



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:00 PM 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

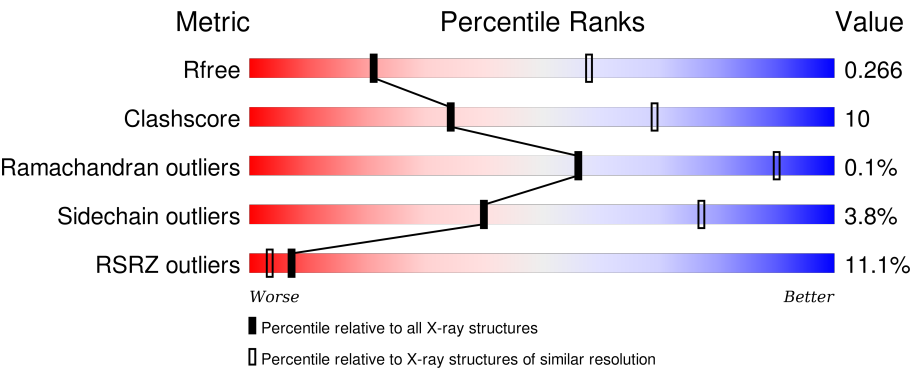
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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}	91344	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (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></div><div></div><div></div><div></div></div><div>57%36%. .</div></div>
1	C	334	<div><div>3%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>60%35%. .</div></div>
1	E	334	<div><div>4%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>69%25%. .</div></div>
1	G	334	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>65%30%. .</div></div>
1	I	334	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>72%21%. .</div></div>

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

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

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

2 Entry composition [i](#)

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		

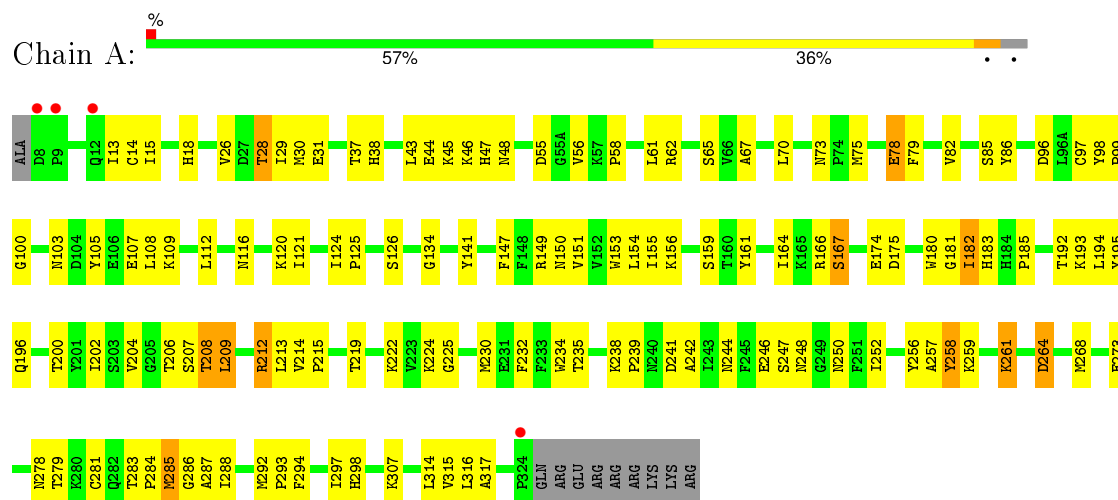
- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

