PHE:N	2.53	0.41
1:Y:124:ILE:HD12	1:Y:254:PRO:HG2	2.02	0.41
4:A:2004:NAG:H3	4:A:2005:NAG:H2	2.03	0.41
1:C:121:ILE:HD11	1:C:176:LEU:HD21	2.03	0.41
1:C:155:ILE:CG2	1:C:156:LYS:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:126:SER:HB2	1:K:166:ARG:NH2	2.34	0.41
1:M:294:PHE:HZ	2:N:59:MET:HG3	1.85	0.41
1:S:252:ILE:HG21	1:S:252:ILE:HD13	1.79	0.41
2:Z:53:ASN:O	2:Z:57:ASP:HB2	2.20	0.41
1:C:247:SER:OG	1:C:248:ASN:N	2.55	0.41
1:C:28:THR:HG22	1:C:31:GLU:N	2.32	0.41
2:F:71:ASN:OD1	2:F:72:ASN:N	2.54	0.41
1:G:125(A):LYS:HE3	1:G:132:ALA:HB1	2.02	0.41
2:B:76:ARG:NH1	2:H:74:GLU:OE1	2.50	0.41
1:I:20:ASN:HB2	1:I:21[A]:ASN:H	1.56	0.41
1:K:117:HIS:HB3	1:K:260(A):VAL:HG12	2.02	0.41
1:S:206:THR:CG2	1:S:207:SER:N	2.84	0.41
1:S:200:THR:HA	1:S:248:ASN:OD1	2.21	0.41
1:S:53:ASP:OD1	1:S:274:TYR:OH	2.25	0.41
1:U:235:THR:OG1	1:U:236:ILE:N	2.53	0.41
1:W:176:LEU:HA	1:W:176:LEU:HD23	1.79	0.41
1:W:187:ASP:OD2	1:W:189:ALA:HB3	2.21	0.41
1:W:73:ASN:HB3	1:W:76:CYS:SG	2.60	0.41
1:A:214:VAL:HA	1:A:215:PRO:HD2	2.08	0.41
1:I:283:THR:HG23	1:I:298:HIS:HB3	2.02	0.41
1:I:44:GLU:HB2	1:I:292:MET:HG3	2.02	0.41
1:M:230:MET:SD	1:M:252:ILE:CD1	3.08	0.41
2:N:129:ASN:HB3	2:N:142:HIS:CE1	2.55	0.41
1:O:222:LYS:HG3	1:O:227:SER:OG	2.20	0.41
2:P:118:LEU:O	2:P:122:VAL:HG23	2.20	0.41
1:S:320:LEU:HD23	2:T:111:HIS:ND1	2.36	0.41
2:T:62:GLN:HG3	2:T:92:TRP:CG	2.55	0.41
1:S:109:LYS:NZ	2:T:69:GLU:OE2	2.50	0.41
1:U:156:LYS:NZ	1:U:193:LYS:O	2.43	0.41
1:W:196:GLN:HE21	1:W:196:GLN:HB2	1.65	0.41
1:W:314:LEU:HD22	2:X:100:VAL:HG21	2.02	0.41
1:A:121:ILE:HD13	1:A:259:LYS:HD3	2.05	0.41
1:A:67:ALA:HB2	1:A:105:TYR:CE1	2.56	0.41
1:E:295:HIS:ND1	1:E:297:ILE:HG12	2.36	0.41
2:B:77:ILE:CD1	2:J:77:ILE:HG21	2.51	0.41
1:K:227:SER:O	1:K:229:ARG:NH1	2.53	0.41
1:K:238:LYS:HD3	1:K:239:PRO:HD2	2.03	0.41
1:M:11:ASP:O	2:N:140:PHE:HB2	2.21	0.41
1:O:124:ILE:HA	1:O:125:PRO:HD3	1.86	0.41
1:U:182:ILE:HB	1:U:202:ILE:HD12	2.01	0.41
2:X:168:LEU:O	2:X:172:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:242:ALA:N	4:Y:2001:NAG:H82	2.36	0.41
1:Y:44:GLU:HB2	1:Y:292:MET:HG3	2.03	0.41
1:Y:28:THR:HG22	1:Y:30:MET:H	1.85	0.41
2:B:71:ASN:OD1	2:B:74:GLU:HG3	2.46	0.41
1:K:115:ILE:CD1	1:K:260:ILE:HG12	2.51	0.41
1:O:105:TYR:CE2	1:O:109:LYS:HE3	2.56	0.41
1:Q:138:ALA:C	1:Q:140:PRO:HD3	2.41	0.41
2:R:149:MET:O	2:R:153:ARG:HG3	2.21	0.41
1:S:169:ASN:O	1:S:171:THR:HG23	2.21	0.41
1:C:44:GLU:OE1	1:C:46:LYS:HG3	2.20	0.41
1:I:277:CYS:HB2	1:I:278:ASN:H	1.73	0.41
2:J:168:LEU:O	2:J:172:GLU:HG3	2.20	0.41
2:J:62:GLN:HG3	2:J:92:TRP:CD2	2.56	0.41
2:L:133:LEU:HD21	2:L:139:GLU:HB2	2.02	0.41
1:O:317:ALA:O	2:P:107:THR:HG21	2.21	0.41
1:Q:122:GLN:NE2	1:Q:255:GLU:OE2	2.54	0.41
1:C:169:ASN:O	1:C:171:THR:HG23	2.21	0.41
1:C:186:ASN:HB2	1:C:190:GLU:OE2	2.39	0.41
1:E:186:ASN:ND2	1:E:227:SER:HB3	2.35	0.41
1:E:206:THR:CG2	1:E:207:SER:N	2.83	0.41
1:G:108:LEU:HB2	1:G:234:TRP:CZ2	2.56	0.41
1:G:226:LEU:HA	1:G:226:LEU:HD23	1.78	0.41
1:G:96:ASP:HB3	1:G:96(A):LEU:H	1.58	0.41
1:M:121:ILE:HD13	1:M:121:ILE:HG21	1.66	0.41
1:O:298:HIS:CE1	1:O:300:LEU:HB2	2.55	0.41
1:W:112:LEU:HD23	1:W:112:LEU:HA	1.70	0.41
1:W:147:PHE:CE2	1:W:148:PHE:HD1	2.39	0.41
1:A:307:LYS:HE2	2:B:64:GLU:OE2	3.58	0.41
2:B:77:ILE:HG13	2:B:77:ILE:H	3.92	0.41
1:C:37:THR:HG22	1:C:38:HIS:CE1	2.55	0.41
2:H:39:GLU:O	2:H:43:LYS:N	2.52	0.41
2:H:94:TYR:CD1	2:H:94:TYR:C	2.94	0.41
1:O:15:ILE:HB	2:P:119:TYR:HD2	1.85	0.41
1:O:202:ILE:HD12	1:O:213:LEU:HD12	2.03	0.41
1:O:295:HIS:CE1	1:O:308:TYR:HD1	2.39	0.41
1:Y:231:GLU:HG2	1:Y:233:PHE:CE1	2.56	0.41
1:A:283:THR:HG23	1:A:298:HIS:HB3	2.05	0.41
2:B:58:LYS:C	2:B:60:ASN:H	2.24	0.41
2:B:5:ALA:HA	2:B:9:PHE:CD1	2.56	0.41
2:B:99:LEU:HD13	2:Z:98:LEU:HD21	83.94	0.41
1:C:154:LEU:HD23	1:C:154:LEU:HA	2.12	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:THR:CG2	1:C:207:SER:N	2.91	0.41
1:G:251:PHE:CE2	1:G:253:ALA:HB2	2.57	0.41
2:J:30:GLN:HE22	2:J:145:ASP:HB2	1.86	0.41
1:K:164:ILE:O	1:K:246:GLU:HA	2.21	0.41
1:U:105:TYR:CE2	1:U:109:LYS:HE3	2.56	0.41
1:Y:98:TYR:CE2	1:Y:226:LEU:HD13	2.56	0.41
1:A:247:SER:OG	1:A:248:ASN:N	2.57	0.40
2:B:50:ASN:O	2:B:54:SER:N	2.94	0.40
1:C:132:ALA:HA	1:C:154:LEU:HD23	2.03	0.40
1:C:242:ALA:H	3:C:2001:NAG:H82	2.04	0.40
1:C:22:SER:O	1:C:322:ASN:ND2	2.66	0.40
1:C:26:VAL:HB	2:D:104:ASN:ND2	2.37	0.40
2:H:84:MET:CE	2:H:85:GLU:HG2	2.51	0.40
1:I:209:LEU:HD12	1:I:209:LEU:HA	1.82	0.40
1:K:105:TYR:CZ	1:K:109:LYS:HE3	2.55	0.40
1:M:111:LEU:HA	1:M:111:LEU:HD12	1.88	0.40
1:M:195:TYR:O	1:M:197:ASN:N	2.51	0.40
2:N:123:ARG:HD2	2:N:132:GLU:OE2	2.21	0.40
1:U:99:PRO:HD2	1:U:226:LEU:HD12	2.01	0.40
2:D:151:SER:HA	2:D:156:THR:HB	2.03	0.40
1:G:138:ALA:O	1:G:140:PRO:HD3	2.21	0.40
1:G:17:TYR:HB2	1:G:320:LEU:HD11	2.04	0.40
2:H:57:ASP:O	2:H:60:ASN:HB2	2.21	0.40
1:K:30:MET:HG2	2:D:47:GLY:O	2.21	0.40
1:O:279:THR:HB	1:O:281:CYS:H	1.87	0.40
1:U:116:ASN:HB2	1:U:261:LYS:HG2	2.03	0.40
1:Y:164:ILE:O	1:Y:246:GLU:HA	2.21	0.40
1:C:18:HIS:CD2	1:C:19:ALA:N	2.89	0.40
1:C:57:LYS:HE2	1:C:274:TYR:CZ	2.55	0.40
2:D:77:ILE:HA	2:D:80:LEU:HB3	2.03	0.40
1:E:226:LEU:HD23	1:E:226:LEU:HA	1.81	0.40
1:G:182:ILE:HD11	1:G:215:PRO:HD3	2.04	0.40
1:G:28:THR:HG22	1:G:31:GLU:N	2.35	0.40
1:G:294:PHE:HZ	2:H:59:MET:HG3	1.85	0.40
1:I:283:THR:HG22	1:I:285:MET:N	2.09	0.40
1:K:135:VAL:HA	1:K:146:SER:O	2.21	0.40
1:M:196:GLN:HB2	1:M:196:GLN:HE21	1.68	0.40
2:N:176:GLY:O	2:N:177:ARG:HG3	2.22	0.40
1:M:307:LYS:HD2	2:N:62:GLN:HB3	2.02	0.40
1:S:70:LEU:HD11	1:S:112:LEU:HD11	2.02	0.40
1:W:141:TYR:CD2	1:W:142:GLN:HG2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:70:LEU:O	1:Y:150:ASN:ND2	2.53	0.40
2:Z:30:GLN:HE21	2:Z:30:GLN:H	1.69	0.40
1:A:175:ASP:OD1	1:A:239:PRO:HD3	2.21	0.40
1:A:258:TYR:N	1:A:258:TYR:HD1	2.20	0.40
1:A:307:LYS:HG2	1:A:307:LYS:HZ2	1.75	0.40
2:F:151:SER:O	2:F:156:THR:N	2.55	0.40
1:G:251:PHE:CZ	1:G:253:ALA:HA	2.56	0.40
2:P:141:TYR:HE1	2:P:173:ILE:HD12	1.87	0.40
2:P:22:TYR:OH	2:P:111:HIS:ND1	2.40	0.40
1:Q:176:LEU:HB2	1:Q:237:LEU:HB3	2.03	0.40
1:Q:266:THR:HG22	1:Q:302:ILE:CD1	2.52	0.40
1:U:187:ASP:OD1	1:U:189:ALA:N	2.55	0.40
1:E:192:THR:HG23	1:U:192:THR:HG21	2.03	0.40
1:U:26:VAL:HB	2:V:104:ASN:ND2	2.36	0.40
1:Y:86:TYR:HB3	1:Y:302:ILE:HD13	2.03	0.40
1:A:232:PHE:CE1	1:A:252:ILE:HG21	2.56	0.40
1:C:283:THR:HG23	1:C:298:HIS:HB3	2.08	0.40
1:E:265:SER:OG	1:E:266:THR:N	2.55	0.40
1:G:185:PRO:HG2	1:G:191:GLN:OE1	2.22	0.40
1:G:17:TYR:CE2	2:H:6:ILE:HA	2.56	0.40
2:H:85:GLU:O	2:H:89:LEU:HG	2.22	0.40
1:I:172:ASN:HB3	1:I:174:GLU:OE2	2.22	0.40
1:K:206:THR:CG2	1:K:207:SER:N	2.84	0.40
1:Q:182:ILE:HB	1:Q:202:ILE:HD12	2.03	0.40
1:C:165:LYS:NZ	1:S:160:THR:HG23	2.36	0.40
1:S:26:VAL:HG21	1:S:317:ALA:HB2	2.04	0.40
2:V:133:LEU:HD12	2:V:137:CYS:CB	2.52	0.40
2:V:106:ARG:NH1	2:X:106:ARG:HH12	2.19	0.40
2:Z:149:MET:O	2:Z:153:ARG:HG3	2.21	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%)	295 (91%)	28 (9%)	0	100	100
1	C	323/334 (97%)	300 (93%)	23 (7%)	0	100	100
1	E	323/334 (97%)	301 (93%)	22 (7%)	0	100	100
1	G	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	I	323/334 (97%)	300 (93%)	23 (7%)	0	100	100
1	K	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	M	323/334 (97%)	298 (92%)	25 (8%)	0	100	100
1	O	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	Q	323/334 (97%)	298 (92%)	25 (8%)	0	100	100
1	S	323/334 (97%)	302 (94%)	20 (6%)	1 (0%)	44	80
1	U	323/334 (97%)	298 (92%)	23 (7%)	2 (1%)	28	70
1	W	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	Y	323/334 (97%)	297 (92%)	25 (8%)	1 (0%)	44	80
1	a	323/334 (97%)	297 (92%)	26 (8%)	0	100	100
1	c	323/334 (97%)	300 (93%)	22 (7%)	1 (0%)	44	80
2	B	175/181 (97%)	163 (93%)	12 (7%)	0	100	100
2	D	175/181 (97%)	162 (93%)	12 (7%)	1 (1%)	28	70
2	F	175/181 (97%)	163 (93%)	11 (6%)	1 (1%)	28	70
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%)	160 (91%)	14 (8%)	1 (1%)	28	70
2	N	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	P	175/181 (97%)	167 (95%)	8 (5%)	0	100	100
2	R	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	T	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	V	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	X	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
2	Z	175/181 (97%)	164 (94%)	11 (6%)	0	100	100
2	b	175/181 (97%)	163 (93%)	12 (7%)	0	100	100
2	d	175/181 (97%)	165 (94%)	10 (6%)	0	100	100
All	All	7470/7725 (97%)	6943 (93%)	519 (7%)	8 (0%)	55	88