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

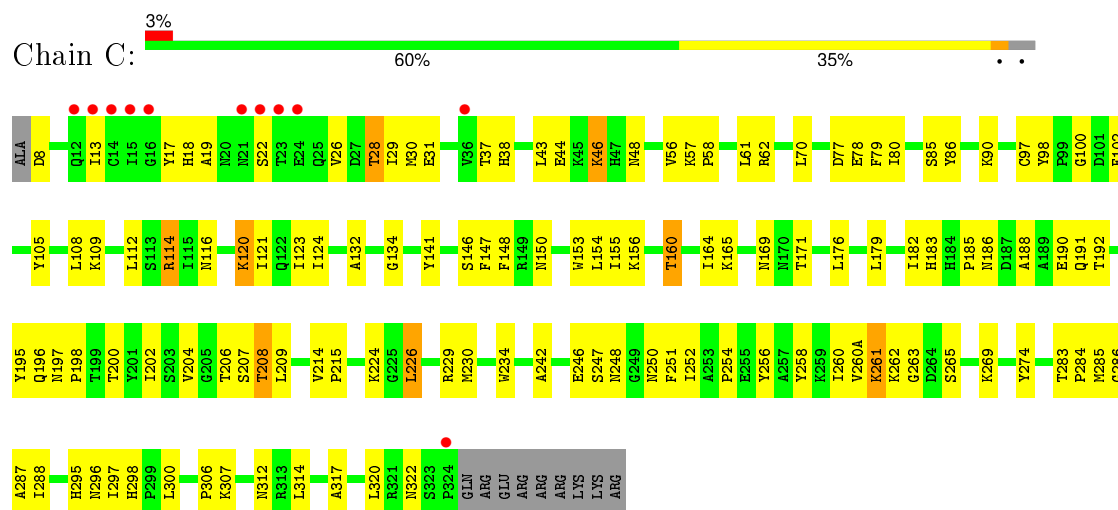
3 Residue-property plots

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

• Molecule 1: Hemagglutinin HA1 chain

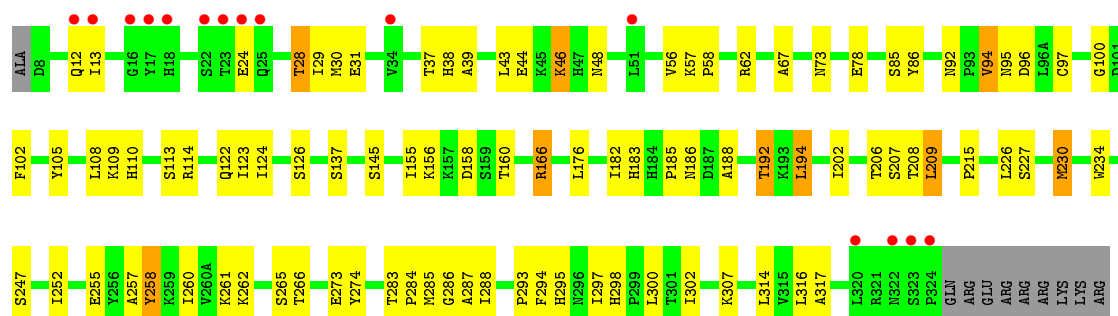


• Molecule 1: Hemagglutinin HA1 chain

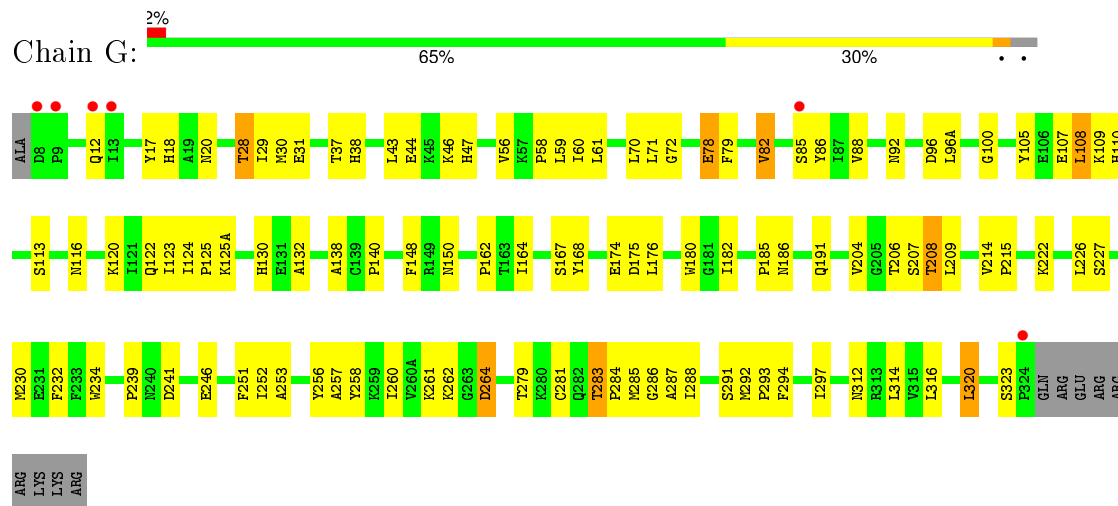


• Molecule 1: Hemagglutinin HA1 chain

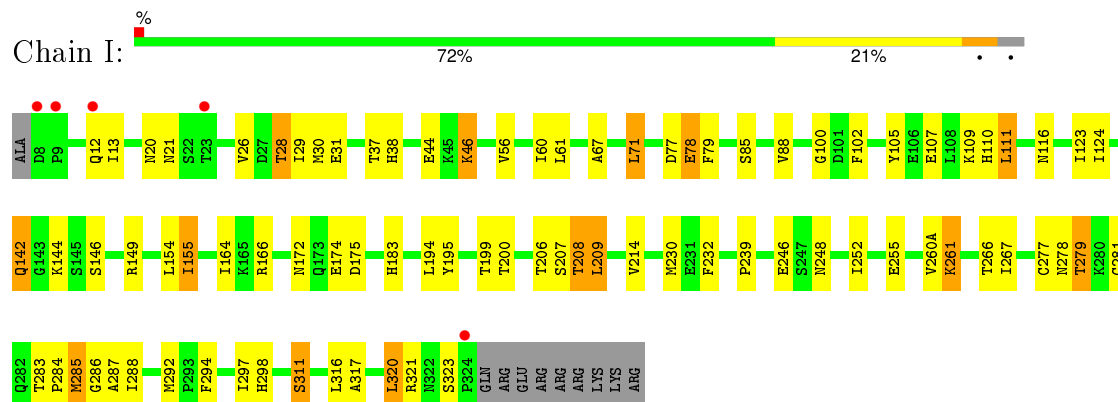




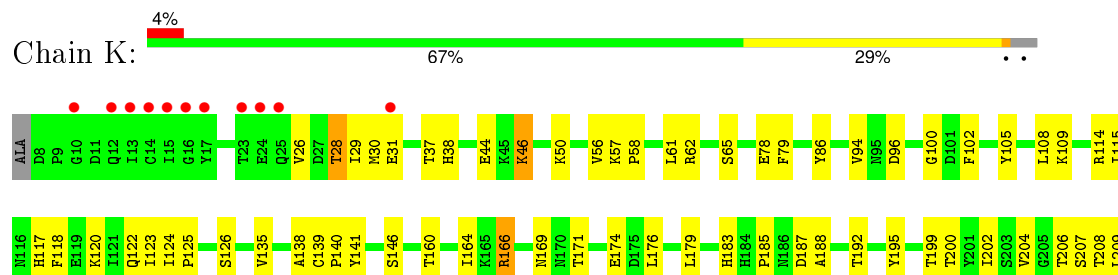
• Molecule 1: Hemagglutinin HA1 chain

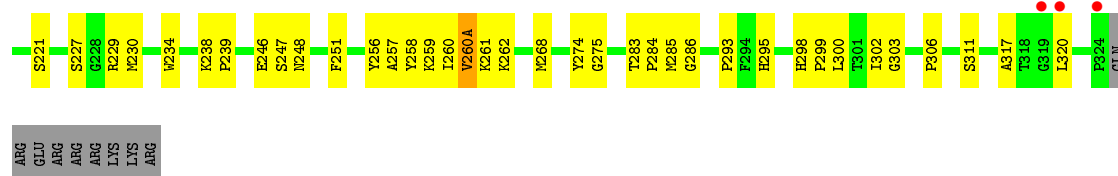


• Molecule 1: Hemagglutinin HA1 chain

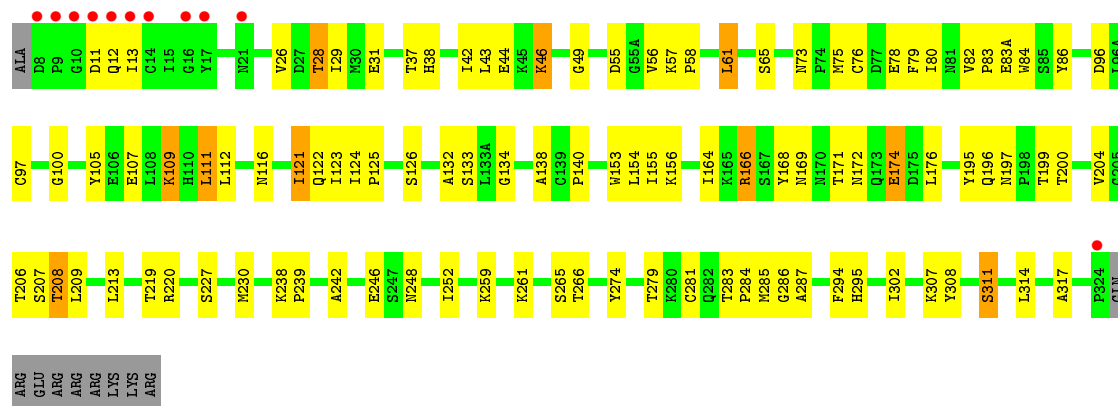


• Molecule 1: Hemagglutinin HA1 chain

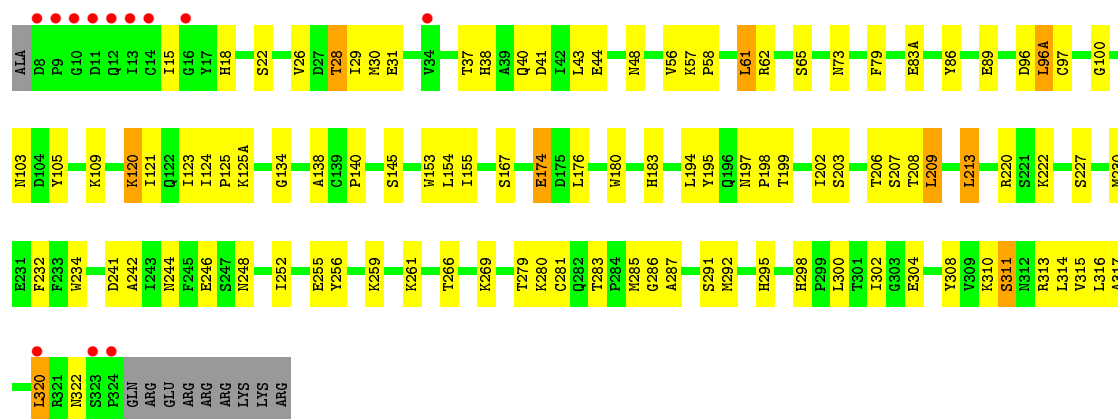




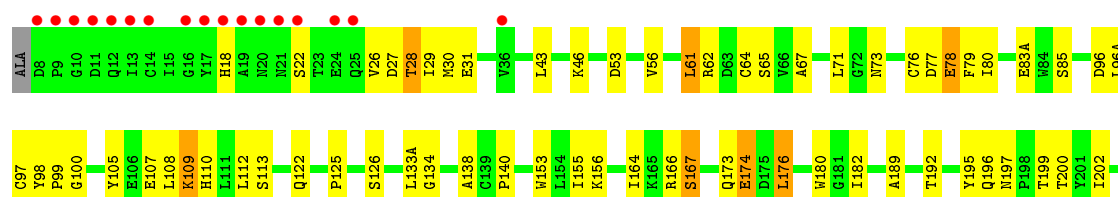
• Molecule 1: Hemagglutinin HA1 chain

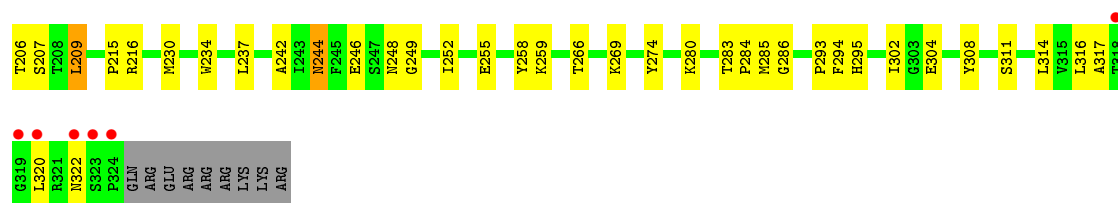


• Molecule 1: Hemagglutinin HA1 chain

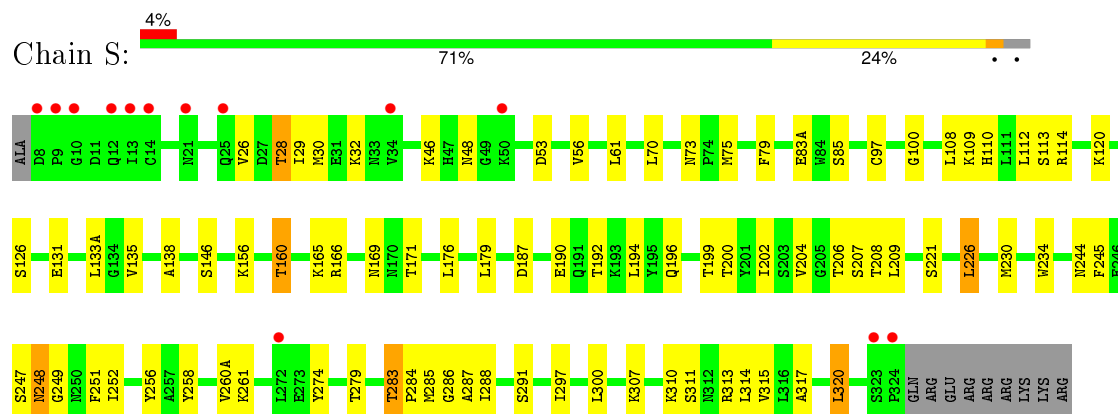


• Molecule 1: Hemagglutinin HA1 chain

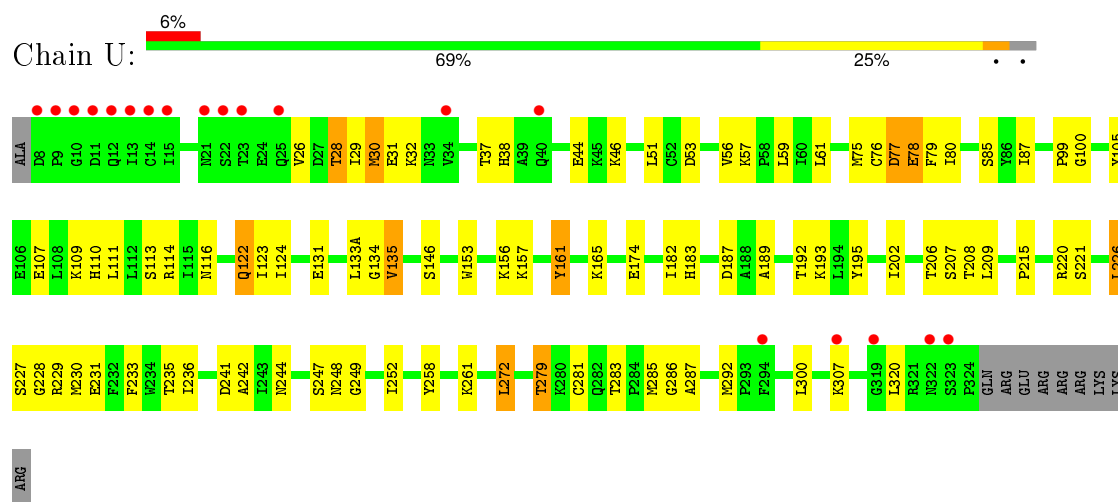




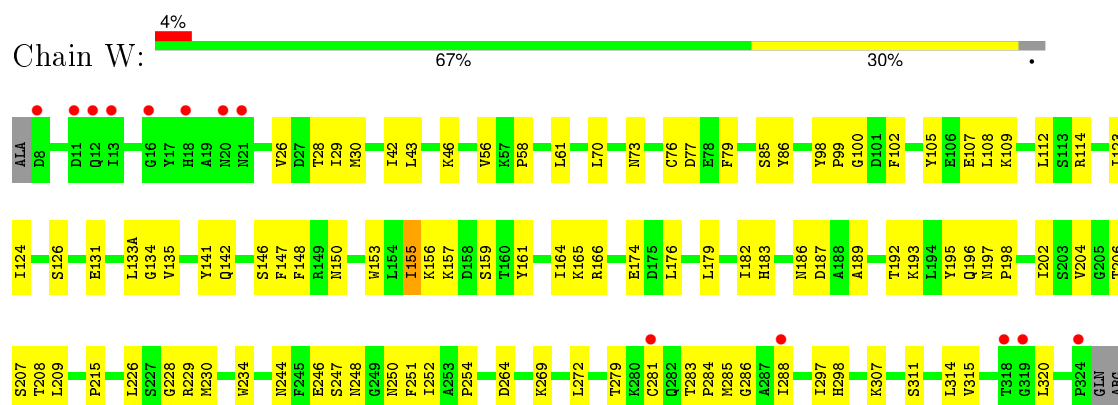
• Molecule 1: Hemagglutinin HA1 chain



• Molecule 1: Hemagglutinin HA1 chain

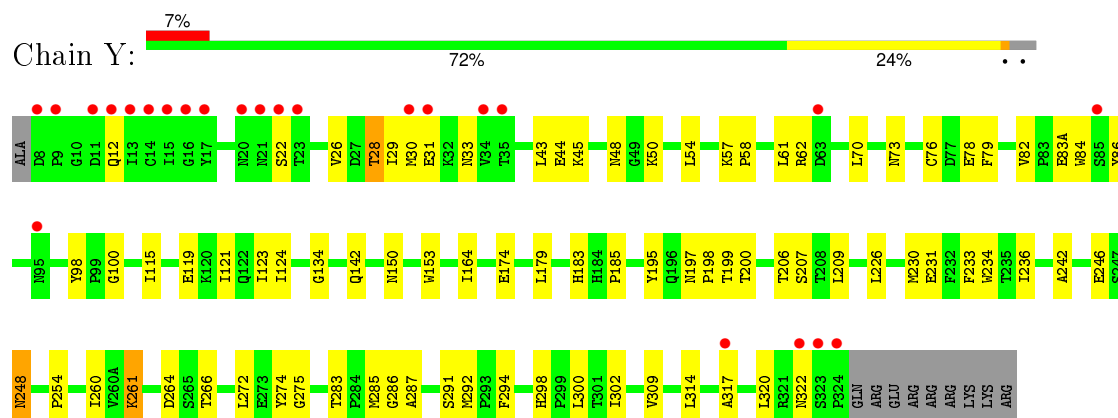


• Molecule 1: Hemagglutinin HA1 chain

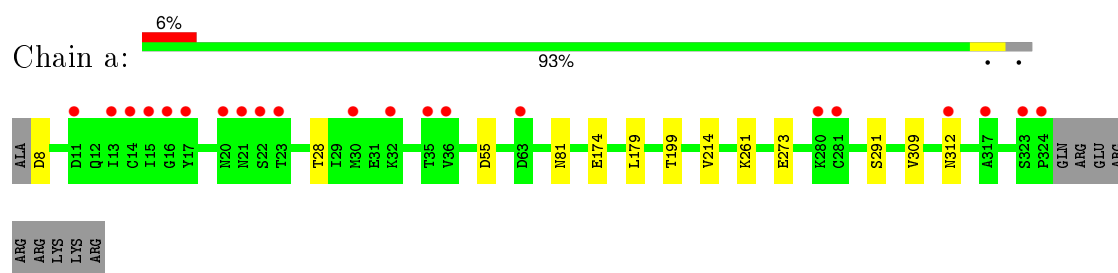


GLU
ARG
ARG
ARG
LYS
LYS
ARG

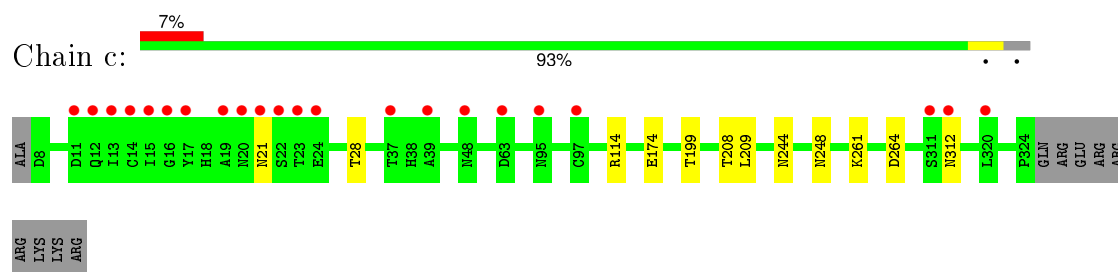
• Molecule 1: Hemagglutinin HA1 chain



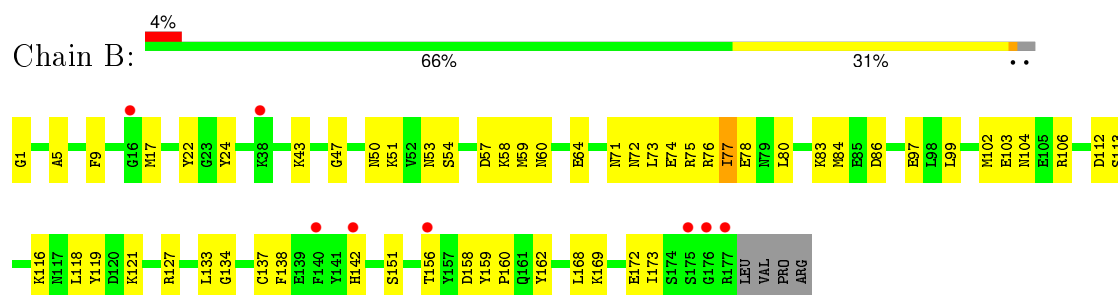
• Molecule 1: Hemagglutinin HA1 chain



• Molecule 1: Hemagglutinin HA1 chain

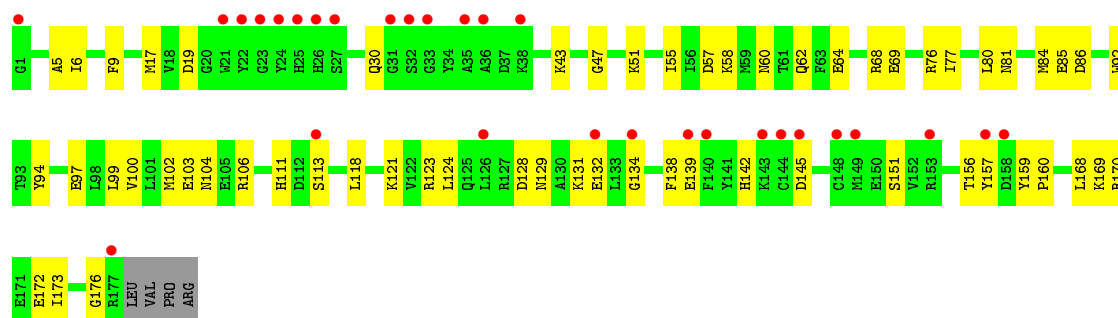


• Molecule 2: Hemagglutinin HA2 chain

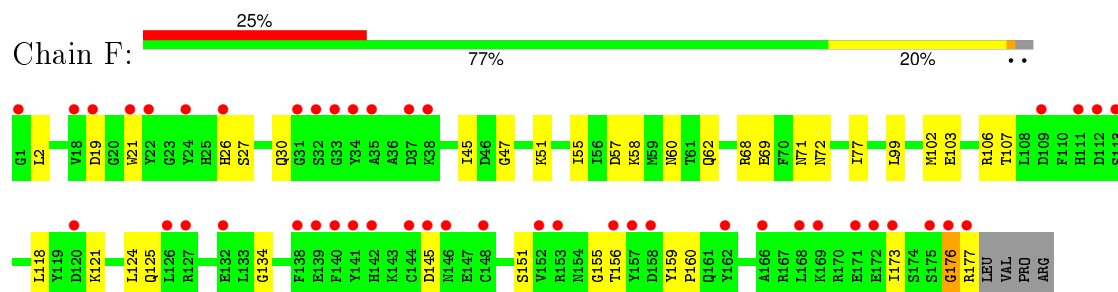


• Molecule 2: Hemagglutinin HA2 chain

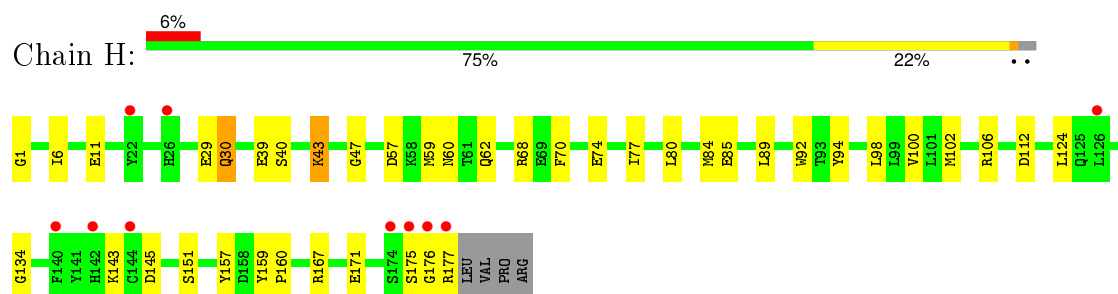




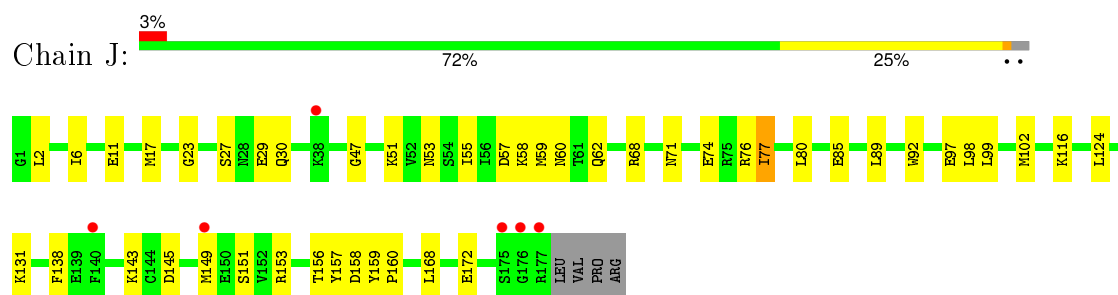
- Molecule 2: Hemagglutinin HA2 chain



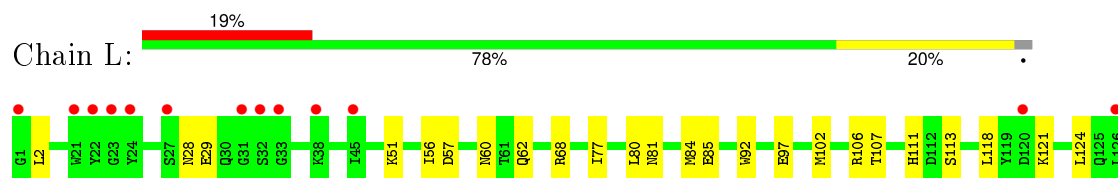
- Molecule 2: Hemagglutinin HA2 chain

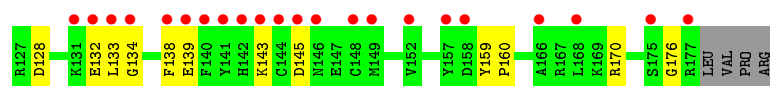


- Molecule 2: Hemagglutinin HA2 chain

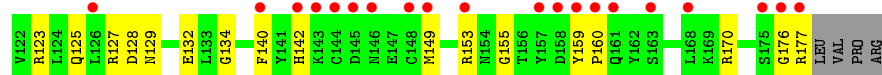
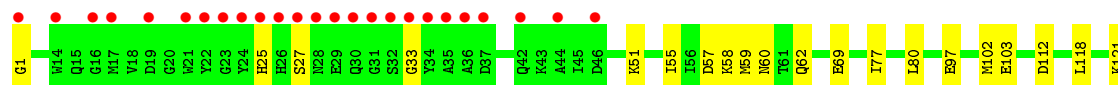
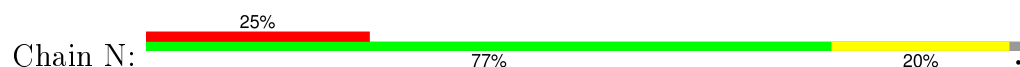