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	77	ASP
1	Y	248	ASN
1	S	248	ASN
1	U	78	GLU
1	c	248	ASN
2	F	176	GLY
2	L	176	GLY
2	D	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%)	273 (94%)	19 (6%)	20	56
1	C	292/300 (97%)	281 (96%)	11 (4%)	38	74
1	E	292/300 (97%)	279 (96%)	13 (4%)	32	69
1	G	292/300 (97%)	277 (95%)	15 (5%)	28	65
1	I	292/300 (97%)	272 (93%)	20 (7%)	18	54
1	K	292/300 (97%)	282 (97%)	10 (3%)	42	76
1	M	292/300 (97%)	274 (94%)	18 (6%)	21	58
1	O	292/300 (97%)	277 (95%)	15 (5%)	28	65
1	Q	292/300 (97%)	275 (94%)	17 (6%)	23	60
1	S	292/300 (97%)	278 (95%)	14 (5%)	30	68
1	U	292/300 (97%)	277 (95%)	15 (5%)	28	65
1	W	292/300 (97%)	285 (98%)	7 (2%)	54	83
1	Y	292/300 (97%)	281 (96%)	11 (4%)	38	74
1	a	292/300 (97%)	279 (96%)	13 (4%)	32	69
1	c	292/300 (97%)	280 (96%)	12 (4%)	35	71
2	B	151/155 (97%)	146 (97%)	5 (3%)	43	77
2	D	151/155 (97%)	149 (99%)	2 (1%)	73	91
2	F	151/155 (97%)	150 (99%)	1 (1%)	87	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	151/155 (97%)	147 (97%)	4 (3%)	51	82
2	J	151/155 (97%)	147 (97%)	4 (3%)	51	82
2	L	151/155 (97%)	151 (100%)	0	100	100
2	N	151/155 (97%)	150 (99%)	1 (1%)	87	96
2	P	151/155 (97%)	150 (99%)	1 (1%)	87	96
2	R	151/155 (97%)	149 (99%)	2 (1%)	73	91
2	T	151/155 (97%)	149 (99%)	2 (1%)	73	91
2	V	151/155 (97%)	148 (98%)	3 (2%)	60	86
2	X	151/155 (97%)	148 (98%)	3 (2%)	60	86
2	Z	151/155 (97%)	147 (97%)	4 (3%)	51	82
2	b	151/155 (97%)	148 (98%)	3 (2%)	60	86
2	d	151/155 (97%)	146 (97%)	5 (3%)	43	77
All	All	6645/6825 (97%)	6395 (96%)	250 (4%)	38	74

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	46	LYS
1	A	75	MET
1	A	78	GLU
1	A	82	VAL
1	A	103	ASN
1	A	112	LEU
1	A	167	SER
1	A	174	GLU
1	A	182	ILE
1	A	208	THR
1	A	219	THR
1	A	235	THR
1	A	258	TYR
1	A	261	LYS
1	A	264	ASP
1	A	268	MET
1	A	273	GLU
1	A	285	MET
1	C	8	ASP
1	C	28	THR

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Mol	Chain	Res	Type
1	C	46	LYS
1	C	102	PHE
1	C	114	ARG
1	C	120	LYS
1	C	160	THR
1	C	208	THR
1	C	260(A)	VAL
1	C	261	LYS
1	C	265	SER
1	E	28	THR
1	E	46	LYS
1	E	92	ASN
1	E	94	VAL
1	E	114	ARG
1	E	156	LYS
1	E	158	ASP
1	E	166	ARG
1	E	192	THR
1	E	230	MET
1	E	258	TYR
1	E	261	LYS
1	E	273	GLU
1	G	12	GLN
1	G	28	THR
1	G	46	LYS
1	G	71	LEU
1	G	78	GLU
1	G	82	VAL
1	G	92	ASN
1	G	174	GLU
1	G	208	THR
1	G	264	ASP
1	G	283	THR
1	G	291	SER
1	G	312	ASN
1	G	320	LEU
1	G	323	SER
1	I	28	THR
1	I	46	LYS
1	I	71	LEU
1	I	78	GLU
1	I	111	LEU

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Mol	Chain	Res	Type
1	I	142	GLN
1	I	146	SER
1	I	155	ILE
1	I	166	ARG
1	I	194	LEU
1	I	199	THR
1	I	208	THR
1	I	214	VAL
1	I	261	LYS
1	I	266	THR
1	I	279	THR
1	I	285	MET
1	I	311	SER
1	I	320	LEU
1	I	323	SER
1	K	28	THR
1	K	46	LYS
1	K	56	VAL
1	K	94	VAL
1	K	114	ARG
1	K	166	ARG
1	K	187	ASP
1	K	199	THR
1	K	260(A)	VAL
1	K	261	LYS
1	M	28	THR
1	M	46	LYS
1	M	55	ASP
1	M	56	VAL
1	M	61	LEU
1	M	75	MET
1	M	109	LYS
1	M	111	LEU
1	M	121	ILE
1	M	133	SER
1	M	166	ARG
1	M	174	GLU
1	M	176	LEU
1	M	199	THR
1	M	208	THR
1	M	219	THR
1	M	265	SER