- Molecule 2: Hemagglutinin HA2 chain

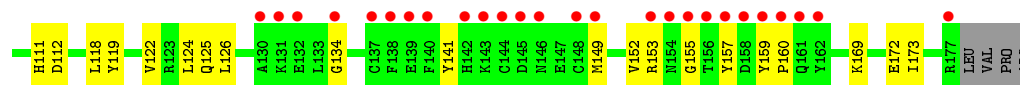
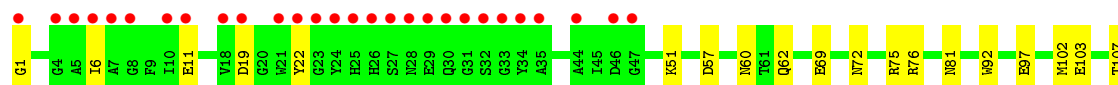
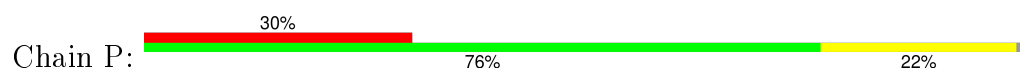




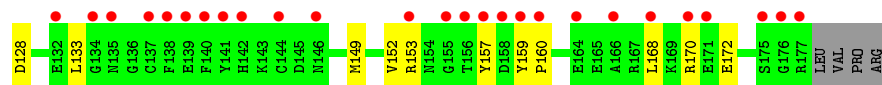
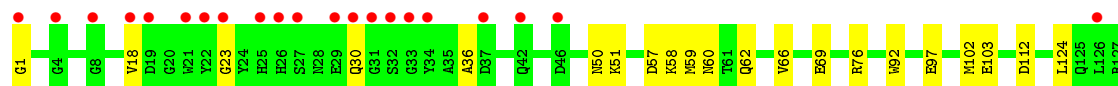
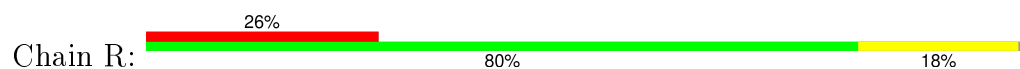
• Molecule 2: Hemagglutinin HA2 chain



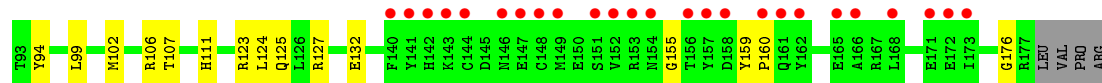
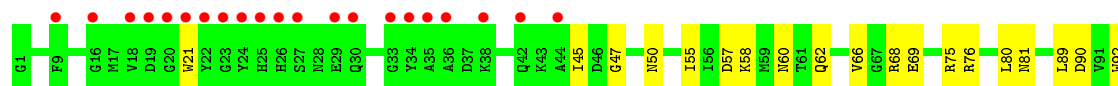
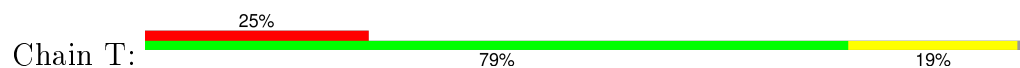
• Molecule 2: Hemagglutinin HA2 chain



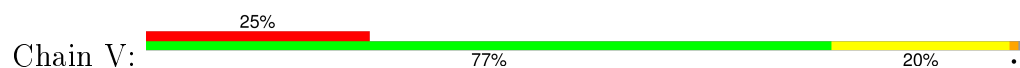
• Molecule 2: Hemagglutinin HA2 chain

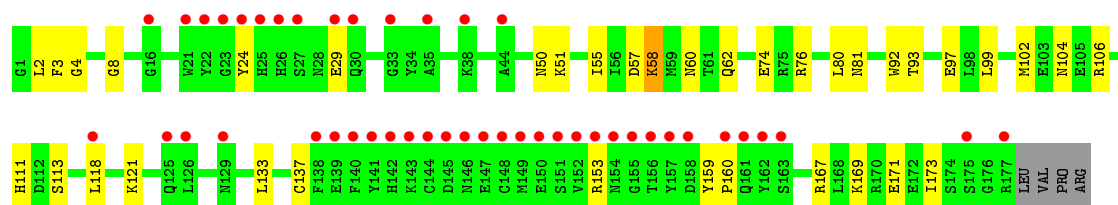


• Molecule 2: Hemagglutinin HA2 chain

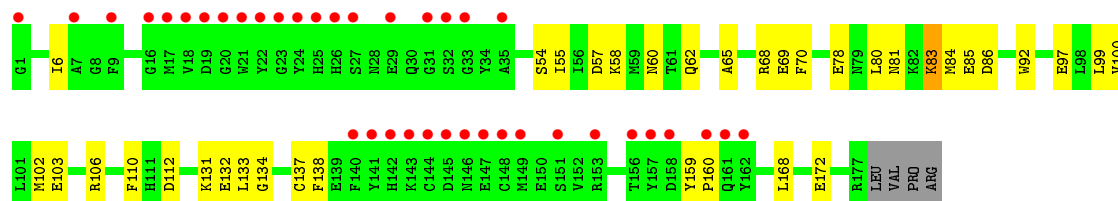
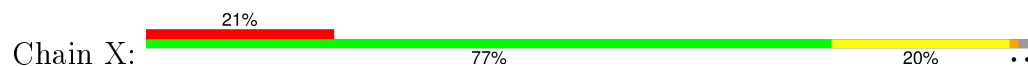


• Molecule 2: Hemagglutinin HA2 chain

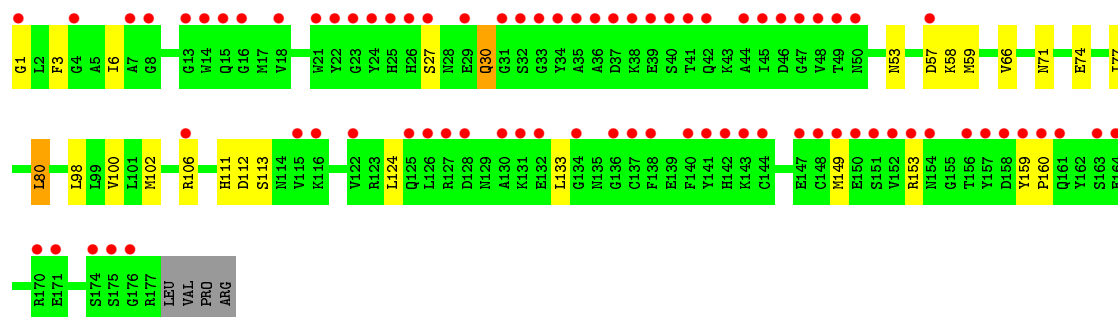
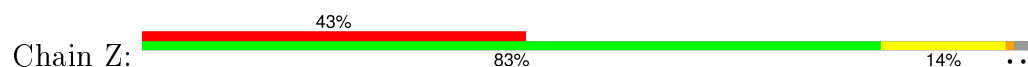




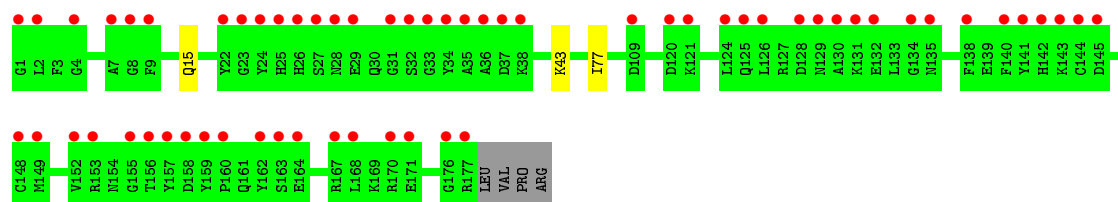
• Molecule 2: Hemagglutinin HA2 chain



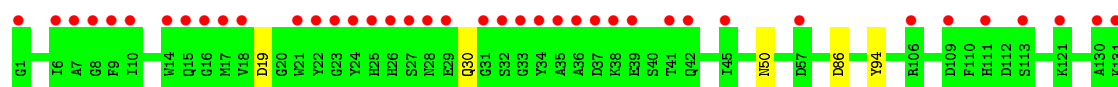
• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



• Molecule 2: Hemagglutinin HA2 chain



E132	E133	G134	N135	G136	G137	F138	E139	F140	Y141	H142	K143	G144	C148	M149	E150	S151	V152	R153	N154	G155	T156	Y157	D158	Y159	P160	Q161	Y162	S163	E164	E165	A166	R167	L168	K169	R170	E171	E172	I173	R177	LEU	VAL	PRO	ARG
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----