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Mol	Chain	Res	Type
1	M	311	SER
1	O	28	THR
1	O	56	VAL
1	O	61	LEU
1	O	96(A)	LEU
1	O	120	LYS
1	O	174	GLU
1	O	176	LEU
1	O	199	THR
1	O	208	THR
1	O	209	LEU
1	O	248	ASN
1	O	291	SER
1	O	310	LYS
1	O	311	SER
1	O	320	LEU
1	Q	27	ASP
1	Q	28	THR
1	Q	46	LYS
1	Q	61	LEU
1	Q	64	CYS
1	Q	78	GLU
1	Q	83(A)	GLU
1	Q	109	LYS
1	Q	112	LEU
1	Q	167	SER
1	Q	173	GLN
1	Q	174	GLU
1	Q	176	LEU
1	Q	199	THR
1	Q	244	ASN
1	Q	248	ASN
1	Q	320	LEU
1	S	28	THR
1	S	46	LYS
1	S	75	MET
1	S	114	ARG
1	S	160	THR
1	S	199	THR
1	S	226	LEU
1	S	244	ASN
1	S	260(A)	VAL

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Mol	Chain	Res	Type
1	S	283	THR
1	S	291	SER
1	S	300	LEU
1	S	311	SER
1	S	320	LEU
1	U	28	THR
1	U	30	MET
1	U	46	LYS
1	U	75	MET
1	U	111	LEU
1	U	114	ARG
1	U	122	GLN
1	U	161	TYR
1	U	174	GLU
1	U	226	LEU
1	U	244	ASN
1	U	258	TYR
1	U	272	LEU
1	U	279	THR
1	U	300	LEU
1	W	46	LYS
1	W	155	ILE
1	W	161	TYR
1	W	174	GLU
1	W	244	ASN
1	W	272	LEU
1	W	320	LEU
1	Y	28	THR
1	Y	54	LEU
1	Y	82	VAL
1	Y	142	GLN
1	Y	174	GLU
1	Y	199	THR
1	Y	261	LYS
1	Y	264	ASP
1	Y	272	LEU
1	Y	291	SER
1	Y	309	VAL
1	a	8	ASP
1	a	28	THR
1	a	55	ASP
1	a	81	ASN

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Mol	Chain	Res	Type
1	a	174	GLU
1	a	179	LEU
1	a	199	THR
1	a	214	VAL
1	a	261	LYS
1	a	273	GLU
1	a	291	SER
1	a	309	VAL
1	a	312	ASN
1	c	21[A]	ASN
1	c	21[B]	ASN
1	c	28	THR
1	c	114	ARG
1	c	174	GLU
1	c	199	THR
1	c	208	THR
1	c	209	LEU
1	c	244	ASN
1	c	261	LYS
1	c	264	ASP
1	c	312	ASN
2	B	22	TYR
2	B	43	LYS
2	B	77	ILE
2	B	84	MET
2	B	86	ASP
2	D	86	ASP
2	D	94	TYR
2	F	77	ILE
2	H	11	GLU
2	H	30	GLN
2	H	43	LYS
2	H	175	SER
2	J	11	GLU
2	J	68	ARG
2	J	77	ILE
2	J	116	LYS
2	N	77	ILE
2	P	11	GLU
2	R	30	GLN
2	R	66	VAL
2	T	50	ASN

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Mol	Chain	Res	Type
2	T	66	VAL
2	V	29	GLU
2	V	58	LYS
2	V	93	THR
2	X	83	LYS
2	X	84	MET
2	X	86	ASP
2	Z	30	GLN
2	Z	66	VAL
2	Z	77	ILE
2	Z	80	LEU
2	b	15	GLN
2	b	43	LYS
2	b	77	ILE
2	d	19	ASP
2	d	30	GLN
2	d	50	ASN
2	d	86	ASP
2	d	94	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	C	18	HIS
1	E	25	GLN
1	E	186	ASN
1	I	38	HIS
1	K	122	GLN
1	M	196	GLN
1	Q	122	GLN
1	S	197	ASN
1	W	186	ASN
1	W	196	GLN
1	Y	110	HIS
1	Y	197	ASN
2	F	62	GLN
2	H	30	GLN
2	H	146	ASN
2	L	42	GLN
2	T	25	HIS
2	T	81	ASN

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Mol	Chain	Res	Type
2	X	30	GLN
2	X	81	ASN
2	b	62	GLN
2	d	81	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

60 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	1.39	2 (14%)	15,19,21	1.21	1 (6%)
3	NAG	A	2002	3	14,14,15	0.50	0	15,19,21	0.60	0
3	BMA	A	2003	3	11,11,12	1.97	3 (27%)	13,15,17	1.98	5 (38%)
4	NAG	A	2004	1,4	14,14,15	1.03	1 (7%)	15,19,21	1.36	2 (13%)
4	NAG	A	2005	4	14,14,15	1.82	2 (14%)	15,19,21	1.23	1 (6%)
3	NAG	C	2001	1,3	14,14,15	0.61	0	15,19,21	0.67	0
3	NAG	C	2002	3	14,14,15	0.64	0	15,19,21	0.86	0
3	BMA	C	2003	3	11,11,12	1.79	2 (18%)	13,15,17	2.89	5 (38%)
3	NAG	E	2001	1,3	14,14,15	0.81	1 (7%)	15,19,21	1.50	1 (6%)
3	NAG	E	2002	3	14,14,15	1.01	1 (7%)	15,19,21	1.47	3 (20%)
3	BMA	E	2003	3	11,11,12	2.52	7 (63%)	13,15,17	1.52	3 (23%)
4	NAG	E	2004	1,4	14,14,15	1.20	1 (7%)	15,19,21	1.39	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	E	2005	4	14,14,15	0.59	1 (7%)	15,19,21	0.43	0
3	NAG	G	2001	1,3	14,14,15	1.74	2 (14%)	15,19,21	1.37	2 (13%)
3	NAG	G	2002	3	14,14,15	1.25	1 (7%)	15,19,21	1.22	2 (13%)
3	BMA	G	2003	3	11,11,12	2.29	5 (45%)	13,15,17	1.77	3 (23%)
4	NAG	G	2004	1,4	14,14,15	1.28	1 (7%)	15,19,21	1.48	2 (13%)
4	NAG	G	2005	4	14,14,15	1.80	3 (21%)	15,19,21	0.96	1 (6%)
3	NAG	I	2001	1,3	14,14,15	1.27	1 (7%)	15,19,21	1.44	2 (13%)
3	NAG	I	2002	3	14,14,15	0.72	1 (7%)	15,19,21	0.64	0
3	BMA	I	2003	3	11,11,12	1.97	3 (27%)	13,15,17	1.64	3 (23%)
4	NAG	I	2004	1,4	14,14,15	0.77	1 (7%)	15,19,21	1.25	1 (6%)
4	NAG	I	2005	4	14,14,15	1.54	2 (14%)	15,19,21	1.04	1 (6%)
3	NAG	K	2001	1,3	14,14,15	0.52	0	15,19,21	0.79	0
3	NAG	K	2002	3	14,14,15	0.92	1 (7%)	15,19,21	1.27	2 (13%)
3	BMA	K	2003	3	11,11,12	2.01	4 (36%)	13,15,17	1.72	3 (23%)
3	NAG	M	2001	1,3	14,14,15	0.67	1 (7%)	15,19,21	0.71	0
3	NAG	M	2002	3	14,14,15	0.85	1 (7%)	15,19,21	0.85	0
3	BMA	M	2003	3	11,11,12	1.92	5 (45%)	13,15,17	2.05	5 (38%)
4	NAG	M	2004	1,4	14,14,15	0.72	0	15,19,21	0.79	0
4	NAG	M	2005	4	14,14,15	1.48	1 (7%)	15,19,21	1.41	3 (20%)
3	NAG	O	2001	1,3	14,14,15	0.94	1 (7%)	15,19,21	0.65	0
3	NAG	O	2002	3	14,14,15	0.32	0	15,19,21	0.48	0
3	BMA	O	2003	3	11,11,12	1.53	2 (18%)	13,15,17	2.30	4 (30%)
4	NAG	O	2004	1,4	14,14,15	0.85	1 (7%)	15,19,21	1.02	1 (6%)
4	NAG	O	2005	4	14,14,15	0.30	0	15,19,21	0.68	1 (6%)
6	NAG	Q	2001	1,6	14,14,15	0.55	0	15,19,21	1.75	5 (33%)
6	NAG	Q	2002	6	14,14,15	0.45	0	15,19,21	1.10	0
6	BMA	Q	2003	6	11,11,12	0.72	0	13,15,17	2.12	4 (30%)
6	MAN	Q	2004	6	11,11,12	0.72	0	13,15,17	1.56	1 (7%)
4	NAG	Q	2005	1,4	14,14,15	1.26	1 (7%)	15,19,21	1.33	3 (20%)
4	NAG	Q	2006	4	14,14,15	1.04	1 (7%)	15,19,21	0.99	1 (6%)
4	NAG	S	2001	1,4	14,14,15	0.25	0	15,19,21	0.47	0
4	NAG	S	2002	4	14,14,15	0.92	1 (7%)	15,19,21	0.92	0
4	NAG	S	2003	1,4	14,14,15	0.95	1 (7%)	15,19,21	1.04	2 (13%)
4	NAG	S	2004	4	14,14,15	1.25	3 (21%)	15,19,21	1.06	1 (6%)
3	NAG	U	2001	1,3	14,14,15	0.30	0	15,19,21	0.63	0
3	NAG	U	2002	3	14,14,15	1.93	1 (7%)	15,19,21	1.41	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	U	2003	3	11,11,12	1.35	2 (18%)	13,15,17	1.46	3 (23%)
4	NAG	U	2004	1,4	14,14,15	1.16	1 (7%)	15,19,21	1.36	2 (13%)
4	NAG	U	2005	4	14,14,15	0.38	0	15,19,21	0.65	0
3	NAG	W	2001	1,3	14,14,15	0.62	0	15,19,21	1.06	2 (13%)
3	NAG	W	2002	3	14,14,15	0.57	0	15,19,21	0.97	0
3	BMA	W	2003	3	11,11,12	0.57	0	13,15,17	0.63	0
4	NAG	W	2004	1,4	14,14,15	1.43	1 (7%)	15,19,21	1.39	3 (20%)
4	NAG	W	2005	4	14,14,15	0.93	1 (7%)	15,19,21	0.82	1 (6%)
4	NAG	Y	2001	1,4	14,14,15	0.38	0	15,19,21	0.50	0
4	NAG	Y	2002	4	14,14,15	0.30	0	15,19,21	0.65	0
4	NAG	a	2001	1,4	14,14,15	0.47	0	15,19,21	1.27	2 (13%)
4	NAG	a	2002	4	14,14,15	0.43	0	15,19,21	0.49	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
4	NAG	M	2004	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	2005	4	-	0/6/23/26	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
4	NAG	O	2005	4	-	0/6/23/26	0/1/1/1
6	NAG	Q	2001	1,6	-	0/6/23/26	0/1/1/1
6	NAG	Q	2002	6	-	0/6/23/26	0/1/1/1
6	BMA	Q	2003	6	-	0/2/19/22	0/1/1/1
6	MAN	Q	2004	6	-	0/2/19/22	0/1/1/1
4	NAG	Q	2005	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Q	2006	4	-	0/6/23/26	0/1/1/1
4	NAG	S	2001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2002	4	-	0/6/23/26	0/1/1/1
4	NAG	S	2003	1,4	-	0/6/23/26	0/1/1/1
4	NAG	S	2004	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	1/1/1/1
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	2001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	Y	2002	4	-	0/6/23/26	0/1/1/1
4	NAG	a	2001	1,4	-	0/6/23/26	0/1/1/1
4	NAG	a	2002	4	-	0/6/23/26	0/1/1/1