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 0.219 , 0.266	Depositor DCC
R_{free} test set	9996 reflections (5.27%)	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 , 67.0	EDS
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
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 199723 reflections	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.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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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
2:R:51:LYS:HD3	2:R:103:GLU:HB3	1.54	0.88
1:G:283:THR:HG22	1:G:285:MET:H	1.35	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
1:Y:29:ILE:HD11	2:Z:102:MET:HG2	1.63	0.79
2:B:134:GLY:HA2	2:D:124:LEU:HD22	198.29	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:206:THR:HG22	1:U:208:THR:H	1.51	0.76
1:U:131:GLU:HB3	1:U:133(A):LEU:HD23	1.67	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: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
2:H:29:GLU:OE1	2:H:143:LYS:NZ	2.20	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:Q:283:THR:HB	1:Q:286:GLY:O	1.92	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:S:206:THR:HB	1:S:209:LEU:H	1.57	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:Q:62:ARG:NH2	1:Q:78:GLU:OE2	2.25	0.69
1:K:283:THR:HB	1:K:286:GLY:O	1.93	0.68
2:D:106:ARG:HG2	2:F:106:ARG:HH22	1.58	0.68
1:M:100:GLY:HA3	1:M:230:MET:O	1.93	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:C:29:ILE:HD11	2:D:102:MET:HG2	1.75	0.68
1:Y:61:LEU:HA	1:Y:79:PHE:CZ	2.29	0.68
1:E:192:THR:HG21	1:U:192:THR:HG21	1.74	0.68
1:S:29:ILE:HD11	2:T:102:MET:HG2	1.74	0.68
4:A:2004:NAG:H4	4:A:2005:NAG:H4	1.76	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:G:175:ASP:OD1	1:G:239:PRO:HD3	1.95	0.67
1:E:73:ASN:HD21	1:E:97:CYS:HB3	1.59	0.67
1:A:206:THR:HB	1:A:209:LEU: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
1:I:279:THR:HB	1:I:281:CYS:H	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:81:ASN:ND2	2:X:80:LEU:HD13	2.10	0.66
1:O:230:MET:SD	1:O:252:ILE:HD11	2.35	0.66
1:A:206:THR:HG22	1:A:208:THR:H	1.60	0.66
1:O:283:THR:HB	1:O:286:GLY:O	1.94	0.66
2:D:97:GLU:OE1	2:Z:58:LYS:NZ	185.86	0.66
1:A:116:ASN:HB2	1:A:261:LYS:HG3	1.75	0.66
2:T:68:ARG:NH1	2:T:81:ASN:HD21	1.92	0.66
1:A:183:HIS:ND1	1:A:195:TYR:OH	2.25	0.66
2:P:134:GLY:HA2	2:R:124:LEU:HD22	1.78	0.66
1:C:183:HIS:ND1	1:C:195:TYR:OH	2.28	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
2:X:68:ARG:NH1	2:X:81:ASN:HD21	1.93	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
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:C:288:ILE:HD11	1:C:297:ILE:HG13	1.78	0.65
1:A:61:LEU:HA	1:A:79:PHE:CZ	2.38	0.65
1:Y:62:ARG:NH1	1:Y:78:GLU:OE2	2.30	0.65
1:K:58:PRO:HB3	1:K:86:TYR:CE1	2.32	0.64
2:D:19:ASP:OD1	2:D:19:ASP:N	2.87	0.64
1:U:135:VAL:HG23	1:U:146:SER:HA	1.77	0.64
1:A:294:PHE:HZ	2:B:59:MET:HG3	1.63	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
1:M:283:THR:HB	1:M:286:GLY:O	1.97	0.64
2:B:106:ARG:HH11	2:H:106:ARG:HH12	1.45	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:E:260:ILE:HG21	1:E:262:LYS:HE3	1.81	0.63
2:D:57:ASP:O	2:D:60:ASN:HB2	1.98	0.63
1:C:28:THR:HG22	1:C:31:GLU:H	1.62	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:O:183:HIS:ND1	1:O:195:TYR:OH	2.26	0.63
1:I:183:HIS:ND1	1:I:195:TYR:OH	2.29	0.63
1:E:206:THR:HG22	1:E:208:THR:H	1.63	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
1:W:61:LEU:HA	1:W:79:PHE:CZ	2.34	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
2:D:169:LYS:HE3	2:D:173:ILE:HD11	1.81	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
1:A:100:GLY:HA3	1:A:230:MET:O	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:Y:22:SER:O	1:Y:322:ASN:ND2	2.32	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: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:Y:83(A):GLU:OE2	1:Y:261:LYS:NZ	2.32	0.62
1:I:37:THR:HG22	1:I:38:HIS:CD2	2.35	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:283:THR:HG22	1:G:285:MET:N	2.13	0.61
1:G:279:THR:HB	1:G:281:CYS:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:83(A):GLU:OE1	1:S:261:LYS:NZ	2.34	0.61
1:I:100:GLY:HA3	1:I:230:MET:O	2.01	0.61
1:C:43:LEU:HB2	1:C:314:LEU:HB2	1.82	0.61
1:O:109:LYS:NZ	2:P:69:GLU:OE2	2.30	0.61
1:K:206:THR:HG22	1:K:208:THR:H	1.64	0.61
1:Q:134:GLY:HA3	1:Q:153:TRP:HB3	1.83	0.60
2:B:5:ALA:HB2	2:B:116:LYS:HB2	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
1:O:174:GLU:HG3	1:O:259:LYS:HB3	1.82	0.60
2:F:118:LEU:HD12	2:F:121:LYS:HD3	1.84	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:Y:283:THR:HB	1:Y:286:GLY:O	2.02	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: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:Q:206:THR:HG22	1:Q:207:SER:N	2.18	0.59
1:E:122:GLN:NE2	1:E:255:GLU:OE2	2.36	0.59
1:Q:61:LEU:HA	1:Q:79:PHE:CZ	2.38	0.59
1:O:206:THR:HB	1:O:209:LEU:H	1.68	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:S:29:ILE:HG22	2:V:51:LYS:HG3	1.85	0.59
1:S:307:LYS:NZ	2:T:60:ASN:O	2.36	0.59
1:W:29:ILE:HD11	2:X:102:MET:HG2	1.84	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:A:212:ARG:HG2	1:A:212:ARG:HH11	1.68	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
1:Q:266:THR:HG22	1:Q:302:ILE:HD12	1.85	0.58
2:D:128:ASP:O	2:D:170:ARG:NH1	2.35	0.58
1:O:22:SER:O	1:O:322:ASN:ND2	2.37	0.58
1:M:206:THR:HG22	1:M:208:THR:H	1.68	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:O:100:GLY:HA3	1:O:230:MET:O	2.03	0.58
1:K:206:THR:HB	1:K:209:LEU:H	1.68	0.58
1:A:108:LEU:HB2	1:A:234:TRP:CZ2	2.39	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:B:169:LYS:HE3	2:B:173:ILE:HD11	1.84	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:K:44:GLU:OE1	1:K:46:LYS:HG3	2.04	0.57
1:I:28:THR:HG22	1:I:31:GLU:H	1.70	0.57
1:C:283:THR:HG22	1:C:285:MET:N	2.11	0.57
2:B:97:GLU:OE1	2:D:58:LYS:NZ	126.87	0.57
1:G:283:THR:CG2	1:G:285:MET:H	2.15	0.57
1:W:29:ILE:HD11	2:X:102:MET:HA	1.85	0.57
1:Q:138:ALA:O	1:Q:140:PRO:HD3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:116:ASN:HB2	1:M:261:LYS:HG3	1.87	0.57
2:H:40:SER:HA	2:H:43:LYS:HB2	1.86	0.57
1:G:204:VAL:HG12	1:G:209:LEU:HD23	1.87	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:59:LEU:HD22	1:G:82:VAL:HG11	1.86	0.57
1:G:28:THR:HG22	1:G:31:GLU:H	1.70	0.56
1:G:316:LEU:HD23	2:H:100:VAL:HG13	1.86	0.56
1:C:18:HIS:ND1	2:D:17:MET:O	3.09	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:S:221:SER:HB2	1:U:207:SER:HA	1.87	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:A:58:PRO:HB3	1:A:86:TYR:CE1	2.39	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
2:V:55:ILE:HG12	2:V:99:LEU:HD21	1.88	0.56
2:F:51:LYS:HD3	2:F:103:GLU:HB3	1.88	0.56
1:A:55:ASP:O	1:A:278:ASN:ND2	3.14	0.56
1:I:279:THR:HG21	1:I:287:ALA:HB1	1.88	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:A:193:LYS:HG2	1:A:194:LEU:HD23	1.87	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
2:J:77:ILE:HA	2:J:80:LEU:HB3	1.88	0.55
2:X:6:ILE:HG13	2:X:112:ASP:HA	1.87	0.55
1:S:288:ILE:HD11	1:S:297:ILE:HG13	1.88	0.55
1:G:78:GLU:O	1:G:78:GLU:HG3	2.05	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:U:221:SER:HB2	1:W:207:SER:HA	1.89	0.55
1:M:156:LYS:HD2	1:M:196:GLN:HB2	1.88	0.55
1:K:320:LEU:HB3	2:L:111:HIS:CG	2.40	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: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:Q:167:SER:HB2	1:Q:244:ASN:CB	2.37	0.55
1:M:83(A):GLU:OE1	1:M:261:LYS:NZ	2.40	0.55
1:K:57:LYS:HE2	1:K:274:TYR:HE2	1.72	0.55
1:I:60:ILE:HG12	1:I:88:VAL:HB	1.89	0.55
1:S:61:LEU:HA	1:S:79:PHE:HZ	1.72	0.54
1:M:29:ILE:HD11	2:N:102:MET:HA	1.88	0.54
1:C:269:LYS:HE3	2:D:69:GLU:OE2	3.30	0.54
2:D:113:SER:OG	2:L:2:LEU:O	2.24	0.54
1:E:307:LYS:HB3	2:F:62:GLN:NE2	2.23	0.54
1:M:58:PRO:HB3	1:M:86:TYR:CE1	2.41	0.54
1:A:44:GLU:HB2	1:A:292:MET:HG3	1.88	0.54
1:K:183:HIS:O	1:K:185:PRO:HD3	2.08	0.54
1:Q:67:ALA:HB3	1:Q:96:ASP:OD1	2.07	0.54
1:O:18:HIS:HD2	1:O:37:THR:HG21	1.72	0.54
1:Q:107:GLU:HG2	2:P:76:ARG:HH21	1.73	0.54
1:M:279:THR:HG21	1:M:287:ALA:HB1	1.88	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
1:Q:283:THR:HG23	1:Q:284:PRO:HD2	1.88	0.54
2:B:58:LYS:NZ	2:J:97:GLU:OE1	2.36	0.54
1:S:247:SER:OG	1:S:248:ASN:N	2.37	0.54
1:Q:182:ILE:HD11	1:Q:215:PRO:HD3	1.90	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:W:126:SER:HB2	1:W:166:ARG:HH22	1.72	0.53
1:Q:295:HIS:CE1	1:Q:308:TYR:HD1	2.26	0.53
1:W:206:THR:HG22	1:W:207:SER:N	2.23	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
2:X:133:LEU:HD12	2:X:137:CYS:HB2	1.89	0.53
1:G:279:THR:HG21	1:G:287:ALA:HB1	1.89	0.53
1:A:43:LEU:HD23	1:A:45:LYS:HE3	2.66	0.53
1:I:311:SER:HB3	2:J:97:GLU:OE2	2.08	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: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:G:56:VAL:HB	1:G:85:SER:HB3	1.89	0.53
1:Q:195:TYR:O	1:Q:197:ASN:N	2.37	0.53
1:O:40:GLN:NE2	1:O:41:ASP:O	2.42	0.53
1:M:138:ALA:O	1:M:140:PRO:HD3	2.09	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:O:37:THR:HG22	1:O:38:HIS:CD2	2.44	0.53
1:G:61:LEU:HA	1:G:79:PHE:CZ	2.43	0.53
1:G:44:GLU:HB2	1:G:292:MET:HG3	1.90	0.53
1:W:42:ILE:HG13	1:W:314:LEU:HB3	1.90	0.53
1:M:73:ASN:HD21	1:M:97:CYS:HB3	1.74	0.53
1:I:78:GLU:HG3	1:I:78:GLU:O	2.05	0.53
1:K:200:THR:HA	1:K:248:ASN:OD1	2.08	0.53
2:B:74:GLU:HB3	2:B:77:ILE:HD12	5.32	0.53
1:K:123:ILE:HG13	1:K:124:ILE:HG13	1.90	0.53
1:M:26:VAL:HG11	1:M:317:ALA:HB2	1.89	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
2:B:159:TYR:HB3	2:B:160:PRO:HD3	1.91	0.53
1:W:26:VAL:HG12	1:W:315:VAL:HG12	1.90	0.53
1:G:206:THR:HB	1:G:209:LEU:HB2	1.91	0.53
2:T:68:ARG:HH22	2:X:83:LYS:HZ2	1.55	0.53
1:U:28:THR:HG22	1:U:31:GLU:H	1.73	0.53
1:G:164:ILE:O	1:G:246:GLU:HA	2.09	0.53
2:B:1:GLY:HA3	2:B:112:ASP:OD2	2.09	0.53
1:K:260:ILE:HG21	1:K:262:LYS:HE3	1.90	0.52
1:I:67:ALA:O	1:I:71:LEU:HD12	2.09	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
2:D:68:ARG:NH1	2:D:81:ASN:HD21	2.89	0.52
1:M:279:THR:HB	1:M:281:CYS:H	1.73	0.52
1:A:65:SER:OG	1:A:96:ASP:OD1	2.29	0.52
1:S:187:ASP:OD1	1:S:190:GLU:N	2.25	0.52
1:A:48:ASN:HD21	1:A:287:ALA:HB3	2.45	0.52
4:I:2004:NAG:H4	4:I:2005:NAG:H4	1.90	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:Q:73:ASN:ND2	1:Q:97:CYS:HB3	2.24	0.52
1:M:123:ILE:O	1:M:124:ILE:HG13	2.10	0.52
1:G:70:LEU:O	1:G:150:ASN:ND2	2.41	0.52
1:M:220:ARG:HD2	1:M:227:SER:O	2.09	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:S:176:LEU:HD23	1:S:258:TYR:O	2.10	0.52
1:K:122:GLN:NE2	1:K:125:PRO:HA	2.24	0.52
1:E:182:ILE:HD11	1:E:215:PRO:HD3	1.91	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:L:159:TYR:HB3	2:L:160:PRO:HD3	1.92	0.52
2:B:127:ARG:HD2	2:J:131:LYS:NZ	2.25	0.52
1:Y:266:THR:HG22	1:Y:302:ILE:HD12	1.92	0.52
1:W:206:THR:HB	1:W:209:LEU:HB2	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:V:159:TYR:HB3	2:V:160:PRO:HD3	1.92	0.52
2:L:84:MET:HE1	2:L:85:GLU:HG2	1.92	0.52
2:X:57:ASP:O	2:X:60:ASN:HB2	2.11	0.51
1:A:37:THR:HG22	1:A:38:HIS:CD2	2.45	0.51
1:I:71:LEU:HD11	1:I:102:PHE:CE2	2.45	0.51
1:A:13:ILE:HG22	2:B:138:PHE:HB2	2.44	0.51
1:Y:28:THR:HG22	1:Y:31:GLU:H	1.75	0.51
1:S:317:ALA:O	2:T:107:THR:HG21	2.11	0.51
1:A:288:ILE:HD11	1:A:297:ILE:HG13	2.25	0.51
1:M:266:THR:HG22	1:M:302:ILE:HD12	1.92	0.51
1:C:314:LEU:HD21	2:D:97:GLU:HA	2.43	0.51
1:K:206:THR:HG22	1:K:207:SER:N	2.25	0.51
1:C:48:ASN:ND2	1:C:287:ALA:HB3	2.30	0.51
1:O:83(A):GLU:OE2	1:O:261:LYS:NZ	2.41	0.51
2:F:30:GLN:HE22	2:F:145:ASP:HA	1.75	0.51
2:D:159:TYR:HB3	2:D:160:PRO:HD3	1.94	0.51
2:L:62:GLN:HG3	2:L:92:TRP:CG	2.45	0.51
1:E:283:THR:HG23	1:E:284:PRO:HD2	1.92	0.51
1:E:100:GLY:HA3	1:E:230:MET:O	2.10	0.51
2:T:21:TRP:CZ3	2:T:45:ILE:HG13	2.46	0.51
2:B:51:LYS:HD3	2:B:103:GLU:HB3	2.32	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
1:U:220:ARG:HD2	1:U:227:SER:O	2.10	0.51
2:N:134:GLY:HA2	2:P:124:LEU:HD22	1.93	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:283:THR:HG22	1:K:285:MET:N	2.17	0.51
1:K:176:LEU:HD22	1:K:257:ALA:HB1	1.93	0.51
2:T:106:ARG:HG3	2:V:106:ARG:HH22	1.76	0.51
1:K:141:TYR:HE2	1:O:62:ARG:HH21	1.57	0.51
1:O:154:LEU:O	1:O:155:ILE:HG13	2.10	0.51
1:C:154:LEU:O	1:C:155:ILE:HG13	2.10	0.51
1:U:110:HIS:O	1:U:113:SER:OG	2.28	0.51
1:O:203:SER:OG	1:O:246:GLU:HB3	2.11	0.51
1:I:175:ASP:OD1	1:I:239:PRO:HD3	2.11	0.51
1:M:12:GLN:HB2	2:N:27:SER:HB3	1.92	0.51
1:Q:26:VAL:HG11	1:Q:317:ALA:HB2	1.93	0.51
1:I:29:ILE:HD11	2:J:102:MET:HA	1.93	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
2:X:62:GLN:NE2	2:X:92:TRP:HB3	2.26	0.50
1:K:37:THR:HG22	1:K:38:HIS:CD2	2.46	0.50
1:C:182:ILE:HD11	1:C:215:PRO:HD3	1.91	0.50
1:M:109:LYS:NZ	2:N:69:GLU:OE2	2.44	0.50
1:Q:230:MET:SD	1:Q:252:ILE:HD11	2.51	0.50
1:Q:206:THR:HG22	1:Q:207:SER:H	1.74	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:A:97:CYS:HA	1:A:224:LYS:NZ	2.92	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:K:299:PRO:HG2	1:K:300:LEU:HD12	1.94	0.50
1:Y:33:ASN:ND2	5:Y:2003:NAG:O7	2.44	0.50
1:A:14:CYS:O	2:B:24:TYR:HA	2.11	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:W:288:ILE:HD11	1:W:297:ILE:HG13	1.94	0.50
1:U:134:GLY:HA3	1:U:153:TRP:HB3	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
2:N:58:LYS:NZ	2:R:97:GLU:OE1	2.45	0.50
1:K:141:TYR:HE2	1:O:62:ARG:NH2	2.10	0.50
2:R:23:GLY:HA3	2:R:36:ALA:HA	1.93	0.50
1:E:108:LEU:HB2	1:E:234:TRP:CE2	2.47	0.50
1:S:156:LYS:HD2	1:S:196:GLN:HB2	1.94	0.50
1:A:156:LYS:NZ	1:A:192:THR:O	2.64	0.50
1:E:12:GLN:N	2:F:27:SER:O	2.41	0.49
2:B:106:ARG:HH22	2:Z:106:ARG:CG	89.41	0.49
1:E:206:THR:HG22	1:E:207:SER:N	2.27	0.49
1:A:73:ASN:ND2	1:A:97:CYS:HB3	2.26	0.49
2:T:94:TYR:CE2	2:V:58:LYS:HB3	2.47	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
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:Y:48:ASN:HD21	1:Y:287:ALA:HB3	1.77	0.49
1:M:206:THR:HB	1:M:209:LEU:H	1.77	0.49
2:X:132:GLU:HG3	2:X:138:PHE:HE1	1.77	0.49
1:U:182:ILE:HD11	1:U:215:PRO:HD3	1.94	0.49
1:C:164:ILE:O	1:C:246:GLU:HA	2.34	0.49
1:E:298:HIS:HE1	1:E:300:LEU:HD12	1.76	0.49
2:D:131:LYS:N	2:D:139:GLU:O	2.38	0.49
1:O:103:ASN:HB2	1:O:232:PHE:O	2.12	0.49
1:A:134:GLY:HA3	1:A:153:TRP:HB3	2.11	0.49
1:S:48:ASN:HD21	1:S:287:ALA:HB3	1.76	0.49
1:C:260:ILE:HG21	1:C:262:LYS:HE3	1.95	0.49
2:J:159:TYR:HB3	2:J:160:PRO:HD3	1.94	0.49
1:W:284:PRO:HG2	1:W:298:HIS:CE1	2.47	0.49
1:G:206:THR:HG22	1:G:207:SER:N	2.27	0.49
1:W:131:GLU:OE2	1:W:157:LYS:HG3	2.12	0.49
1:U:320:LEU:HB3	2:V:111:HIS:CG	2.47	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:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:204:VAL:HG22	1:S:245:PHE:HD1	1.77	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:I:30:MET:HG2	2:B:47:GLY:O	2.12	0.49
1:M:116:ASN:HB2	1:M:261:LYS:CG	2.43	0.49
1:K:100:GLY:HA3	1:K:230:MET:O	2.13	0.49
1:C:57:LYS:HE2	1:C:274:TYR:CE2	2.48	0.49
1:U:122:GLN:HB2	1:U:122:GLN:HE21	1.39	0.49
2:J:51:LYS:O	2:J:55:ILE:HD12	2.12	0.49
1:E:137:SER:HA	1:E:145:SER:CB	2.42	0.49
2:V:62:GLN:HG3	2:V:92:TRP:CG	2.48	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
1:G:58:PRO:HB3	1:G:86:TYR:CE1	2.47	0.49
1:U:206:THR:HB	1:U:209:LEU:N	2.22	0.49
1:A:182:ILE:HD12	1:A:202:ILE:HD12	1.95	0.49
1:W:43:LEU:HB2	1:W:314:LEU:HB2	1.95	0.49
2:B:133:LEU:HD12	2:B:137:CYS:HB2	2.47	0.49
1:Q:189:ALA:HA	1:Q:192:THR:HG22	1.95	0.49
1:C:134:GLY:HA3	1:C:153:TRP:HB3	2.33	0.49
1:K:58:PRO:HB3	1:K:86:TYR:CZ	2.48	0.48
1:Y:50:LYS:HD3	1:Y:275:GLY:CA	2.42	0.48
2:V:4:GLY:O	2:V:8:GLY:HA3	2.12	0.48
1:I:123:ILE:HG13	1:I:124:ILE:HG13	1.95	0.48
2:N:159:TYR:HB3	2:N:160:PRO:HD3	1.94	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
1:Q:78:GLU:O	1:Q:78:GLU:HG3	2.10	0.48
1:E:29:ILE:HG22	2:L:51:LYS:HG3	1.96	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
4:W:2004:NAG:H3	4:W:2005:NAG:O7	2.14	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
2:L:84:MET:CE	2:L:85:GLU:HG2	2.43	0.48
1:G:138:ALA:HB2	1:G:226:LEU:HD12	1.95	0.48
1:I:56:VAL:HB	1:I:85:SER:HB3	1.94	0.48
1:G:72:GLY:O	1:G:148:PHE:HA	2.14	0.48
1:Q:164:ILE:O	1:Q:246:GLU:HA	2.13	0.48
1:E:109:LYS:NZ	2:F:69:GLU:OE2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:98:TYR:CD1	1:W:99:PRO:HD2	2.48	0.48
2:V:169:LYS:HE3	2:V:173:ILE:HD11	1.94	0.48
2:N:57:ASP:O	2:N:60:ASN:HB2	2.13	0.48
1:I:78:GLU:HG2	1:I:79:PHE:CE2	2.48	0.48
1:C:100:GLY:HA3	1:C:230:MET:O	2.13	0.48
1:C:43:LEU:HD21	1:C:296:ASN:HD22	3.47	0.48
1:C:108:LEU:HB2	1:C:234:TRP:CE2	2.48	0.48
1:Y:195:TYR:O	1:Y:197:ASN:N	2.43	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:O:48:ASN:ND2	1:O:287:ALA:HB3	2.28	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: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:293:PRO:HG2	1:A:294:PHE:HD1	5.00	0.48
1:M:58:PRO:HB3	1:M:86:TYR:CZ	2.49	0.48
1:A:164:ILE:O	1:A:246:GLU:HA	2.14	0.48
1:I:320:LEU:HD12	1:I:321:ARG:N	2.28	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:206:THR:HG22	1:A:207:SER:N	2.29	0.47
1:A:182:ILE:HG13	1:A:183:HIS: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:65:SER:OG	1:Q:96:ASP:HA	2.14	0.47
1:Q:126:SER:HB2	1:Q:166:ARG:HH22	1.78	0.47
2:T:159:TYR:HB3	2:T:160:PRO:HD3	1.96	0.47
1:C:204:VAL:HG12	1:C:209:LEU:HD23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:ALA:H	3:A:2001:NAG:H82	2.66	0.47
1:M:123:ILE:C	1:M:124:ILE:HG13	2.34	0.47
1:O:120:LYS:HD3	1:O:256:TYR:CD2	2.49	0.47
1:E:58:PRO:HB3	1:E:86:TYR:CE1	2.49	0.47
2:Z:159:TYR:HB3	2:Z:160:PRO:HD3	1.96	0.47
2:N:1:GLY:HA3	2:N:112:ASP:OD2	2.14	0.47
1:W:283:THR:HG23	1:W:284:PRO:HD2	1.94	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
6:Q:2003:BMA:O2	6:Q:2004:MAN:H3	2.15	0.47
1:K:274:TYR:HD1	1:K:275:GLY:N	2.12	0.47
2:V:106:ARG:HH11	2:X:106:ARG:HH12	1.62	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:293:PRO:HG2	1:Q:294:PHE:CD2	2.49	0.47
1:Q:18:HIS:CE1	2:R:18:VAL:HA	2.48	0.47
1:W:100:GLY:HA3	1:W:230:MET:O	2.14	0.47
2:R:168:LEU:O	2:R:172:GLU:HG3	2.14	0.47
1:M:295:HIS:CE1	1:M:308:TYR:HD2	2.32	0.47
1:Y:179:LEU:HD23	1:Y:234:TRP:HB3	1.96	0.47
1:Q:98:TYR:CD1	1:Q:99:PRO:HD2	2.49	0.47
1:A:200:THR:HA	1:A:248:ASN:OD1	2.27	0.47
1:A:116:ASN:HB2	1:A:261:LYS:CG	2.45	0.47
1:O:123:ILE:O	1:O:124:ILE:HG13	2.15	0.47
1:C:147:PHE:CG	1:C:148:PHE:N	2.83	0.47
2:R:128:ASP:O	2:R:170:ARG:NH1	2.47	0.47
2:J:17:MET:SD	2:J:23:GLY:HA3	2.55	0.47
1:Q:78:GLU:HG2	1:Q:79:PHE:CE2	2.50	0.47
1:K:28:THR:HG23	1:K:30:MET:H	1.78	0.47
1:I:29:ILE:HD11	2:J:102:MET:HG2	1.97	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:A:182:ILE:HD12	1:A:202:ILE:CD1	2.44	0.47
1:U:59:LEU:HD23	1:U:87:ILE:HG12	1.97	0.47
1:O:58:PRO:HB3	1:O:86:TYR:CE1	2.50	0.47
2:N:25:HIS:HA	2:N:33:GLY:O	2.15	0.47
1:A:47:HIS:ND1	1:A:286:GLY:HA3	2.30	0.47
1:U:133(A):LEU:O	1:U:135:VAL:HG12	2.15	0.47
1:I:77:ASP:OD2	1:I:149:ARG:NH2	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:168:LEU:O	2:D:172:GLU:HG3	2.15	0.47
1:E:57:LYS:HE2	1:E:274:TYR:CE2	2.50	0.47
1:E:317:ALA:O	2:F:107:THR:HG21	2.15	0.47
1:C:312:ASN:OD1	1:C:312:ASN:N	3.22	0.47
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: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:Y:98:TYR:CZ	1:Y:226:LEU:HD13	2.50	0.46
1:K:188:ALA:O	1:K:192:THR:HG22	2.15	0.46
2:B:106:ARG:HG2	2:D:106:ARG:HH12	149.26	0.46
1:M:172:ASN:HB3	1:M:174:GLU:OE2	2.15	0.46
2:B:127:ARG:NH1	2:Z:133:LEU:O	85.44	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:G:214:VAL:HG13	1:G:215:PRO:HD2	1.96	0.46
1:C:26:VAL:HG21	1:C:317:ALA:HB2	2.14	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:G:123:ILE:HG13	1:G:124:ILE:HG13	1.97	0.46
1:W:58:PRO:HB3	1:W:86:TYR:CE1	2.50	0.46
1:C:197:ASN:HA	1:C:198:PRO:HD3	1.83	0.46
2:J:158:ASP:OD1	2:J:160:PRO:HD2	2.15	0.46
1:E:24:GLU:OE1	1:E:39:ALA:HB3	2.16	0.46
2:P:1:GLY:HA3	2:P:112:ASP:OD2	2.15	0.46
1:C:70:LEU:O	1:C:150:ASN:ND2	2.47	0.46
2:F:21:TRP:HZ3	2:F:45:ILE:HG13	1.80	0.46
1:U:56:VAL:HB	1:U:85:SER:HB3	1.97	0.46
1:K:293:PRO:HB3	2:L:56:ILE:HG12	1.96	0.46
1:C:56:VAL:HB	1:C:85:SER:HB3	2.22	0.46
2:H:167:ARG:O	2:H:171:GLU:HG3	2.16	0.46
1:Y:57:LYS:HE2	1:Y:274:TYR:CE2	2.50	0.46
2:R:58:LYS:HD3	2:R:58:LYS:HA	1.76	0.46
1:C:183:HIS:O	1:C:185:PRO:HD3	2.15	0.46
1:K:247:SER:OG	1:K:248:ASN:N	2.46	0.46
2:B:77:ILE:HD12	2:J:77:ILE:HG21	1.98	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:O:89:GLU:OE1	1:O:269:LYS:HE2	2.15	0.46
1:M:230:MET:SD	1:M:252:ILE:HD11	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:206:THR:HG22	1:O:207:SER:H	1.81	0.46