All (71) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	2002	NAG	O5-C1	-7.05	1.32	1.43
3	G	2001	NAG	O5-C1	-5.93	1.34	1.43
4	M	2005	NAG	O5-C1	-4.96	1.35	1.43
4	W	2004	NAG	O5-C1	-4.94	1.35	1.43
4	G	2004	NAG	O5-C1	-4.56	1.36	1.43
3	G	2002	NAG	O5-C1	-4.44	1.36	1.43
4	Q	2005	NAG	O5-C1	-4.25	1.36	1.43
4	G	2005	NAG	O5-C1	-4.22	1.36	1.43
4	E	2004	NAG	O5-C1	-4.20	1.36	1.43
4	U	2004	NAG	O5-C1	-4.03	1.37	1.43
3	I	2001	NAG	O5-C1	-3.90	1.37	1.43
4	A	2004	NAG	O5-C1	-3.56	1.37	1.43
3	I	2003	BMA	O5-C1	-3.38	1.38	1.43
3	E	2002	NAG	O5-C1	-3.38	1.38	1.43
3	M	2003	BMA	O5-C1	-3.28	1.38	1.43
3	G	2003	BMA	O5-C1	-3.20	1.38	1.43
4	Q	2006	NAG	O5-C1	-3.19	1.38	1.43
3	O	2001	NAG	O5-C1	-3.10	1.38	1.43
4	S	2002	NAG	O5-C1	-3.02	1.38	1.43
4	S	2004	NAG	O5-C1	-2.92	1.38	1.43
4	S	2003	NAG	O5-C1	-2.90	1.39	1.43
4	O	2004	NAG	O5-C1	-2.69	1.39	1.43
3	K	2002	NAG	O5-C1	-2.65	1.39	1.43
4	I	2004	NAG	O5-C1	-2.60	1.39	1.43
3	A	2001	NAG	O5-C1	-2.57	1.39	1.43
3	I	2002	NAG	O5-C1	-2.54	1.39	1.43
3	M	2002	NAG	O5-C1	-2.49	1.39	1.43
4	S	2004	NAG	C3-C2	2.02	1.56	1.52
4	E	2005	NAG	C1-C2	2.03	1.55	1.52
3	G	2001	NAG	C3-C2	2.06	1.57	1.52
3	K	2003	BMA	C4-C3	2.08	1.57	1.52
3	M	2001	NAG	C1-C2	2.10	1.55	1.52
3	E	2003	BMA	O5-C1	2.15	1.47	1.43
3	G	2003	BMA	C1-C2	2.20	1.57	1.52
4	G	2005	NAG	C3-C2	2.20	1.57	1.52
3	M	2003	BMA	C2-C3	2.21	1.55	1.52
3	K	2003	BMA	C6-C5	2.23	1.59	1.51
3	M	2003	BMA	C1-C2	2.24	1.57	1.52
3	M	2003	BMA	C4-C3	2.29	1.58	1.52
3	O	2003	BMA	C1-C2	2.32	1.57	1.52
3	G	2003	BMA	C2-C3	2.34	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	U	2003	BMA	O5-C5	2.36	1.48	1.43
3	E	2003	BMA	C6-C5	2.45	1.60	1.51
4	W	2005	NAG	C1-C2	2.53	1.55	1.52
3	C	2003	BMA	C6-C5	2.56	1.60	1.51
3	E	2003	BMA	C4-C3	2.81	1.59	1.52
3	E	2003	BMA	O3-C3	2.81	1.49	1.43
3	U	2003	BMA	C1-C2	2.93	1.59	1.52
4	S	2004	NAG	C1-C2	2.94	1.56	1.52
3	E	2001	NAG	O5-C1	2.94	1.48	1.43
3	A	2003	BMA	C2-C3	2.99	1.56	1.52
3	K	2003	BMA	O3-C3	3.10	1.50	1.43
3	E	2003	BMA	C1-C2	3.11	1.59	1.52
3	K	2003	BMA	C4-C5	3.14	1.59	1.53
3	I	2003	BMA	C4-C3	3.22	1.60	1.52
3	E	2003	BMA	C4-C5	3.25	1.59	1.53
3	G	2003	BMA	C4-C5	3.37	1.60	1.53
3	I	2003	BMA	C4-C5	3.37	1.60	1.53
3	M	2003	BMA	C4-C5	3.40	1.60	1.53
3	C	2003	BMA	C4-C3	3.40	1.61	1.52
3	O	2003	BMA	C4-C5	3.46	1.60	1.53
3	A	2003	BMA	C1-C2	3.61	1.60	1.52
3	A	2003	BMA	C4-C3	3.74	1.61	1.52
4	I	2005	NAG	O5-C1	3.78	1.49	1.43
3	A	2001	NAG	C1-C2	3.94	1.57	1.52
3	E	2003	BMA	C2-C3	3.95	1.57	1.52
4	I	2005	NAG	C1-C2	4.19	1.58	1.52
3	G	2003	BMA	C4-C3	4.44	1.63	1.52
4	A	2005	NAG	C1-C2	4.65	1.58	1.52
4	G	2005	NAG	C1-C2	4.65	1.58	1.52
4	A	2005	NAG	O5-C1	4.82	1.51	1.43

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	2001	NAG	O5-C1-C2	-3.55	106.53	111.47
6	Q	2003	BMA	O3-C3-C4	-3.47	102.81	110.36
6	Q	2003	BMA	O5-C1-C2	-3.47	105.36	110.79
3	I	2001	NAG	C1-O5-C5	-3.14	107.84	112.17
4	M	2005	NAG	C1-O5-C5	-2.98	108.06	112.17
3	U	2003	BMA	O2-C2-C3	-2.93	104.41	110.17
3	A	2003	BMA	C1-O5-C5	-2.84	108.25	112.17
3	O	2003	BMA	O2-C2-C3	-2.50	105.27	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	2003	BMA	O2-C2-C3	-2.49	105.29	110.17
4	Q	2005	NAG	C1-O5-C5	-2.45	108.79	112.17
4	E	2004	NAG	C1-O5-C5	-2.40	108.86	112.17
6	Q	2001	NAG	C3-C4-C5	-2.36	106.06	110.22
3	K	2002	NAG	C1-O5-C5	-2.36	108.92	112.17
3	W	2001	NAG	O5-C1-C2	-2.34	108.22	111.47
4	W	2004	NAG	C1-O5-C5	-2.28	109.02	112.17
6	Q	2001	NAG	C2-N2-C7	-2.09	119.90	122.94
3	E	2003	BMA	C1-O5-C5	2.01	114.93	112.17
4	O	2005	NAG	C1-O5-C5	2.01	114.94	112.17
4	Q	2005	NAG	C3-C4-C5	2.04	113.82	110.22
6	Q	2001	NAG	C1-O5-C5	2.11	115.08	112.17
3	A	2003	BMA	C1-C2-C3	2.18	112.41	109.65
3	W	2001	NAG	C1-O5-C5	2.18	115.17	112.17
4	M	2005	NAG	C3-C4-C5	2.21	114.11	110.22
3	E	2002	NAG	O4-C4-C5	2.21	114.86	109.28
4	S	2003	NAG	C3-C4-C5	2.22	114.12	110.22
3	K	2003	BMA	O5-C1-C2	2.26	114.32	110.79
4	Q	2006	NAG	C4-C3-C2	2.26	114.33	111.02
4	E	2004	NAG	C3-C4-C5	2.33	114.31	110.22
3	E	2003	BMA	C3-C4-C5	2.34	114.33	110.22
4	S	2003	NAG	C4-C3-C2	2.36	114.48	111.02
4	W	2005	NAG	C4-C3-C2	2.40	114.53	111.02
3	M	2003	BMA	C2-C3-C4	2.42	115.09	110.88
3	G	2001	NAG	C3-C4-C5	2.42	114.48	110.22
3	I	2003	BMA	C2-C3-C4	2.48	115.21	110.88
3	G	2003	BMA	C2-C3-C4	2.50	115.24	110.88
3	U	2003	BMA	O2-C2-C1	2.55	114.37	109.18
4	O	2004	NAG	C4-C3-C2	2.56	114.77	111.02
4	a	2001	NAG	C3-C4-C5	2.57	114.74	110.22
4	G	2004	NAG	C4-C3-C2	2.57	114.78	111.02
3	G	2002	NAG	C4-C3-C2	2.57	114.79	111.02
3	K	2003	BMA	O3-C3-C2	2.60	114.76	110.02
3	A	2003	BMA	C2-C3-C4	2.65	115.49	110.88
4	A	2004	NAG	C4-C3-C2	2.65	114.91	111.02
3	E	2002	NAG	C1-O5-C5	2.66	115.83	112.17
3	U	2003	BMA	C1-O5-C5	2.68	115.85	112.17
3	G	2002	NAG	C3-C4-C5	2.70	114.98	110.22
4	W	2004	NAG	C3-C4-C5	2.76	115.08	110.22
3	O	2003	BMA	O5-C1-C2	2.76	115.12	110.79
3	G	2003	BMA	O2-C2-C1	2.80	114.88	109.18
3	I	2003	BMA	O2-C2-C1	2.87	115.01	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	2004	NAG	C3-C4-C5	2.93	115.39	110.22
3	E	2003	BMA	O3-C3-C2	2.96	115.41	110.02
3	K	2002	NAG	C4-C3-C2	2.96	115.36	111.02
3	U	2002	NAG	C3-C4-C5	2.99	115.48	110.22
3	M	2003	BMA	C1-C2-C3	3.02	113.48	109.65
4	U	2004	NAG	C4-C3-C2	3.15	115.64	111.02
3	M	2003	BMA	C3-C4-C5	3.15	115.77	110.22
3	U	2002	NAG	C4-C3-C2	3.21	115.73	111.02
6	Q	2001	NAG	C1-C2-N2	3.22	116.00	110.49
4	G	2005	NAG	C4-C3-C2	3.25	115.78	111.02
4	Q	2005	NAG	C4-C3-C2	3.27	115.81	111.02
3	A	2003	BMA	O2-C2-C1	3.27	115.83	109.18
3	C	2003	BMA	C2-C3-C4	3.32	116.67	110.88
3	A	2003	BMA	O5-C1-C2	3.36	116.05	110.79
3	C	2003	BMA	C3-C4-C5	3.37	116.15	110.22
4	a	2001	NAG	C1-O5-C5	3.39	116.83	112.17
3	I	2003	BMA	C3-C4-C5	3.40	116.21	110.22
6	Q	2003	BMA	O3-C3-C2	3.40	116.21	110.02
4	E	2004	NAG	C4-C3-C2	3.46	116.09	111.02
3	O	2003	BMA	C3-C4-C5	3.47	116.34	110.22
3	G	2003	BMA	C3-C4-C5	3.51	116.41	110.22
3	K	2003	BMA	C1-O5-C5	3.52	117.01	112.17
4	S	2004	NAG	C4-C3-C2	3.55	116.21	111.02
4	W	2004	NAG	C4-C3-C2	3.56	116.23	111.02
4	M	2005	NAG	C4-C3-C2	3.57	116.25	111.02
4	I	2004	NAG	C3-C4-C5	3.58	116.53	110.22
4	I	2005	NAG	C1-O5-C5	3.66	117.21	112.17
3	E	2002	NAG	C3-C4-C5	3.67	116.68	110.22
3	M	2003	BMA	C1-O5-C5	3.73	117.31	112.17
3	C	2003	BMA	C1-C2-C3	3.75	114.40	109.65
3	A	2001	NAG	C4-C3-C2	3.86	116.67	111.02
4	A	2004	NAG	C3-C4-C5	3.95	117.17	110.22
3	G	2001	NAG	C4-C3-C2	4.00	116.88	111.02
3	I	2001	NAG	C4-C3-C2	4.05	116.95	111.02
6	Q	2003	BMA	C3-C4-C5	4.29	117.78	110.22
4	G	2004	NAG	C3-C4-C5	4.30	117.79	110.22
4	A	2005	NAG	C1-O5-C5	4.42	118.26	112.17
3	E	2001	NAG	C1-O5-C5	4.94	118.98	112.17
6	Q	2004	MAN	O5-C1-C2	4.98	118.59	110.79
3	O	2003	BMA	C1-O5-C5	5.23	119.37	112.17
3	C	2003	BMA	O5-C1-C2	5.64	119.63	110.79
3	C	2003	BMA	C1-O5-C5	5.86	120.24	112.17