1:M:84:TRP:O	1:M:116:ASN:ND2	2.43	0.46
1:C:17:TYR:CE2	2:D:6:ILE:HA	3.13	0.46
1:K:139:CYS:O	1:K:146:SER:HB3	2.16	0.46
1:E:44:GLU:OE1	1:E:46:LYS:HG3	2.15	0.46
1:O:167:SER:HB2	1:O:244:ASN:OD1	2.15	0.46
1:W:186:ASN:HD21	1:W:228:GLY:N	2.14	0.46
1:W:134:GLY:HA3	1:W:153:TRP:HB3	1.98	0.46
1:G:108:LEU:HB2	1:G:234:TRP:CE2	2.50	0.46
1:I:28:THR:CG2	1:I:30:MET:H	2.28	0.46
1:U:242:ALA:N	3:U:2001:NAG:H82	2.31	0.46
2:N:149:MET:O	2:N:153:ARG:HG3	2.16	0.46
2:H:30:GLN:HE22	2:H:145:ASP:HA	1.80	0.46
1:K:105:TYR:CE2	1:K:109:LYS:HE3	2.50	0.46
1:A:175:ASP:OD1	1:A:238:LYS:HE2	2.16	0.46
2:R:1:GLY:HA3	2:R:112:ASP:OD2	2.16	0.46
2:J:53:ASN:O	2:J:57:ASP:HB2	2.16	0.46
1:E:206:THR:HB	1:E:209:LEU:H	1.81	0.46
1:A:73:ASN:HD21	1:A:97:CYS:HB3	1.81	0.46
1:C:320:LEU:HD13	2:D:6:ILE:HD13	2.88	0.46
1:C:295:HIS:CD2	1:C:306:PRO:HG2	2.51	0.46
2:P:62:GLN:HG3	2:P:92:TRP:CG	2.50	0.46
1:S:313:ARG:CZ	1:S:315:VAL:HG21	2.45	0.46
2:R:62:GLN:HG3	2:R:92:TRP:CG	2.51	0.46
1:I:316:LEU:HD23	1:I:316:LEU:HA	1.68	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
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.66	0.46
1:O:283:THR:HG23	1:O:298:HIS:HB3	1.98	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: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:W:179:LEU:O	1:W:254:PRO:HG3	2.15	0.45
1:E:37:THR:HG22	1:E:38:HIS:CD2	2.52	0.45
1:W:164:ILE:O	1:W:246:GLU:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:102:PHE:O	1:I:105:TYR:HB2	2.16	0.45
1:E:13:ILE:HA	2:F:26:HIS:HA	1.99	0.45
1:E:288:ILE:HD11	1:E:297:ILE:HG13	1.97	0.45
2:P:125:GLN:OE1	2:P:155:GLY:HA2	2.17	0.45
2:J:85:GLU:O	2:J:89:LEU:HG	2.17	0.45
1:C:242:ALA:N	3:C:2001:NAG:H82	2.48	0.45
1:W:56:VAL:HB	1:W:85:SER:HB3	1.98	0.45
1:C:176:LEU:HD23	1:C:258:TYR:O	2.56	0.45
2:H:1:GLY:HA3	2:H:112:ASP:OD2	2.16	0.45
2:N:118:LEU:HD12	2:N:121:LYS:HD3	1.97	0.45
1:G:43:LEU:HB2	1:G:314:LEU:HB2	1.98	0.45
1:C:185:PRO:HG3	1:C:191:GLN:OE1	2.17	0.45
1:A:58:PRO:HB3	1:A:86:TYR:CZ	2.51	0.45
1:S:176:LEU:HA	1:S:176:LEU:HD23	1.75	0.45
1:A:15:ILE:HD13	2:B:119:TYR:HD1	1.81	0.45
2:T:127:ARG:NH1	2:X:131:LYS:HE2	2.31	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: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
1:G:47:HIS:ND1	1:G:286:GLY:HA3	2.31	0.45
1:E:12:GLN:O	2:F:27:SER:N	2.41	0.45
1:U:107:GLU:HG2	2:T:76:ARG:HH21	1.82	0.45
1:A:141:TYR:CE1	1:A:149:ARG:NH2	3.73	0.45
1:M:13:ILE:HD12	2:N:149:MET:SD	2.56	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
1:G:232:PHE:HE1	1:G:252:ILE:HG21	1.81	0.45
1:O:220:ARG:HD2	1:O:227:SER:O	2.16	0.45
1:I:142:GLN:C	1:I:144:LYS:H	2.19	0.45
1:O:242:ALA:H	3:O:2001:NAG:H82	1.80	0.45
1:O:242:ALA:N	3:O:2001:NAG:H82	2.32	0.45
1:Y:123:ILE:HG13	1:Y:124:ILE:HG13	1.98	0.45
2:F:58:LYS:HD3	2:F:58:LYS:HA	1.80	0.45
1:I:260(A):VAL:O	1:I:260(A):VAL:HG13	2.16	0.45
1:M:283:THR:HG23	1:M:284:PRO:HD2	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
2:B:53:ASN:O	2:B:57:ASP:HB2	2.17	0.45
1:Q:73:ASN:HB3	1:Q:76:CYS:SG	2.57	0.45
1:I:294:PHE:HZ	2:J:59:MET:HG3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:173:ILE:HG23	2:F:177:ARG:HG2	1.99	0.45
1:O:134:GLY:HA3	1:O:153:TRP:HB3	1.98	0.45
1:W:105:TYR:CE2	1:W:109:LYS:HE3	2.51	0.45
2:B:151:SER:O	2:B:156:THR:N	2.50	0.45
1:G:293:PRO:HG2	1:G:294:PHE:CD2	2.52	0.45
1:O:29:ILE:HD11	2:P:102:MET:HA	1.98	0.45
1:I:206:THR:HG22	1:I:207:SER:N	2.32	0.45
1:M:49:GLY:HA2	1:M:285:MET:O	2.17	0.45
1:W:206:THR:CG2	1:W:207:SER:N	2.80	0.45
1:S:108:LEU:HB2	1:S:234:TRP:CZ2	2.52	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
2:X:65:ALA:HB1	2:X:85:GLU:OE1	2.17	0.45
1:U:53:ASP:OD1	1:U:57:LYS:HA	2.17	0.45
1:G:110:HIS:O	1:G:113:SER:OG	2.26	0.45
2:D:124:LEU:HD22	2:L:134:GLY:HA2	1.98	0.45
1:K:160:THR:HG21	1:U:165:LYS:CE	2.43	0.45
1:I:124:ILE:O	1:I:255:GLU:HG3	2.17	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
2:N:129:ASN:HB3	2:N:142:HIS:HE1	1.80	0.45
1:A:105:TYR:CE2	1:A:109:LYS:HE3	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:S:202:ILE:HD11	1:S:251:PHE:HA	1.99	0.44
1:Y:12:GLN:HB2	2:Z:27:SER:HB3	1.99	0.44
1:O:311:SER:HB3	2:P:97:GLU:OE2	2.17	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:S:206:THR:HG22	1:S:207:SER:N	2.32	0.44
1:I:105:TYR:CE2	1:I:109:LYS:HE3	2.53	0.44
2:X:103:GLU:OE2	2:X:106:ARG:HD3	2.16	0.44
1:K:102:PHE:O	1:K:105:TYR:HB2	2.17	0.44
1:U:51:LEU:HG	1:U:272:LEU:HD12	1.99	0.44
1:M:42:ILE:HG13	1:M:314:LEU:HB3	1.99	0.44
1:Q:206:THR:CG2	1:Q:207:SER:N	2.80	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
2:N:127:ARG:NH1	2:R:133:LEU:HA	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:280:LYS:O	1:O:304:GLU:N	2.51	0.44
1:S:194:LEU:HD23	1:S:194:LEU:HA	1.77	0.44
1:W:283:THR:HB	1:W:286:GLY:O	2.17	0.44
1:U:206:THR:CG2	1:U:207:SER:N	2.80	0.44
1:C:214:VAL:HA	1:C:215:PRO:HD2	2.00	0.44
1:W:107:GLU:HG2	2:V:76:ARG:HH21	1.82	0.44
1:C:141:TYR:HB2	1:C:146:SER:HB2	2.45	0.44
1:E:110:HIS:O	1:E:113:SER:OG	2.28	0.44
1:A:120:LYS:HG2	1:A:256:TYR:HB3	2.00	0.44
1:K:174:GLU:HG3	1:K:259:LYS:HB3	1.99	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:A:43:LEU:HB2	1:A:314:LEU:HB2	1.98	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:Q:269:LYS:HE3	2:R:69:GLU:OE1	2.18	0.44
1:Q:53:ASP:OD1	1:Q:274:TYR:OH	2.23	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:U:161:TYR:CE2	1:U:249:GLY:HA2	2.53	0.44
1:O:316:LEU:HD23	1:O:316:LEU:HA	1.84	0.44
1:Q:316:LEU:HD23	1:Q:316:LEU:HA	1.87	0.44
2:B:58:LYS:HG3	2:J:98:LEU:CD1	2.48	0.44
1:W:30:MET:HG2	2:T:47:GLY:O	2.16	0.44
1:E:108:LEU:HB2	1:E:234:TRP:CZ2	2.52	0.44
1:C:226:LEU:HD23	1:C:226:LEU:HA	1.70	0.44
2:B:72:ASN:O	2:B:75:ARG:HG2	2.18	0.44
1:A:98:TYR:CD1	1:A:99:PRO:HD2	2.88	0.44
1:A:147:PHE:HE2	1:A:151:VAL:HG23	1.82	0.44
1:Q:200:THR:HG21	1:Q:249:GLY:HA3	1.99	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: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:A:56:VAL:HB	1:A:85:SER:HB3	2.22	0.44
1:A:107:GLU:HG2	2:J:76:ARG:HH21	1.83	0.44
1:G:18:HIS:HD2	1:G:37:THR:HG21	1.83	0.44
2:T:124:LEU:HD22	2:X:134:GLY:HA2	1.99	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:J:58:LYS:HA	2:J:58:LYS:HD3	1.57	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:O:283:THR:HG22	1:O:285:MET:N	2.11	0.43
1:A:78:GLU:HG2	1:A:79:PHE:CE2	2.53	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
2:Z:3:PHE:CE2	2:Z:113:SER:HB2	2.52	0.43
1:Y:84:TRP:NE1	1:Y:115:ILE:O	2.51	0.43
1:M:57:LYS:HE2	1:M:274:TYR:CE2	2.52	0.43
2:H:98:LEU:HD21	2:J:99:LEU:HD13	2.00	0.43
1:S:283:THR:HB	1:S:286:GLY:O	2.17	0.43
1:M:61:LEU:H	1:M:61:LEU:HG	1.57	0.43
2:T:94:TYR:HE2	2:V:58:LYS:HB3	1.82	0.43
1:C:26:VAL:HG11	1:C:317:ALA:HB2	2.03	0.43
2:V:3:PHE:CE1	2:V:113:SER:HB3	2.53	0.43
2:F:55:ILE:HG12	2:F:99:LEU:HD21	2.00	0.43
1:A:18:HIS:ND1	2:B:17:MET:O	4.28	0.43
1:W:108:LEU:HB2	1:W:234:TRP:CZ2	2.53	0.43
1:E:176:LEU:HA	1:E:176:LEU:HD23	1.81	0.43
1:M:28:THR:HG22	1:M:31:GLU:N	2.26	0.43
1:O:314:LEU:HD23	1:O:314:LEU:HA	1.73	0.43
2:B:158:ASP:OD1	2:B:160:PRO:HD2	2.44	0.43
1:O:138:ALA:O	1:O:140:PRO:HD3	2.18	0.43
1:M:242:ALA:N	3:M:2001:NAG:H82	2.32	0.43
1:I:20:ASN:HB2	1:I:21[B]:ASN:H	1.60	0.43
1:S:206:THR:HB	1:S:209:LEU:HB2	2.00	0.43
1:W:204:VAL:HG12	1:W:209:LEU:HD23	1.99	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:U:230:MET:SD	1:U:252:ILE:HD11	2.59	0.43
2:T:123:ARG:HD2	2:T:132:GLU:OE2	2.18	0.43
1:W:279:THR:HB	1:W:281:CYS:H	1.83	0.43
1:G:120:LYS:HD3	1:G:256:TYR:CD2	2.53	0.43
2:D:129:ASN:HB3	2:D:142:HIS:CE1	4.31	0.43
1:E:137:SER:HA	1:E:145:SER:HB2	2.01	0.43
1:S:249:GLY:O	1:S:251:PHE:N	2.51	0.43
1:Q:108:LEU:HD13	1:Q:234:TRP:CD2	2.54	0.43
1:C:114:ARG:HH21	1:C:263:GLY:C	2.21	0.43
1:Y:320:LEU:HB3	2:Z:111:HIS:CD2	2.53	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
2:H:70:PHE:CD1	2:H:70:PHE:N	2.87	0.43
1:M:78:GLU:O	1:M:78:GLU:HG2	2.19	0.43
1:M:132:ALA:HA	1:M:154:LEU:HD23	2.01	0.43
1:S:283:THR:HG23	1:S:284:PRO:HD2	2.01	0.43
1:K:28:THR:CG2	1:K:30:MET:H	2.32	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:G:176:LEU:HD22	1:G:257:ALA:HB1	2.00	0.43
1:C:13:ILE:HG22	2:D:138:PHE:HB2	2.35	0.43
1:K:118:PHE:CD1	1:K:258:TYR:HB3	2.54	0.43
1:Y:314:LEU:HA	1:Y:314:LEU:HD23	1.80	0.43
2:F:19:ASP:N	2:F:19:ASP:OD1	2.50	0.43
1:O:28:THR:HG22	1:O:31:GLU:N	2.28	0.43
1:A:126:SER:HB2	1:A:166:ARG:NH2	2.93	0.43
1:S:32:LYS:HE2	2:V:50:ASN:ND2	2.33	0.43
1:A:214:VAL:HG13	1:A:215:PRO:HD2	2.00	0.43
1:O:28:THR:CG2	1:O:30:MET:H	2.31	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: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
2:P:19:ASP:OD1	2:P:19:ASP:N	2.51	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:Y:197:ASN:HA	1:Y:198:PRO:HD3	1.86	0.43
1:G:100:GLY:HA3	1:G:230:MET:O	2.19	0.43
1:U:228:GLY:O	1:U:229:ARG:HD3	2.19	0.43
2:H:151:SER:O	2:H:157:TYR:N	2.50	0.43
1:W:202:ILE:HD11	1:W:251:PHE:HA	2.01	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:E:284:PRO:HG2	1:E:298:HIS:CE1	2.54	0.43
1:A:181:GLY:O	1:A:252:ILE:HB	2.46	0.43
1:M:204:VAL:HG12	1:M:209:LEU:HD23	2.01	0.43
1:W:99:PRO:HD2	1:W:226:LEU:HD12	2.00	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
2:D:5:ALA:HA	2:D:9:PHE:CE1	2.53	0.43
2:P:122:VAL:O	2:P:126:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:264:ASP:OD1	1:A:264:ASP:N	2.51	0.43
2:V:57:ASP:O	2:V:60:ASN:HB2	2.19	0.42
2:Z:71:ASN:OD1	2:Z:74:GLU:HG3	2.19	0.42
1:G:222:LYS:HA	1:G:226:LEU:O	2.18	0.42
1:Y:115:ILE:HD13	1:Y:260:ILE:HG12	2.00	0.42
1:E:293:PRO:HG2	1:E:294:PHE:HD1	1.84	0.42
1:E:257:ALA:C	1:E:258:TYR:HD1	2.23	0.42
1:I:206:THR:HB	1:I:209:LEU:CB	2.49	0.42
2:B:106:ARG:HH11	2:H:106:ARG:NH1	2.13	0.42
1:Y:83(A):GLU:CD	1:Y:261:LYS:HZ3	2.21	0.42
1:A:258:TYR:CD1	1:A:258:TYR:N	2.86	0.42
1:W:159:SER:O	1:W:196:GLN:NE2	2.51	0.42
2:H:62:GLN:HG3	2:H:92:TRP:CG	2.54	0.42
1:O:313:ARG:NH2	1:O:315:VAL:HG21	2.34	0.42
1:I:200:THR:HA	1:I:248:ASN:OD1	2.19	0.42
2:B:83:LYS:HG3	2:H:68:ARG:HH21	1.83	0.42
1:A:283:THR:HG23	1:A:284:PRO:HD2	2.02	0.42
1:M:283:THR:HG22	1:M:285:MET:N	2.17	0.42
1:E:188:ALA:O	1:E:192:THR:HG22	2.19	0.42
1:A:26:VAL:HB	2:B:104:ASN:ND2	2.87	0.42
1:S:135:VAL:HG22	1:S:146:SER:CA	2.49	0.42
1:O:65:SER:OG	1:O:96:ASP:HA	2.19	0.42
2:V:133:LEU:HD12	2:V:137:CYS:HB2	2.01	0.42
2:J:149:MET:O	2:J:153:ARG:HG3	2.19	0.42
1:I:12:GLN:HB2	2:J:27:SER:HB3	2.00	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:S:126:SER:HB2	1:S:166:ARG:HH22	1.84	0.42
1:O:121:ILE:HD13	1:O:121:ILE:HG21	1.66	0.42
1:M:122:GLN:NE2	1:M:125:PRO:HA	2.34	0.42
1:I:206:THR:HB	1:I:209:LEU:N	2.29	0.42
2:T:68:ARG:HH22	2:X:83:LYS:NZ	2.18	0.42
2:D:106:ARG:HH22	2:L:106:ARG:CG	2.32	0.42
1:I:107:GLU:O	1:I:110:HIS:HB3	2.18	0.42
1:W:197:ASN:HA	1:W:198:PRO:HD3	1.87	0.42
1:Y:298:HIS:HE1	1:Y:300:LEU:HD12	1.85	0.42
1:W:311:SER:HB3	2:X:97:GLU:OE2	2.19	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:Y:314:LEU:HD22	2:Z:100:VAL:HG21	2.01	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
1:S:314:LEU:HA	1:S:314:LEU:HD23	1.94	0.42
2:R:152:VAL:HG22	2:R:157:TYR:CD1	2.54	0.42
1:U:135:VAL:HG23	1:U:146:SER:CA	2.48	0.42
1:G:316:LEU:HD23	1:G:316:LEU:HA	1.78	0.42
2:V:106:ARG:CG	2:X:106:ARG:HH22	2.33	0.42
2:T:80:LEU:HD13	2:V:81:ASN:OD1	2.20	0.42
1:Q:280:LYS:O	1:Q:304:GLU:N	2.52	0.42
1:Y:183:HIS:O	1:Y:185:PRO:HD3	2.20	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:A:47:HIS:CE1	1:A:285:MET:O	2.72	0.42
1:Q:28:THR:HG23	1:Q:30:MET:H	1.84	0.42
1:U:131:GLU:OE2	1:U:157:LYS:HG3	2.20	0.42
1:K:61:LEU:HA	1:K:79:PHE:CE1	2.53	0.42
1:S:108:LEU:HB2	1:S:234:TRP:CE2	2.55	0.42
1:W:314:LEU:HA	1:W:314:LEU:HD23	1.79	0.42
2:D:118:LEU:HD12	2:D:121:LYS:HD3	2.01	0.42
2:T:55:ILE:HG12	2:T:99:LEU:HD21	2.01	0.42
1:G:28:THR:HG23	1:G:30:MET:H	1.84	0.42
1:A:278:ASN:OD1	1:A:279:THR:N	2.64	0.42
2:Z:6:ILE:HD11	2:Z:111:HIS:HB3	2.02	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:D:123:ARG:HD2	2:D:132:GLU:OE2	2.19	0.42
1:K:65:SER:OG	1:K:96:ASP:OD1	2.28	0.42
2:Z:1:GLY:HA3	2:Z:112:ASP:OD2	2.19	0.42
1:C:206:THR:HG22	1:C:207:SER:H	1.84	0.42
1:O:30:MET:O	2:R:50:ASN:ND2	2.43	0.42
1:A:195:TYR:O	1:A:196:GLN:HB3	2.19	0.42
2:V:58:LYS:HD3	2:V:58:LYS:HA	1.44	0.42
3:U:2001:NAG:H61	3:U:2002:NAG:HN2	1.85	0.42
2:P:6:ILE:HG13	2:P:112:ASP:HA	2.02	0.42
1:W:102:PHE:O	1:W:105:TYR:HB2	2.20	0.42
2:B:75:ARG:O	2:B:78:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:80:LEU:HD13	2:P:81:ASN:OD1	2.20	0.42
1:W:156:LYS:NZ	1:W:193:LYS:O	2.51	0.42
1:A:154:LEU:O	1:A:155:ILE:HG13	2.20	0.42
1:G:167:SER:OG	1:G:168:TYR:N	2.51	0.42
1:Q:105:TYR:CE2	1:Q:109:LYS:HE3	2.55	0.42
1:O:180:TRP:CZ3	1:O:234:TRP:HA	2.54	0.42
1:W:77:ASP:OD2	1:W:141:TYR:HE1	2.03	0.42
2:B:142:HIS:CE1	2:B:162:TYR:CD2	3.08	0.42
2:P:169:LYS:HD2	2:P:172:GLU:OE1	2.20	0.42
1:C:207:SER:HA	1:K:221:SER:HB2	2.02	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:E:183:HIS:O	1:E:185:PRO:HD3	2.20	0.42
1:O:26:VAL:HG21	1:O:317:ALA:HB2	2.01	0.42
1:A:124:ILE:HA	1:A:125:PRO:HD3	1.73	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
2:T:89:LEU:HD23	2:T:89:LEU:HA	1.91	0.42
1:C:283:THR:HG23	1:C:284:PRO:HD2	2.02	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:C:156:LYS:HD2	1:C:196:GLN:HB2	2.15	0.41
2:N:125:GLN:OE1	2:N:155:GLY:HA2	2.20	0.41
1:A:180:TRP:NE1	1:A:204:VAL:HG21	2.34	0.41
1:K:302:ILE:HG13	1:K:303:GLY:N	2.35	0.41
1:C:202:ILE:HD11	1:C:251:PHE:HA	2.52	0.41
1:Y:236:ILE:HA	1:Y:236:ILE:HD13	1.86	0.41
1:I:111:LEU:HD12	1:I:111:LEU:HA	1.92	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:K:50:LYS:HB3	1:K:275:GLY:HA3	2.03	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
1:K:108:LEU:HB2	1:K:234:TRP:CZ2	2.55	0.41
2:T:75:ARG:HA	2:T:75:ARG:HD3	1.88	0.41
1:O:197:ASN:HA	1:O:198:PRO:HD3	1.88	0.41
1:G:60:ILE:HG12	1:G:88:VAL:HB	2.03	0.41
1:K:126:SER:HB2	1:K:166:ARG:NH2	2.34	0.41
4:A:2004:NAG:H3	4:A:2005:NAG:H2	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:C:121:ILE:HD11	1:C:176:LEU:HD21	2.03	0.41
1:M:294:PHE:HZ	2:N:59:MET:HG3	1.85	0.41
2:Z:53:ASN:O	2:Z:57:ASP:HB2	2.20	0.41
1:S:252:ILE:HG21	1:S:252:ILE:HD13	1.79	0.41
1:S:206:THR:CG2	1:S:207:SER:N	2.84	0.41
2:B:76:ARG:NH1	2:H:74:GLU:OE1	2.50	0.41
1:C:28:THR:HG22	1:C:31:GLU:N	2.32	0.41
1:C:247:SER:OG	1:C:248:ASN:N	2.55	0.41
1:S:200:THR:HA	1:S:248:ASN:OD1	2.21	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:W:187:ASP:OD2	1:W:189:ALA:HB3	2.21	0.41
1:U:235:THR:OG1	1:U:236:ILE:N	2.53	0.41
1:G:125(A):LYS:HE3	1:G:132:ALA:HB1	2.02	0.41
1:W:73:ASN:HB3	1:W:76:CYS:SG	2.60	0.41
1:S:53:ASP:OD1	1:S:274:TYR:OH	2.25	0.41
2:F:71:ASN:OD1	2:F:72:ASN:N	2.54	0.41
1:W:176:LEU:HA	1:W:176:LEU:HD23	1.79	0.41
1:I:283:THR:HG23	1:I:298:HIS:HB3	2.02	0.41
1:M:230:MET:SD	1:M:252:ILE:CD1	3.08	0.41
1:I:44:GLU:HB2	1:I:292:MET:HG3	2.02	0.41
1:W:314:LEU:HD22	2:X:100:VAL:HG21	2.02	0.41
1:O:222:LYS:HG3	1:O:227:SER:OG	2.20	0.41
2:T:62:GLN:HG3	2:T:92:TRP:CG	2.55	0.41
2:N:129:ASN:HB3	2:N:142:HIS:CE1	2.55	0.41
1:A:214:VAL:HA	1:A:215:PRO:HD2	2.08	0.41
2:P:118:LEU:O	2:P:122:VAL:HG23	2.20	0.41
1:W:196:GLN:HB2	1:W:196:GLN:HE21	1.65	0.41
1:S:320:LEU:HD23	2:T:111:HIS:ND1	2.36	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:O:124:ILE:HA	1:O:125:PRO:HD3	1.86	0.41
2:B:77:ILE:CD1	2:J:77:ILE:HG21	2.51	0.41
1:Y:28:THR:HG22	1:Y:30:MET:H	1.85	0.41
1:U:182:ILE:HB	1:U:202:ILE:HD12	2.01	0.41
1:E:295:HIS:ND1	1:E:297:ILE:HG12	2.36	0.41
1:A:67:ALA:HB2	1:A:105:TYR:CE1	2.56	0.41
2:X:168:LEU:O	2:X:172:GLU:HG3	2.20	0.41
1:Y:242:ALA:N	4:Y:2001:NAG:H82	2.36	0.41
1:M:11:ASP:O	2:N:140:PHE:HB2	2.21	0.41
1:A:121:ILE:HD13	1:A:259:LYS:HD3	2.05	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:44:GLU:HB2	1:Y:292:MET:HG3	2.03	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: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: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
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
2:J:62:GLN:HG3	2:J:92:TRP:CD2	2.56	0.41
1:Q:122:GLN:NE2	1:Q:255:GLU:OE2	2.54	0.41
1:O:317:ALA:O	2:P:107:THR:HG21	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:L:133:LEU:HD21	2:L:139:GLU:HB2	2.02	0.41
2:J:168:LEU:O	2:J:172:GLU:HG3	2.20	0.41
1:O:298:HIS:CE1	1:O:300:LEU:HB2	2.55	0.41
1:E:206:THR:CG2	1:E:207:SER:N	2.83	0.41
2:H:39:GLU:O	2:H:43:LYS:N	2.52	0.41
2:B:77:ILE:HG13	2:B:77:ILE:H	3.92	0.41
1:G:226:LEU:HA	1:G:226:LEU:HD23	1.78	0.41
1:G:108:LEU:HB2	1:G:234:TRP:CZ2	2.56	0.41
1:G:96:ASP:HB3	1:G:96(A):LEU:H	1.58	0.41
1:E:186:ASN:ND2	1:E:227:SER:HB3	2.35	0.41
1:W:147:PHE:CE2	1:W:148:PHE:HD1	2.39	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:M:121:ILE:HD13	1:M:121:ILE:HG21	1.66	0.41
1:W:112:LEU:HD23	1:W:112:LEU:HA	1.70	0.41
1:Y:231:GLU:HG2	1:Y:233:PHE:CE1	2.56	0.41
1:O:202:ILE:HD12	1:O:213:LEU:HD12	2.03	0.41
1:O:15:ILE:HB	2:P:119:TYR:HD2	1.85	0.41
1:C:37:THR:HG22	1:C:38:HIS:CE1	2.55	0.41
2:H:94:TYR:CD1	2:H:94:TYR:C	2.94	0.41
1:A:307:LYS:HE2	2:B:64:GLU:OE2	3.58	0.41
1:O:295:HIS:CE1	1:O:308:TYR:HD1	2.39	0.41
1:A:283:THR:HG23	1:A:298:HIS:HB3	2.05	0.41
1:C:206:THR:CG2	1:C:207:SER:N	2.91	0.41
2:B:58:LYS:C	2:B:60:ASN:H	2.24	0.41
2:B:99:LEU:HD13	2:Z:98:LEU:HD21	83.94	0.41
2:B:5:ALA:HA	2:B:9:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:LEU:HD23	1:C:154:LEU:HA	2.12	0.41
1:Y:98:TYR:CE2	1:Y:226:LEU:HD13	2.56	0.41
1:U:105:TYR:CE2	1:U:109:LYS:HE3	2.56	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:I:209:LEU:HD12	1:I:209:LEU:HA	1.82	0.40
1:C:132:ALA:HA	1:C:154:LEU:HD23	2.03	0.40
1:A:247:SER:OG	1:A:248:ASN:N	2.57	0.40
1:C:26:VAL:HB	2:D:104:ASN:ND2	2.37	0.40
1:K:105:TYR:CZ	1:K:109:LYS:HE3	2.55	0.40
1:C:242:ALA:H	3:C:2001:NAG:H82	2.04	0.40
2:H:84:MET:CE	2:H:85:GLU:HG2	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
1:C:22:SER:O	1:C:322:ASN:ND2	2.66	0.40
1:M:195:TYR:O	1:M:197:ASN:N	2.51	0.40
2:B:50:ASN:O	2:B:54:SER:N	2.94	0.40
1:M:111:LEU:HA	1:M:111:LEU:HD12	1.88	0.40
1:K:30:MET:HG2	2:D:47:GLY:O	2.21	0.40
1:U:116:ASN:HB2	1:U:261:LYS:HG2	2.03	0.40
1:G:138:ALA:O	1:G:140:PRO:HD3	2.21	0.40
2:D:151:SER:HA	2:D:156:THR:HB	2.03	0.40
1:Y:164:ILE:O	1:Y:246:GLU:HA	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:O:279:THR:HB	1:O:281:CYS:H	1.87	0.40
1:I:283:THR:HG22	1:I:285:MET:N	2.09	0.40
1:G:28:THR:HG22	1:G:31:GLU:N	2.35	0.40
1:C:18:HIS:CD2	1:C:19:ALA:N	2.89	0.40
1:M:307:LYS:HD2	2:N:62:GLN:HB3	2.02	0.40
1:M:196:GLN:HB2	1:M:196:GLN:HE21	1.68	0.40
1:C:57:LYS:HE2	1:C:274:TYR:CZ	2.55	0.40
1:G:182:ILE:HD11	1:G:215:PRO:HD3	2.04	0.40
1:K:135:VAL:HA	1:K:146:SER:O	2.21	0.40
1:G:294:PHE:HZ	2:H:59:MET:HG3	1.85	0.40
1:W:141:TYR:CD2	1:W:142:GLN:HG2	2.56	0.40
2:Z:30:GLN:HE21	2:Z:30:GLN:H	1.69	0.40
2:D:77:ILE:HA	2:D:80:LEU:HB3	2.03	0.40
2:N:176:GLY:O	2:N:177:ARG:HG3	2.22	0.40
1:S:70:LEU:HD11	1:S:112:LEU:HD11	2.02	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
1:E:226:LEU:HD23	1:E:226:LEU:HA	1.81	0.40
2:P:22:TYR:OH	2:P:111:HIS:ND1	2.40	0.40
1:E:192:THR:HG23	1:U:192:THR:HG21	2.03	0.40
1:Q:266:THR:HG22	1:Q:302:ILE:CD1	2.52	0.40
1:Y:86:TYR:HB3	1:Y:302:ILE:HD13	2.03	0.40
1:Q:176:LEU:HB2	1:Q:237:LEU:HB3	2.03	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
1:G:251:PHE:CZ	1:G:253:ALA:HA	2.56	0.40
2:F:151:SER:O	2:F:156:THR:N	2.55	0.40
2:P:141:TYR:HE1	2:P:173:ILE:HD12	1.87	0.40
1:U:26:VAL:HB	2:V:104:ASN:ND2	2.36	0.40
1:U:187:ASP:OD1	1:U:189:ALA:N	2.55	0.40
1:C:283:THR:HG23	1:C:298:HIS:HB3	2.08	0.40
1:A:232:PHE:CE1	1:A:252:ILE:HG21	2.56	0.40
1:K:206:THR:CG2	1:K:207:SER:N	2.84	0.40
1:E:265:SER:OG	1:E:266:THR:N	2.55	0.40
1:Q:182:ILE:HB	1:Q:202:ILE:HD12	2.03	0.40
1:S:26:VAL:HG21	1:S:317:ALA:HB2	2.04	0.40
2:V:106:ARG:NH1	2:X:106:ARG:HH12	2.19	0.40
2:V:133:LEU:HD12	2:V:137:CYS:CB	2.52	0.40
2:H:85:GLU:O	2:H:89:LEU:HG	2.22	0.40
1:G:17:TYR:CE2	2:H:6:ILE:HA	2.56	0.40
2:Z:149:MET:O	2:Z:153:ARG:HG3	2.21	0.40
1:C:165:LYS:NZ	1:S:160:THR:HG23	2.36	0.40
1:G:185:PRO:HG2	1:G:191:GLN:OE1	2.22	0.40
1:I:172:ASN:HB3	1:I:174:GLU:OE2	2.22	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%)	46	84
1	U	323/334 (97%)	298 (92%)	23 (7%)	2 (1%)	30	74
1	W	323/334 (97%)	299 (93%)	24 (7%)	0	100	100
1	Y	323/334 (97%)	297 (92%)	25 (8%)	1 (0%)	46	84
1	a	323/334 (97%)	297 (92%)	26 (8%)	0	100	100
1	c	323/334 (97%)	300 (93%)	22 (7%)	1 (0%)	46	84
2	B	175/181 (97%)	163 (93%)	12 (7%)	0	100	100
2	D	175/181 (97%)	162 (93%)	12 (7%)	1 (1%)	30	74
2	F	175/181 (97%)	163 (93%)	11 (6%)	1 (1%)	30	74
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%)	30	74
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%)	56	90

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%)	21	60
1	C	292/300 (97%)	281 (96%)	11 (4%)	40	77
1	E	292/300 (97%)	279 (96%)	13 (4%)	34	73
1	G	292/300 (97%)	277 (95%)	15 (5%)	29	69
1	I	292/300 (97%)	272 (93%)	20 (7%)	20	57
1	K	292/300 (97%)	282 (97%)	10 (3%)	44	80
1	M	292/300 (97%)	274 (94%)	18 (6%)	23	62
1	O	292/300 (97%)	277 (95%)	15 (5%)	29	69
1	Q	292/300 (97%)	275 (94%)	17 (6%)	25	64
1	S	292/300 (97%)	278 (95%)	14 (5%)	31	71
1	U	292/300 (97%)	277 (95%)	15 (5%)	29	69
1	W	292/300 (97%)	285 (98%)	7 (2%)	57	86
1	Y	292/300 (97%)	281 (96%)	11 (4%)	40	77
1	a	292/300 (97%)	279 (96%)	13 (4%)	34	73
1	c	292/300 (97%)	280 (96%)	12 (4%)	37	75
2	B	151/155 (97%)	146 (97%)	5 (3%)	45	80
2	D	151/155 (97%)	149 (99%)	2 (1%)	76	92
2	F	151/155 (97%)	150 (99%)	1 (1%)	88	97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	151/155 (97%)	147 (97%)	4 (3%)	54	85
2	J	151/155 (97%)	147 (97%)	4 (3%)	54	85
2	L	151/155 (97%)	151 (100%)	0	100	100
2	N	151/155 (97%)	150 (99%)	1 (1%)	88	97
2	P	151/155 (97%)	150 (99%)	1 (1%)	88	97
2	R	151/155 (97%)	149 (99%)	2 (1%)	76	92
2	T	151/155 (97%)	149 (99%)	2 (1%)	76	92
2	V	151/155 (97%)	148 (98%)	3 (2%)	63	88
2	X	151/155 (97%)	148 (98%)	3 (2%)	63	88
2	Z	151/155 (97%)	147 (97%)	4 (3%)	54	85
2	b	151/155 (97%)	148 (98%)	3 (2%)	63	88
2	d	151/155 (97%)	146 (97%)	5 (3%)	45	80
All	All	6645/6825 (97%)	6395 (96%)	250 (4%)	40	77