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	U	2003	BMA	C1-C2-C3-C4-C5-O5

19 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	NAG	3	0
4	A	2004	NAG	2	0
4	A	2005	NAG	2	0
3	C	2001	NAG	2	0
3	G	2001	NAG	1	0
4	I	2004	NAG	1	0
4	I	2005	NAG	1	0
3	M	2001	NAG	1	0
3	O	2001	NAG	2	0
4	O	2004	NAG	1	0
4	O	2005	NAG	1	0
6	Q	2001	NAG	1	0
6	Q	2003	BMA	4	0
6	Q	2004	MAN	4	0
3	U	2001	NAG	2	0
3	U	2002	NAG	1	0
4	W	2004	NAG	1	0
4	W	2005	NAG	1	0
4	Y	2001	NAG	1	0

5.6 Ligand geometry

5 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	K	2004	1	14,14,15	0.70	1 (7%)	15,19,21	0.58	0
5	NAG	O	2006	1	14,14,15	1.18	2 (14%)	15,19,21	1.13	2 (13%)
5	NAG	Y	2003	1	14,14,15	0.57	0	15,19,21	0.49	0
5	NAG	c	2001	1	14,14,15	0.55	0	15,19,21	0.51	0
5	NAG	c	2002	1	14,14,15	1.16	2 (14%)	15,19,21	1.25	1 (6%)

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	K	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	2003	1	-	0/6/23/26	0/1/1/1
5	NAG	c	2001	1	-	0/6/23/26	0/1/1/1
5	NAG	c	2002	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	c	2002	NAG	O5-C1	-3.45	1.38	1.43
5	O	2006	NAG	O5-C1	-3.05	1.38	1.43
5	K	2004	NAG	C1-C2	2.06	1.55	1.52
5	c	2002	NAG	C1-C2	2.16	1.55	1.52
5	O	2006	NAG	C1-C2	2.77	1.56	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	2006	NAG	C3-C4-C5	2.23	114.15	110.22
5	O	2006	NAG	C4-C3-C2	2.75	115.04	111.02
5	c	2002	NAG	C4-C3-C2	3.36	115.95	111.02

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	2003	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.25	4 (1%) 79 66	22, 45, 101, 176	0
1	C	324/334 (97%)	-0.09	11 (3%) 46 29	30, 56, 143, 199	0
1	E	324/334 (97%)	-0.08	15 (4%) 33 19	30, 56, 144, 203	0
1	G	324/334 (97%)	-0.26	6 (1%) 67 51	19, 46, 102, 183	0
1	I	324/334 (97%)	-0.33	5 (1%) 74 60	24, 44, 100, 186	0
1	K	324/334 (97%)	-0.02	14 (4%) 36 21	33, 57, 143, 218	0
1	M	324/334 (97%)	-0.16	10 (3%) 49 32	26, 50, 152, 220	0
1	O	324/334 (97%)	-0.10	12 (3%) 42 26	25, 50, 140, 226	0
1	Q	324/334 (97%)	-0.08	22 (6%) 18 10	25, 49, 151, 212	0
1	S	324/334 (97%)	-0.05	11 (3%) 46 29	35, 64, 158, 195	0
1	U	324/334 (97%)	-0.03	19 (5%) 23 12	31, 64, 158, 214	0
1	W	324/334 (97%)	-0.08	13 (4%) 39 24	35, 64, 148, 211	0
1	Y	324/334 (97%)	0.29	23 (7%) 17 9	55, 91, 189, 248	0
1	a	324/334 (97%)	0.27	17 (5%) 28 14	55, 87, 184, 263	0
1	c	324/334 (97%)	0.33	21 (6%) 20 11	59, 90, 185, 253	0
2	B	177/181 (97%)	0.36	8 (4%) 34 20	26, 113, 153, 173	0
2	D	177/181 (97%)	0.81	29 (16%) 2 1	41, 155, 195, 210	0
2	F	177/181 (97%)	1.11	44 (24%) 1 0	42, 154, 196, 206	0
2	H	177/181 (97%)	0.31	10 (5%) 25 13	23, 113, 154, 174	0
2	J	177/181 (97%)	0.17	4 (2%) 61 45	27, 113, 153, 166	0
2	L	177/181 (97%)	1.07	35 (19%) 1 1	42, 148, 195, 206	0
2	N	177/181 (97%)	1.23	44 (24%) 1 0	38, 158, 213, 231	0
2	P	177/181 (97%)	1.38	53 (29%) 1 0	38, 163, 213, 231	0
2	R	177/181 (97%)	1.26	44 (24%) 1 0	34, 163, 210, 222	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9	
2	T	177/181 (97%)	1.09	46 (25%)	1	0	45, 153, 201, 209	0
2	V	177/181 (97%)	1.22	40 (22%)	1	1	49, 153, 213, 228	0
2	X	177/181 (97%)	1.06	37 (20%)	1	1	50, 155, 204, 220	0
2	Z	177/181 (97%)	2.04	72 (40%)	0	0	74, 191, 237, 256	0
2	b	177/181 (97%)	1.85	60 (33%)	0	0	73, 187, 239, 254	0
2	d	177/181 (97%)	2.08	69 (38%)	0	0	78, 194, 247, 269	0
All	All	7515/7725 (97%)	0.37	798 (10%)	7	4	19, 79, 201, 269	0

All (798) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	c	16	GLY	18.0
2	d	23	GLY	15.5
1	O	13	ILE	15.1
2	b	141	TYR	14.3
1	U	12	GLN	14.0
2	P	140	PHE	10.8
1	O	12	GLN	10.7
2	d	141	TYR	9.9
1	Q	16	GLY	9.8
1	a	16	GLY	9.7
2	P	27	SER	9.5
2	d	8	GLY	9.3
2	V	157	TYR	9.3
2	d	153	ARG	9.1
2	X	142	HIS	9.0
2	R	32	SER	8.8
2	b	153	ARG	8.7
1	c	23	THR	8.7
2	Z	22	TYR	8.6
1	Y	12	GLN	8.6
2	P	32	SER	8.6
2	P	33	GLY	8.4
2	Z	23	GLY	8.2
1	Y	23	THR	8.2
2	d	32	SER	8.1
2	Z	157	TYR	8.0
2	N	22	TYR	8.0
2	F	157	TYR	8.0
1	Q	14	CYS	7.9

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Mol	Chain	Res	Type	RSRZ
1	O	14	CYS	7.9
2	V	158	ASP	7.9
2	V	140	PHE	7.8
1	a	23	THR	7.8
2	X	27	SER	7.7
2	b	35	ALA	7.7
2	b	37	ASP	7.7
1	M	9	PRO	7.6
2	d	152	VAL	7.6
2	V	22	TYR	7.5
2	N	29	GLU	7.3
1	Q	13	ILE	7.3
1	S	12	GLN	7.2
1	W	12	GLN	7.2
1	K	12	GLN	7.2
2	P	26	HIS	7.2
2	F	1	GLY	7.1
2	X	140	PHE	7.1
1	M	8	ASP	7.1
2	R	22	TYR	7.1
2	Z	140	PHE	7.1
1	M	10	GLY	7.0
2	b	142	HIS	7.0
2	Z	37	ASP	7.0
2	b	130	ALA	6.9
1	M	16	GLY	6.9
2	Z	152	VAL	6.9
2	Z	153	ARG	6.9
2	Z	35	ALA	6.8
1	Q	12	GLN	6.8
1	O	324	PRO	6.8
1	c	15	ILE	6.7
1	M	14	CYS	6.6
2	Z	130	ALA	6.6
2	b	24	TYR	6.6
2	F	140	PHE	6.5
2	P	25	HIS	6.5
2	Z	38	LYS	6.5
2	Z	1	GLY	6.5
2	T	140	PHE	6.5
1	K	13	ILE	6.4
2	N	160	PRO	6.4