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	1.36	2 (14%)	15,19,21	1.13	1 (6%)
3	NAG	A	2002	3	14,14,15	0.49	0	15,19,21	0.44	0
3	BMA	A	2003	3	11,11,12	1.93	3 (27%)	14,15,17	1.95	5 (35%)
4	NAG	A	2004	1,4	14,14,15	1.01	1 (7%)	15,19,21	1.27	2 (13%)
4	NAG	A	2005	4	14,14,15	1.79	2 (14%)	15,19,21	1.27	1 (6%)
3	NAG	C	2001	1,3	14,14,15	0.61	0	15,19,21	0.61	0
3	NAG	C	2002	3	14,14,15	0.63	0	15,19,21	0.79	0
3	BMA	C	2003	3	11,11,12	1.74	2 (18%)	14,15,17	2.86	5 (35%)
3	NAG	E	2001	1,3	14,14,15	0.79	1 (7%)	15,19,21	1.57	1 (6%)
3	NAG	E	2002	3	14,14,15	0.99	1 (7%)	15,19,21	1.43	3 (20%)
3	BMA	E	2003	3	11,11,12	2.46	7 (63%)	14,15,17	1.51	3 (21%)
4	NAG	E	2004	1,4	14,14,15	1.18	1 (7%)	15,19,21	1.33	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	0.58	1 (7%)	15,19,21	0.35	0
3	NAG	G	2001	1,3	14,14,15	1.70	1 (7%)	15,19,21	1.31	3 (20%)
3	NAG	G	2002	3	14,14,15	1.22	1 (7%)	15,19,21	1.18	3 (20%)
3	BMA	G	2003	3	11,11,12	2.24	5 (45%)	14,15,17	1.71	3 (21%)
4	NAG	G	2004	1,4	14,14,15	1.25	1 (7%)	15,19,21	1.38	2 (13%)
4	NAG	G	2005	4	14,14,15	1.77	3 (21%)	15,19,21	0.89	1 (6%)
3	NAG	I	2001	1,3	14,14,15	1.25	1 (7%)	15,19,21	1.42	2 (13%)
3	NAG	I	2002	3	14,14,15	0.71	1 (7%)	15,19,21	0.48	0
3	BMA	I	2003	3	11,11,12	1.93	3 (27%)	14,15,17	1.59	3 (21%)
4	NAG	I	2004	1,4	14,14,15	0.75	1 (7%)	15,19,21	1.17	1 (6%)
4	NAG	I	2005	4	14,14,15	1.52	2 (14%)	15,19,21	1.07	1 (6%)
3	NAG	K	2001	1,3	14,14,15	0.51	0	15,19,21	0.74	0
3	NAG	K	2002	3	14,14,15	0.90	1 (7%)	15,19,21	1.22	2 (13%)
3	BMA	K	2003	3	11,11,12	1.96	4 (36%)	14,15,17	1.69	3 (21%)
3	NAG	M	2001	1,3	14,14,15	0.66	1 (7%)	15,19,21	0.66	0
3	NAG	M	2002	3	14,14,15	0.83	1 (7%)	15,19,21	0.68	0
3	BMA	M	2003	3	11,11,12	1.89	5 (45%)	14,15,17	2.08	5 (35%)
4	NAG	M	2004	1,4	14,14,15	0.71	0	15,19,21	0.71	0
4	NAG	M	2005	4	14,14,15	1.45	1 (7%)	15,19,21	1.37	3 (20%)
3	NAG	O	2001	1,3	14,14,15	0.92	1 (7%)	15,19,21	0.55	0
3	NAG	O	2002	3	14,14,15	0.32	0	15,19,21	0.33	0
3	BMA	O	2003	3	11,11,12	1.51	2 (18%)	14,15,17	2.30	4 (28%)
4	NAG	O	2004	1,4	14,14,15	0.83	1 (7%)	15,19,21	0.94	1 (6%)
4	NAG	O	2005	4	14,14,15	0.30	0	15,19,21	0.64	1 (6%)
6	NAG	Q	2001	1,6	14,14,15	0.54	0	15,19,21	1.34	3 (20%)
6	NAG	Q	2002	6	14,14,15	0.44	0	15,19,21	1.01	0
6	BMA	Q	2003	6	11,11,12	0.70	0	14,15,17	2.03	4 (28%)
6	MAN	Q	2004	6	11,11,12	0.70	0	14,15,17	1.49	1 (7%)
4	NAG	Q	2005	1,4	14,14,15	1.23	1 (7%)	15,19,21	1.28	3 (20%)
4	NAG	Q	2006	4	14,14,15	1.02	1 (7%)	15,19,21	0.94	1 (6%)
4	NAG	S	2001	1,4	14,14,15	0.26	0	15,19,21	0.34	0
4	NAG	S	2002	4	14,14,15	0.91	1 (7%)	15,19,21	0.84	0
4	NAG	S	2003	1,4	14,14,15	0.93	1 (7%)	15,19,21	0.98	2 (13%)
4	NAG	S	2004	4	14,14,15	1.23	2 (14%)	15,19,21	0.97	1 (6%)
3	NAG	U	2001	1,3	14,14,15	0.30	0	15,19,21	0.55	0
3	NAG	U	2002	3	14,14,15	1.89	1 (7%)	15,19,21	1.35	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	1.32	2 (18%)	14,15,17	1.46	3 (21%)
4	NAG	U	2004	1,4	14,14,15	1.13	1 (7%)	15,19,21	1.29	3 (20%)
4	NAG	U	2005	4	14,14,15	0.38	0	15,19,21	0.57	1 (6%)
3	NAG	W	2001	1,3	14,14,15	0.61	0	15,19,21	1.05	2 (13%)
3	NAG	W	2002	3	14,14,15	0.56	0	15,19,21	0.88	0
3	BMA	W	2003	3	11,11,12	0.56	0	14,15,17	0.78	0
4	NAG	W	2004	1,4	14,14,15	1.39	1 (7%)	15,19,21	1.33	3 (20%)
4	NAG	W	2005	4	14,14,15	0.91	1 (7%)	15,19,21	0.73	1 (6%)
4	NAG	Y	2001	1,4	14,14,15	0.37	0	15,19,21	0.40	0
4	NAG	Y	2002	4	14,14,15	0.29	0	15,19,21	0.52	0
4	NAG	a	2001	1,4	14,14,15	0.46	0	15,19,21	1.25	2 (13%)
4	NAG	a	2002	4	14,14,15	0.42	0	15,19,21	0.35	0