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Mol	Chain	Res	Type	RSRZ
2	D	26	HIS	6.4
2	b	23	GLY	6.4
2	Z	159	TYR	6.4
1	Q	18	HIS	6.4
2	b	1	GLY	6.3
2	L	1	GLY	6.3
1	Y	14	CYS	6.3
1	O	16	GLY	6.3
1	M	13	ILE	6.2
1	Y	13	ILE	6.2
2	R	27	SER	6.2
2	b	36	ALA	6.2
1	M	12	GLN	6.2
2	b	129	ASN	6.2
2	V	149	MET	6.2
2	d	24	TYR	6.2
1	K	16	GLY	6.2
2	d	157	TYR	6.1
2	d	37	ASP	6.1
2	b	26	HIS	6.1
2	X	143	LYS	6.1
2	P	31	GLY	6.0
2	V	143	LYS	6.0
2	L	142	HIS	6.0
2	N	140	PHE	6.0
2	Z	41	THR	6.0
2	Z	125	GLN	6.0
2	b	140	PHE	6.0
1	I	324	PRO	6.0
2	P	22	TYR	6.0
1	E	324	PRO	5.9
2	d	154	ASN	5.9
1	U	8	ASP	5.9
2	F	158	ASP	5.8
2	d	36	ALA	5.8
2	R	176	GLY	5.8
2	d	38	LYS	5.8
2	N	27	SER	5.8
2	N	23	GLY	5.8
1	Q	320	LEU	5.7
2	L	138	PHE	5.7
1	Y	16	GLY	5.7

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Mol	Chain	Res	Type	RSRZ
2	b	157	TYR	5.7
2	X	22	TYR	5.6
2	b	128	ASP	5.6
1	O	10	GLY	5.6
2	L	140	PHE	5.6
2	L	22	TYR	5.5
2	L	144	CYS	5.5
2	b	143	LYS	5.5
2	Z	24	TYR	5.5
1	U	13	ILE	5.5
2	X	26	HIS	5.5
1	a	13	ILE	5.4
2	V	27	SER	5.4
2	V	161	GLN	5.4
1	M	11	ASP	5.4
1	O	11	ASP	5.4
2	F	33	GLY	5.3
2	X	157	TYR	5.3
2	d	143	LYS	5.3
2	V	35	ALA	5.3
2	d	144	CYS	5.3
2	N	144	CYS	5.3
2	D	22	TYR	5.2
2	d	156	THR	5.2
2	L	134	GLY	5.2
2	T	22	TYR	5.2
2	V	144	CYS	5.2
2	d	170	ARG	5.2
1	Y	21[A]	ASN	5.2
2	d	22	TYR	5.2
2	Z	176	GLY	5.1
2	b	32	SER	5.1
1	c	14	CYS	5.1
2	Z	148	CYS	5.1
1	G	324	PRO	5.1
2	X	160	PRO	5.1
2	T	35	ALA	5.1
2	d	16	GLY	5.1
2	D	140	PHE	5.1
2	T	157	TYR	5.1
2	Z	42	GLN	5.1
1	Q	10	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	c	13	ILE	5.0
2	d	155	GLY	5.0
2	b	152	VAL	5.0
2	D	1	GLY	5.0
1	a	11	ASP	4.9
1	C	12	GLN	4.9
2	X	23	GLY	4.9
2	d	132	GLU	4.9
2	P	23	GLY	4.9
2	P	10	ILE	4.8
2	d	158	ASP	4.8
2	P	160	PRO	4.8
2	R	33	GLY	4.8
2	N	157	TYR	4.8
2	V	24	TYR	4.8
2	d	163	SER	4.8
2	P	29	GLU	4.8
2	T	158	ASP	4.8
2	Z	36	ALA	4.8
2	d	35	ALA	4.8
2	T	143	LYS	4.8
2	R	138	PHE	4.7
2	D	144	CYS	4.7
2	R	171	GLU	4.7
1	K	15	ILE	4.7
1	Q	319	GLY	4.7
2	V	141	TYR	4.7
2	b	38	LYS	4.7
1	C	13	ILE	4.7
2	P	144	CYS	4.7
2	T	141	TYR	4.7
2	P	148	CYS	4.7
2	V	148	CYS	4.7
2	H	175	SER	4.7
1	U	14	CYS	4.7
1	a	22	SER	4.7
2	Z	16	GLY	4.6
2	b	160	PRO	4.6
2	N	32	SER	4.6
2	X	149	MET	4.6
2	F	141	TYR	4.6
2	F	142	HIS	4.6

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Mol	Chain	Res	Type	RSRZ
2	R	31	GLY	4.6
2	R	25	HIS	4.6
2	Z	4	GLY	4.6
2	N	24	TYR	4.6
2	R	160	PRO	4.6
1	Y	15	ILE	4.5
2	d	31	GLY	4.5
2	T	24	TYR	4.5
2	N	21	TRP	4.5
1	S	13	ILE	4.5
2	N	159	TYR	4.5
2	X	24	TYR	4.5
2	T	21	TRP	4.5
2	X	32	SER	4.5
2	b	7	ALA	4.5
2	X	158	ASP	4.5
2	T	38	LYS	4.5
2	N	176	GLY	4.5
1	c	22	SER	4.4
1	E	322	ASN	4.4
2	L	133	LEU	4.4
2	Z	136	GLY	4.4
2	b	144	CYS	4.4
2	V	156	THR	4.4
2	d	164	GLU	4.4
2	P	7	ALA	4.4
2	b	149	MET	4.4
2	b	22	TYR	4.4
2	L	132	GLU	4.3
2	Z	26	HIS	4.3
2	b	148	CYS	4.3
2	d	148	CYS	4.3
1	c	320	LEU	4.3
2	T	144	CYS	4.3
2	L	145	ASP	4.3
2	Z	126	LEU	4.3
1	Y	323	SER	4.3
2	F	32	SER	4.3
2	P	139	GLU	4.2
1	Y	22	SER	4.2
2	Z	32	SER	4.2
2	X	141	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
2	d	168	LEU	4.2
2	b	27	SER	4.2
1	O	9	PRO	4.2
2	T	149	MET	4.2
2	d	26	HIS	4.2
2	D	134	GLY	4.2
2	b	31	GLY	4.2
2	Z	29	GLU	4.2
1	S	8	ASP	4.1
2	H	177	ARG	4.1
2	R	175	SER	4.1
1	C	24	GLU	4.1
2	F	126	LEU	4.1
1	c	21[A]	ASN	4.1
2	R	157	TYR	4.1
1	I	8	ASP	4.1
1	C	324	PRO	4.0
2	F	22	TYR	4.0
2	V	21	TRP	4.0
2	Z	128	ASP	4.0
2	P	138	PHE	4.0
2	N	46	ASP	4.0
2	d	9	PHE	4.0
2	H	176	GLY	4.0
1	E	25	GLN	4.0
2	b	168	LEU	4.0
2	b	138	PHE	4.0
2	P	142	HIS	4.0
2	Z	154	ASN	4.0
2	b	34	TYR	4.0
1	Y	317	ALA	4.0
2	P	157	TYR	4.0
2	V	152	VAL	4.0
2	d	27	SER	4.0
2	R	177	ARG	4.0
2	N	35	ALA	4.0
2	N	33	GLY	3.9
1	K	319	GLY	3.9
2	d	121	LYS	3.9
2	Z	151	SER	3.9
2	d	15	GLN	3.9
2	Z	143	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	Q	24	GLU	3.9
1	Y	30	MET	3.9
2	d	25	HIS	3.9
2	F	177	ARG	3.9
2	V	23	GLY	3.9
2	T	156	THR	3.9
1	K	17	TYR	3.9
2	Z	40	SER	3.9
2	b	33	GLY	3.9
2	T	172	GLU	3.9
2	d	172	GLU	3.9
1	Y	11	ASP	3.9
2	Z	46	ASP	3.9
2	d	18	VAL	3.8
2	V	153	ARG	3.8
1	G	9	PRO	3.8
1	S	324	PRO	3.8
1	c	20	ASN	3.8
2	N	148	CYS	3.8
1	K	324	PRO	3.8
2	D	27	SER	3.8
2	X	16	GLY	3.8
2	Z	25	HIS	3.8
2	d	1	GLY	3.8
2	d	142	HIS	3.8
1	A	8	ASP	3.8
2	L	141	TYR	3.8
2	Z	39	GLU	3.8
1	K	14	CYS	3.8
1	Q	324	PRO	3.8
2	P	5	ALA	3.8
2	X	156	THR	3.8
2	N	142	HIS	3.8
2	N	143	LYS	3.8
1	Q	11	ASP	3.8
1	E	24	GLU	3.8
1	a	15	ILE	3.8
2	F	38	LYS	3.7
2	V	139	GLU	3.7
2	R	140	PHE	3.7
2	B	176	GLY	3.7
2	R	26	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
2	L	24	TYR	3.7
2	B	175	SER	3.7
2	V	126	LEU	3.7
2	R	134	GLY	3.7
2	N	25	HIS	3.7
1	c	37	THR	3.7
2	Z	141	TYR	3.7
2	D	139	GLU	3.7
2	d	136	GLY	3.7
2	X	7	ALA	3.7
2	X	25	HIS	3.7
2	N	158	ASP	3.7
2	b	177	ARG	3.7
2	V	151	SER	3.7
2	T	26	HIS	3.7
2	P	158	ASP	3.6
2	X	161	GLN	3.6
2	X	151	SER	3.6
2	D	157	TYR	3.6
2	R	19	ASP	3.6
2	D	33	GLY	3.6
1	W	8	ASP	3.6
2	V	25	HIS	3.6
2	P	6	ILE	3.6
2	d	166	ALA	3.6
1	c	11	ASP	3.6
2	V	162	TYR	3.6
1	E	23	THR	3.6
2	b	170	ARG	3.6
2	F	35	ALA	3.6
2	P	4	GLY	3.6
2	R	158	ASP	3.6
2	d	171	GLU	3.6
2	P	162	TYR	3.6
2	N	30	GLN	3.5
2	R	1	GLY	3.5
2	L	146	ASN	3.5
1	U	11	ASP	3.5
1	W	288	ILE	3.5
2	R	137	CYS	3.5
2	T	27	SER	3.5
2	Z	160	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
2	d	140	PHE	3.5
1	a	323	SER	3.5
1	A	324	PRO	3.5
2	X	35	ALA	3.5
2	F	21	TRP	3.5
2	R	18	VAL	3.5
2	b	158	ASP	3.5
2	d	149	MET	3.5
2	V	147	GLU	3.5
2	V	155	GLY	3.5
2	Z	47	GLY	3.5
1	Y	9	PRO	3.4
2	N	26	HIS	3.4
1	Q	8	ASP	3.4
1	W	11	ASP	3.4
1	U	9	PRO	3.4
2	Z	127	ARG	3.4
2	F	156	THR	3.4
1	a	20	ASN	3.4
2	b	9	PHE	3.4
2	d	106	ARG	3.4
2	b	156	THR	3.4
2	F	138	PHE	3.4
2	V	150	GLU	3.4
1	Y	322	ASN	3.4
2	R	159	TYR	3.4
2	Z	175	SER	3.4
2	D	25	HIS	3.4
2	F	26	HIS	3.4
1	a	63	ASP	3.4
2	N	19	ASP	3.4
2	X	153	ARG	3.4
1	E	13	ILE	3.4
2	d	29	GLU	3.4
2	d	151	SER	3.4
2	B	140	PHE	3.3
2	D	158	ASP	3.3
2	Z	45	ILE	3.3
2	d	17	MET	3.3
2	Z	144	CYS	3.3
2	X	162	TYR	3.3
1	O	34	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	Z	156	THR	3.3
1	S	9	PRO	3.3
2	F	145	ASP	3.3
2	L	177	ARG	3.3
2	R	29	GLU	3.3
2	Z	171	GLU	3.3
2	N	161	GLN	3.3
1	c	63	ASP	3.3
1	Q	20	ASN	3.3
2	Z	13	GLY	3.3
2	Z	131	LYS	3.3
2	V	26	HIS	3.3
1	O	323	SER	3.3
2	P	137	CYS	3.3
2	X	144	CYS	3.3
2	P	132	GLU	3.3
2	b	132	GLU	3.3
2	T	23	GLY	3.3
1	Y	34	VAL	3.3
1	c	312	ASN	3.2
2	F	171	GLU	3.2
2	N	36	ALA	3.2
2	X	21	TRP	3.2
2	P	156	THR	3.2
1	c	24	GLU	3.2
1	W	13	ILE	3.2
2	X	31	GLY	3.2
2	T	18	VAL	3.2
2	b	109	ASP	3.2
1	G	12	GLN	3.2
2	F	166	ALA	3.2
2	Z	149	MET	3.2
2	F	24	TYR	3.2
2	X	29	GLU	3.2
1	E	16	GLY	3.2
1	W	16	GLY	3.2
2	P	145	ASP	3.2
2	R	141	TYR	3.2
2	L	148	CYS	3.2
2	D	145	ASP	3.2
2	b	163	SER	3.2
2	V	16	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
2	Z	34	TYR	3.2
2	V	29	GLU	3.1
2	d	135	ASN	3.1
2	F	176	GLY	3.1
2	N	42	GLN	3.1
2	B	156	THR	3.1
2	Z	33	GLY	3.1
2	b	155	GLY	3.1
2	R	21	TRP	3.1
2	V	118	LEU	3.1
2	N	146	ASN	3.1
2	P	154	ASN	3.1
1	G	8	ASP	3.1
1	O	8	ASP	3.1
2	T	161	GLN	3.1
2	F	31	GLY	3.1
2	Z	147	GLU	3.1
2	b	2	LEU	3.1
2	V	125	GLN	3.1
1	K	24	GLU	3.1
2	R	132	GLU	3.1
2	L	23	GLY	3.1
2	N	177	ARG	3.1
1	Q	9	PRO	3.1
1	U	21[A]	ASN	3.1
2	T	19	ASP	3.1
2	d	130	ALA	3.1
1	I	9	PRO	3.0
2	N	175	SER	3.0
1	A	9	PRO	3.0
2	P	131	LYS	3.0
2	D	153	ARG	3.0
1	Q	17	TYR	3.0
2	D	32	SER	3.0
2	P	161	GLN	3.0
2	P	28	ASN	3.0
2	R	168	LEU	3.0
1	W	324	PRO	3.0
2	F	144	CYS	3.0
2	P	155	GLY	3.0
2	L	168	LEU	3.0
2	N	31	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	c	17	TYR	3.0
2	N	44	ALA	3.0
2	b	159	TYR	3.0
1	E	12	GLN	3.0
2	J	38	LYS	3.0
1	U	322	ASN	3.0
2	L	175	SER	3.0
2	Z	18	VAL	3.0
2	Z	132	GLU	3.0
2	d	33	GLY	3.0
2	L	158	ASP	3.0
2	D	177	ARG	3.0
2	X	33	GLY	2.9
2	B	177	ARG	2.9
1	S	21[A]	ASN	2.9
1	U	22	SER	2.9
2	F	175	SER	2.9
2	T	160	PRO	2.9
2	Z	158	ASP	2.9
1	C	21[A]	ASN	2.9
2	d	111	HIS	2.9
2	V	38	LYS	2.9
2	L	126	LEU	2.9
2	P	146	ASN	2.9
2	X	147	GLU	2.9
2	L	21	TRP	2.9
2	L	31	GLY	2.9
2	R	142	HIS	2.9
2	R	139	GLU	2.9
2	Z	14	TRP	2.9
1	K	10	GLY	2.9
2	L	38	LYS	2.9
2	P	143	LYS	2.9
2	T	173	ILE	2.9
2	P	177	ARG	2.9
2	V	160	PRO	2.9
2	D	149	MET	2.9
2	Z	142	HIS	2.9
2	L	139	GLU	2.9
2	L	143	LYS	2.9
2	P	46	ASP	2.9
2	V	145	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	13	ILE	2.8
2	B	16	GLY	2.8
2	T	25	HIS	2.8
2	F	127	ARG	2.8
2	L	157	TYR	2.8
2	R	164	GLU	2.8
2	R	166	ALA	2.8
2	P	34	TYR	2.8
2	T	16	GLY	2.8
2	T	142	HIS	2.8
2	D	126	LEU	2.8
1	U	34	VAL	2.8
1	c	12	GLN	2.8
1	W	21[A]	ASN	2.8
2	d	131	LYS	2.8
2	d	134	GLY	2.8
2	d	34	TYR	2.8
1	K	31	GLU	2.8
2	V	154	ASN	2.8
1	Y	324	PRO	2.8
2	b	8	GLY	2.8
1	S	323	SER	2.8
1	K	23	THR	2.8
2	D	31	GLY	2.8
2	b	25	HIS	2.8
2	R	144	CYS	2.8
1	C	23	THR	2.8
2	T	33	GLY	2.8
1	Y	20	ASN	2.8
2	T	168	LEU	2.8
2	V	142	HIS	2.8
1	Q	322	ASN	2.7
1	a	21[A]	ASN	2.7
1	a	317	ALA	2.7
2	L	166	ALA	2.7
2	P	153	ARG	2.7
2	L	27	SER	2.7
2	T	171	GLU	2.7
2	R	4	GLY	2.7
2	N	34	TYR	2.7
2	T	29	GLU	2.7
2	J	177	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
2	P	47	GLY	2.7
2	b	164	GLU	2.7
1	G	85	SER	2.7
2	D	143	LYS	2.7
2	d	28	ASN	2.7
2	N	145	ASP	2.7
2	T	42	GLN	2.7
1	Q	36	VAL	2.7
1	a	17	TYR	2.7
2	F	19	ASP	2.7
2	P	35	ALA	2.7
2	b	145	ASP	2.7
2	L	152	VAL	2.7
2	N	1	GLY	2.7
2	Z	137	CYS	2.7
2	F	173	ILE	2.7
2	X	148	CYS	2.6
1	c	19	ALA	2.6
2	P	44	ALA	2.6
2	P	130	ALA	2.6
1	U	294	PHE	2.6
2	H	22	TYR	2.6
2	R	34	TYR	2.6
1	Q	22	SER	2.6
2	P	134	GLY	2.6
2	Z	48	VAL	2.6
1	C	15	ILE	2.6
1	W	318	THR	2.6
2	L	131	LYS	2.6
2	b	124	LEU	2.6
2	V	177	ARG	2.6
2	d	14	TRP	2.6
2	Z	170	ARG	2.6
2	P	159	TYR	2.6
2	X	145	ASP	2.6
2	R	135	ASN	2.6
2	Z	49	THR	2.6
2	T	36	ALA	2.6
2	N	28	ASN	2.6
1	E	320	LEU	2.6
2	R	170	ARG	2.6
2	T	153	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
2	b	126	LEU	2.6
2	P	30	GLN	2.6
2	T	165	GLU	2.5
2	T	166	ALA	2.5
1	Y	63	ASP	2.5
2	B	38	LYS	2.5
2	F	146	ASN	2.5
2	N	17	MET	2.5
1	Q	323	SER	2.5
2	P	1	GLY	2.5
2	X	1	GLY	2.5
2	d	42	GLN	2.5
2	T	146	ASN	2.5
1	E	323	SER	2.5
1	O	320	LEU	2.5
2	F	120	ASP	2.5
2	T	34	TYR	2.5
2	B	142	HIS	2.5
2	D	21	TRP	2.5
2	V	146	ASN	2.5
2	b	29	GLU	2.5
2	F	37	ASP	2.5
2	T	9	PHE	2.5
2	F	168	LEU	2.5
2	d	160	PRO	2.5
2	F	152	VAL	2.5
2	T	162	TYR	2.5
2	Z	174	SER	2.5
1	A	12	GLN	2.4
2	d	10	ILE	2.4
1	Y	17	TYR	2.4
2	D	148	CYS	2.4
2	P	19	ASP	2.4
2	J	140	PHE	2.4
1	W	20	ASN	2.4
1	Y	35	THR	2.4
2	P	24	TYR	2.4
2	L	149	MET	2.4
1	E	51	LEU	2.4
2	R	42	GLN	2.4
2	R	156	THR	2.4
1	Y	31	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	162	TYR	2.4
2	F	153	ARG	2.4
2	Z	8	GLY	2.4
2	F	169	LYS	2.4
2	d	41	THR	2.4
2	N	16	GLY	2.4
2	d	139	GLU	2.4
2	T	44	ALA	2.4
1	U	23	THR	2.4
2	L	33	GLY	2.3
2	R	23	GLY	2.3
2	Z	106	ARG	2.3
2	d	173	ILE	2.3
1	c	95	ASN	2.3
1	Q	25	GLN	2.3
2	d	162	TYR	2.3
2	R	155	GLY	2.3
2	Z	122	VAL	2.3
2	F	139	GLU	2.3
1	K	320	LEU	2.3
1	a	324	PRO	2.3
1	I	12	GLN	2.3
1	M	21[A]	ASN	2.3
2	Z	164	GLU	2.3
1	c	39	ALA	2.3
2	Z	27	SER	2.3
2	Z	163	SER	2.3
1	C	14	CYS	2.3
2	F	18	VAL	2.3
2	T	152	VAL	2.3
1	S	25	GLN	2.3
1	c	311	SER	2.3
2	T	148	CYS	2.3
2	d	45	ILE	2.3
2	D	35	ALA	2.3
1	a	280	LYS	2.3
2	Z	21	TRP	2.3
1	E	22	SER	2.3
2	b	125	GLN	2.3
2	b	167	ARG	2.3
1	E	18	HIS	2.3
2	H	140	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	142	HIS	2.3
1	S	50	LYS	2.3
2	d	6	ILE	2.3
2	T	151	SER	2.3
2	Z	7	ALA	2.3
1	Q	21[A]	ASN	2.2
2	V	30	GLN	2.2
2	P	21	TRP	2.2
2	Z	50	ASN	2.2
2	T	20	GLY	2.2
1	C	22	SER	2.2
2	N	168	LEU	2.2
1	C	16	GLY	2.2
2	Z	161	GLN	2.2
2	V	163	SER	2.2
2	X	19	ASP	2.2
2	D	23	GLY	2.2
1	W	18	HIS	2.2
1	Y	95	ASN	2.2
2	F	34	TYR	2.2
1	U	307	LYS	2.2
2	D	113	SER	2.2
2	L	32	SER	2.2
2	R	8	GLY	2.2
1	U	25	GLN	2.2
2	R	126	LEU	2.2
2	d	133	LEU	2.2
1	a	312	ASN	2.2
2	X	146	ASN	2.2
2	b	135	ASN	2.2
2	D	36	ALA	2.2
1	K	25	GLN	2.2
2	N	126	LEU	2.2
2	F	109	ASP	2.2
2	L	120	ASP	2.2
1	C	36	VAL	2.2
2	H	26	HIS	2.2
2	N	14	TRP	2.2
1	a	32	LYS	2.2
2	H	174	SER	2.2
1	c	48	ASN	2.2
2	b	171	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	132	GLU	2.2
2	X	20	GLY	2.2
2	F	112	ASP	2.1
2	T	147	GLU	2.1
2	d	57	ASP	2.1
2	b	176	GLY	2.1
1	E	17	TYR	2.1
2	P	18	VAL	2.1
2	b	121	LYS	2.1
1	Q	19	ALA	2.1
2	D	24	TYR	2.1
2	b	131	LYS	2.1
1	U	15	ILE	2.1
2	Z	44	ALA	2.1
2	b	162	TYR	2.1
2	R	153	ARG	2.1
1	U	319	GLY	2.1
2	N	37	ASP	2.1
2	R	37	ASP	2.1
2	b	28	ASN	2.1
2	N	149	MET	2.1
2	d	109	ASP	2.1
1	a	14	CYS	2.1
1	U	323	SER	2.1
2	N	163	SER	2.1
2	T	30	GLN	2.1
2	T	154	ASN	2.1
2	d	39	GLU	2.1
1	U	10	GLY	2.1
1	W	319	GLY	2.1
2	L	45	ILE	2.1
2	Z	31	GLY	2.1
1	W	281	CYS	2.0
2	F	172	GLU	2.0
2	J	149	MET	2.0
2	P	11	GLU	2.0
2	F	148	CYS	2.0
1	S	10	GLY	2.0
2	Z	116	LYS	2.0
1	Y	85	SER	2.0
2	F	111	HIS	2.0
1	E	34	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	38	LYS	2.0
2	H	126	LEU	2.0
1	I	23	THR	2.0
2	P	149	MET	2.0
1	M	17	TYR	2.0
2	b	120	ASP	2.0
2	b	4	GLY	2.0
1	U	40	GLN	2.0
1	S	34	VAL	2.0
2	d	21	TRP	2.0
2	X	9	PHE	2.0
2	H	144	CYS	2.0
2	X	18	VAL	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	C	2001	14/15	0.84	0.32	2.99	56,75,85,89	0
3	NAG	O	2001	14/15	0.95	0.28	1.59	39,57,67,74	0
3	NAG	A	2001	14/15	0.93	0.22	1.14	61,66,70,73	0
3	NAG	I	2001	14/15	0.93	0.22	0.88	50,59,64,64	0
3	NAG	E	2001	14/15	0.89	0.22	0.51	54,72,97,102	0
3	NAG	U	2001	14/15	0.91	0.20	0.46	54,66,81,92	0
4	NAG	a	2001	14/15	0.88	0.28	0.16	86,95,107,111	0
3	NAG	W	2001	14/15	0.87	0.17	0.03	64,71,80,92	0
3	BMA	K	2003	11/12	0.78	0.21	-0.19	32,49,59,61	0
3	NAG	G	2001	14/15	0.95	0.18	-0.19	54,63,66,66	0
4	NAG	S	2001	14/15	0.90	0.18	-0.20	50,69,87,102	0
4	NAG	Y	2001	14/15	0.90	0.19	-1.37	95,100,108,119	0
4	NAG	Y	2002	14/15	0.79	0.24	-	115,131,144,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	A	2005	14/15	0.67	0.26	-	119,129,135,136	0
3	NAG	W	2002	14/15	0.86	0.29	-	77,96,107,119	0
3	NAG	I	2002	14/15	0.92	0.27	-	65,75,86,89	0
3	BMA	W	2003	11/12	0.47	0.44	-	113,124,130,135	0
3	NAG	O	2002	14/15	0.88	0.26	-	61,90,101,113	0
3	BMA	U	2003	11/12	0.76	0.23	-	114,122,125,127	0
4	NAG	E	2004	14/15	0.90	0.20	-	126,134,144,151	0
3	NAG	K	2001	14/15	0.87	0.28	-	59,73,92,93	0
3	BMA	M	2003	11/12	0.65	0.21	-	102,115,128,131	0
4	NAG	a	2002	14/15	0.89	0.31	-	96,118,126,129	0
4	NAG	M	2004	14/15	0.85	0.12	-	128,145,151,160	0
4	NAG	S	2003	14/15	0.77	0.19	-	133,146,152,153	0
4	NAG	O	2004	14/15	0.84	0.18	-	142,148,151,153	0
3	BMA	C	2003	11/12	0.84	0.17	-	35,55,68,70	0
4	NAG	A	2004	14/15	0.82	0.20	-	104,114,123,124	0
4	NAG	U	2005	14/15	0.78	0.20	-	156,166,172,172	0
3	NAG	G	2002	14/15	0.90	0.24	-	53,70,85,96	0
4	NAG	G	2004	14/15	0.83	0.20	-	87,103,110,112	0
4	NAG	Q	2006	14/15	0.81	0.23	-	124,153,157,160	0
4	NAG	W	2005	14/15	0.86	0.21	-	139,152,158,160	0
6	NAG	Q	2002	14/15	0.91	0.21	-	94,99,105,115	0
6	MAN	Q	2004	11/12	0.70	0.29	-	111,129,131,135	0
6	BMA	Q	2003	11/12	0.79	0.18	-	116,120,126,127	0
4	NAG	O	2005	14/15	0.81	0.20	-	138,149,152,152	0
4	NAG	M	2005	14/15	0.75	0.26	-	137,162,176,177	0
3	BMA	I	2003	11/12	0.81	0.39	-	83,95,103,110	0
3	NAG	E	2002	14/15	0.71	0.26	-	79,102,115,117	0
3	NAG	A	2002	14/15	0.96	0.19	-	52,75,87,93	0
3	NAG	M	2001	14/15	0.94	0.16	-	42,57,74,81	0
3	NAG	C	2002	14/15	0.91	0.24	-	69,81,86,90	0
3	NAG	U	2002	14/15	0.82	0.22	-	95,102,117,127	0
4	NAG	W	2004	14/15	0.81	0.23	-	145,151,158,159	0
6	NAG	Q	2001	14/15	0.82	0.23	-	68,80,90,103	0
4	NAG	S	2002	14/15	0.70	0.25	-	96,108,125,129	0
4	NAG	Q	2005	14/15	0.90	0.13	-	122,138,141,145	0
3	NAG	M	2002	14/15	0.84	0.23	-	64,91,98,106	0
3	BMA	O	2003	11/12	0.78	0.14	-	102,115,125,130	0
4	NAG	S	2004	14/15	0.79	0.17	-	116,143,150,154	0
3	BMA	G	2003	11/12	0.75	0.30	-	80,97,103,107	0
3	NAG	K	2002	14/15	0.91	0.21	-	61,76,88,94	0
4	NAG	I	2005	14/15	0.83	0.14	-	109,125,128,129	0
4	NAG	G	2005	14/15	0.89	0.13	-	106,115,120,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	I	2004	14/15	0.82	0.20	-	94,108,117,122	0
4	NAG	E	2005	14/15	0.68	0.36	-	129,148,157,159	0
3	BMA	E	2003	11/12	0.74	0.20	-	43,57,80,88	0
4	NAG	U	2004	14/15	0.82	0.15	-	141,148,158,159	0
3	BMA	A	2003	11/12	0.83	0.23	-	65,90,98,98	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	c	2001	14/15	0.80	0.28	-0.31	94,106,117,123	0
5	NAG	c	2002	14/15	0.66	0.19	-	143,162,169,170	0
5	NAG	K	2004	14/15	0.88	0.10	-	127,140,146,149	0
5	NAG	Y	2003	14/15	0.65	0.27	-	149,160,166,170	0
5	NAG	O	2006	14/15	0.87	0.24	-	87,95,100,102	0

6.5 Other polymers [i](#)

There are no such residues in this entry.