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

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

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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 (69) 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	-6.89	1.32	1.43
3	G	2001	NAG	O5-C1	-5.80	1.34	1.43
4	M	2005	NAG	O5-C1	-4.85	1.35	1.43
4	W	2004	NAG	O5-C1	-4.83	1.35	1.43
4	G	2004	NAG	O5-C1	-4.46	1.36	1.43
3	G	2002	NAG	O5-C1	-4.34	1.36	1.43
4	Q	2005	NAG	O5-C1	-4.16	1.36	1.43
4	G	2005	NAG	O5-C1	-4.13	1.36	1.43
4	E	2004	NAG	O5-C1	-4.11	1.36	1.43
4	U	2004	NAG	O5-C1	-3.94	1.37	1.43
3	I	2001	NAG	O5-C1	-3.82	1.37	1.43
4	A	2004	NAG	O5-C1	-3.48	1.37	1.43
3	I	2003	BMA	O5-C1	-3.31	1.38	1.43
3	E	2002	NAG	O5-C1	-3.30	1.38	1.43
3	M	2003	BMA	O5-C1	-3.21	1.38	1.43
3	G	2003	BMA	O5-C1	-3.13	1.38	1.43
4	Q	2006	NAG	O5-C1	-3.12	1.38	1.43
3	O	2001	NAG	O5-C1	-3.03	1.38	1.43
4	S	2002	NAG	O5-C1	-2.95	1.38	1.43
4	S	2004	NAG	O5-C1	-2.86	1.38	1.43
4	S	2003	NAG	O5-C1	-2.83	1.39	1.43
4	O	2004	NAG	O5-C1	-2.64	1.39	1.43
3	K	2002	NAG	O5-C1	-2.59	1.39	1.43
4	I	2004	NAG	O5-C1	-2.54	1.39	1.43
3	A	2001	NAG	O5-C1	-2.51	1.39	1.43
3	I	2002	NAG	O5-C1	-2.49	1.39	1.43
3	M	2002	NAG	O5-C1	-2.43	1.39	1.43
3	K	2003	BMA	C4-C3	2.01	1.57	1.52
4	E	2005	NAG	C1-C2	2.01	1.55	1.52
3	M	2001	NAG	C1-C2	2.08	1.55	1.52
3	E	2003	BMA	O5-C1	2.10	1.47	1.43
4	G	2005	NAG	C3-C2	2.11	1.57	1.52
3	K	2003	BMA	C6-C5	2.13	1.59	1.51
3	G	2003	BMA	C1-C2	2.18	1.57	1.52
3	M	2003	BMA	C2-C3	2.19	1.55	1.52
3	M	2003	BMA	C4-C3	2.21	1.58	1.52
3	M	2003	BMA	C1-C2	2.22	1.57	1.52
3	U	2003	BMA	O5-C5	2.25	1.48	1.43
3	O	2003	BMA	C1-C2	2.30	1.57	1.52
3	G	2003	BMA	C2-C3	2.31	1.55	1.52
3	E	2003	BMA	C6-C5	2.35	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2003	BMA	C6-C5	2.44	1.60	1.51
4	W	2005	NAG	C1-C2	2.51	1.55	1.52
3	E	2003	BMA	O3-C3	2.70	1.49	1.43
3	E	2003	BMA	C4-C3	2.71	1.59	1.52
3	E	2001	NAG	O5-C1	2.88	1.48	1.43
3	U	2003	BMA	C1-C2	2.90	1.59	1.52
4	S	2004	NAG	C1-C2	2.92	1.56	1.52
3	A	2003	BMA	C2-C3	2.95	1.56	1.52
3	K	2003	BMA	O3-C3	2.97	1.50	1.43
3	E	2003	BMA	C1-C2	3.08	1.59	1.52
3	I	2003	BMA	C4-C3	3.11	1.60	1.52
3	K	2003	BMA	C4-C5	3.12	1.59	1.53
3	E	2003	BMA	C4-C5	3.23	1.59	1.53
3	C	2003	BMA	C4-C3	3.29	1.61	1.52
3	G	2003	BMA	C4-C5	3.35	1.60	1.53
3	I	2003	BMA	C4-C5	3.36	1.60	1.53
3	M	2003	BMA	C4-C5	3.39	1.60	1.53
3	O	2003	BMA	C4-C5	3.45	1.60	1.53
3	A	2003	BMA	C1-C2	3.57	1.60	1.52
3	A	2003	BMA	C4-C3	3.62	1.61	1.52
4	I	2005	NAG	O5-C1	3.69	1.49	1.43
3	E	2003	BMA	C2-C3	3.90	1.57	1.52
3	A	2001	NAG	C1-C2	3.92	1.57	1.52
4	I	2005	NAG	C1-C2	4.17	1.58	1.52
3	G	2003	BMA	C4-C3	4.30	1.63	1.52
4	A	2005	NAG	C1-C2	4.62	1.58	1.52
4	G	2005	NAG	C1-C2	4.62	1.58	1.52
4	A	2005	NAG	O5-C1	4.71	1.51	1.43

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2001	NAG	C1-O5-C5	-3.47	107.84	112.25
6	Q	2003	BMA	O5-C1-C2	-3.39	105.36	110.86
6	Q	2003	BMA	O3-C3-C4	-3.34	102.81	110.34
4	M	2005	NAG	C1-O5-C5	-3.30	108.06	112.25
3	A	2003	BMA	C1-O5-C5	-3.15	108.25	112.25
3	U	2003	BMA	O2-C2-C3	-2.84	104.41	110.12
4	Q	2005	NAG	C1-O5-C5	-2.72	108.79	112.25
4	E	2004	NAG	C1-O5-C5	-2.67	108.86	112.25
3	K	2002	NAG	C1-O5-C5	-2.62	108.92	112.25
4	W	2004	NAG	C1-O5-C5	-2.54	109.02	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	2001	NAG	C2-N2-C7	-2.44	119.90	123.04
3	O	2003	BMA	O2-C2-C3	-2.41	105.27	110.12
3	M	2003	BMA	O2-C2-C3	-2.40	105.29	110.12
6	Q	2001	NAG	C3-C4-C5	-2.37	106.06	110.20
3	W	2001	NAG	C3-C2-N2	-2.24	105.20	110.56
4	Q	2006	NAG	C1-O5-C5	-2.16	109.51	112.25
4	U	2004	NAG	C1-O5-C5	-2.14	109.53	112.25
3	G	2001	NAG	C1-O5-C5	-2.08	109.61	112.25
3	G	2002	NAG	C1-O5-C5	-2.07	109.62	112.25
4	U	2005	NAG	C1-O5-C5	2.01	114.81	112.25
4	Q	2005	NAG	C3-C4-C5	2.08	113.82	110.20
4	S	2003	NAG	C4-C3-C2	2.09	114.48	111.23
3	E	2003	BMA	C1-O5-C5	2.12	114.93	112.25
3	E	2002	NAG	O4-C4-C5	2.12	114.86	109.24
4	O	2005	NAG	C1-O5-C5	2.12	114.94	112.25
4	W	2005	NAG	C4-C3-C2	2.13	114.53	111.23
3	K	2003	BMA	O5-C1-C2	2.14	114.32	110.86
6	Q	2001	NAG	C1-O5-C5	2.23	115.08	112.25
4	M	2005	NAG	C3-C4-C5	2.25	114.11	110.20
4	S	2003	NAG	C3-C4-C5	2.25	114.12	110.20
4	O	2004	NAG	C4-C3-C2	2.28	114.77	111.23
4	G	2004	NAG	C4-C3-C2	2.29	114.78	111.23
3	G	2002	NAG	C4-C3-C2	2.29	114.79	111.23
3	W	2001	NAG	C1-O5-C5	2.30	115.17	112.25
4	E	2004	NAG	C3-C4-C5	2.36	114.31	110.20
4	A	2004	NAG	C4-C3-C2	2.37	114.91	111.23
3	E	2003	BMA	C3-C4-C5	2.37	114.33	110.20
3	M	2003	BMA	C2-C3-C4	2.38	115.09	111.04
3	A	2003	BMA	C1-C2-C3	2.42	112.41	109.54
3	I	2003	BMA	C2-C3-C4	2.45	115.21	111.04
3	G	2001	NAG	C3-C4-C5	2.46	114.48	110.20
3	G	2003	BMA	C2-C3-C4	2.47	115.24	111.04
3	U	2003	BMA	O2-C2-C1	2.58	114.37	109.21
4	a	2001	NAG	C3-C4-C5	2.61	114.74	110.20
3	A	2003	BMA	C2-C3-C4	2.62	115.49	111.04
3	O	2003	BMA	O5-C1-C2	2.63	115.12	110.86
3	K	2003	BMA	O3-C3-C2	2.63	114.76	110.00
3	K	2002	NAG	C4-C3-C2	2.66	115.36	111.23
3	G	2002	NAG	C3-C4-C5	2.74	114.98	110.20
4	W	2004	NAG	C3-C4-C5	2.80	115.08	110.20
3	E	2002	NAG	C1-O5-C5	2.82	115.83	112.25
3	G	2003	BMA	O2-C2-C1	2.83	114.88	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	U	2004	NAG	C4-C3-C2	2.83	115.64	111.23
3	U	2003	BMA	C1-O5-C5	2.84	115.85	112.25
3	I	2003	BMA	O2-C2-C1	2.89	115.01	109.21
3	U	2002	NAG	C4-C3-C2	2.89	115.73	111.23
4	G	2005	NAG	C4-C3-C2	2.93	115.78	111.23
4	Q	2005	NAG	C4-C3-C2	2.95	115.81	111.23
4	U	2004	NAG	C3-C4-C5	2.98	115.39	110.20
3	E	2003	BMA	O3-C3-C2	2.99	115.41	110.00
3	U	2002	NAG	C3-C4-C5	3.03	115.48	110.20
4	E	2004	NAG	C4-C3-C2	3.12	116.09	111.23
3	M	2003	BMA	C3-C4-C5	3.20	115.77	110.20
3	A	2003	BMA	O5-C1-C2	3.20	116.05	110.86
4	S	2004	NAG	C4-C3-C2	3.21	116.21	111.23
4	W	2004	NAG	C4-C3-C2	3.22	116.23	111.23
4	M	2005	NAG	C4-C3-C2	3.23	116.25	111.23
3	A	2003	BMA	O2-C2-C1	3.30	115.83	109.21
3	C	2003	BMA	C2-C3-C4	3.31	116.67	111.04
3	M	2003	BMA	C1-C2-C3	3.33	113.48	109.54
3	C	2003	BMA	C3-C4-C5	3.41	116.15	110.20
6	Q	2003	BMA	O3-C3-C2	3.44	116.21	110.00
3	I	2003	BMA	C3-C4-C5	3.45	116.21	110.20
3	A	2001	NAG	C4-C3-C2	3.50	116.67	111.23
3	O	2003	BMA	C3-C4-C5	3.52	116.34	110.20
3	G	2003	BMA	C3-C4-C5	3.56	116.41	110.20
4	a	2001	NAG	C1-O5-C5	3.61	116.83	112.25
4	I	2004	NAG	C3-C4-C5	3.63	116.53	110.20
3	G	2001	NAG	C4-C3-C2	3.63	116.88	111.23
3	I	2001	NAG	C4-C3-C2	3.68	116.95	111.23
3	E	2002	NAG	C3-C4-C5	3.72	116.68	110.20
3	K	2003	BMA	C1-O5-C5	3.75	117.01	112.25
4	I	2005	NAG	C1-O5-C5	3.91	117.21	112.25
3	M	2003	BMA	C1-O5-C5	3.99	117.31	112.25
4	A	2004	NAG	C3-C4-C5	4.00	117.17	110.20
3	C	2003	BMA	C1-C2-C3	4.11	114.40	109.54
6	Q	2003	BMA	C3-C4-C5	4.35	117.78	110.20
4	G	2004	NAG	C3-C4-C5	4.35	117.79	110.20
4	A	2005	NAG	C1-O5-C5	4.74	118.26	112.25
6	Q	2004	MAN	O5-C1-C2	4.77	118.59	110.86
3	E	2001	NAG	C1-O5-C5	5.30	118.98	112.25
3	C	2003	BMA	O5-C1-C2	5.41	119.63	110.86
3	O	2003	BMA	C1-O5-C5	5.61	119.37	112.25
3	C	2003	BMA	C1-O5-C5	6.30	120.24	112.25

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	0.69	1 (7%)	15,19,21	0.44	0
5	NAG	O	2006	1	14,14,15	1.16	2 (14%)	15,19,21	1.02	2 (13%)
5	NAG	Y	2003	1	14,14,15	0.56	0	15,19,21	0.36	0
5	NAG	c	2001	1	14,14,15	0.54	0	15,19,21	0.38	0
5	NAG	c	2002	1	14,14,15	1.13	2 (14%)	15,19,21	1.19	2 (13%)

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	-3.37	1.38	1.43
5	O	2006	NAG	O5-C1	-2.98	1.38	1.43
5	K	2004	NAG	C1-C2	2.03	1.55	1.52
5	c	2002	NAG	C1-C2	2.14	1.55	1.52
5	O	2006	NAG	C1-C2	2.75	1.56	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	c	2002	NAG	C1-O5-C5	-2.18	109.49	112.25
5	O	2006	NAG	C3-C4-C5	2.27	114.15	110.20
5	O	2006	NAG	C4-C3-C2	2.45	115.04	111.23
5	c	2002	NAG	C4-C3-C2	3.03	115.95	111.23

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%)	-0.23	4 (1%) 81 69	22, 45, 101, 176	0
1	C	324/334 (97%)	-0.07	11 (3%) 49 32	30, 56, 143, 199	0
1	E	324/334 (97%)	-0.06	15 (4%) 36 21	30, 56, 144, 203	0
1	G	324/334 (97%)	-0.25	6 (1%) 70 54	19, 46, 102, 183	0
1	I	324/334 (97%)	-0.31	5 (1%) 76 62	24, 44, 100, 186	0
1	K	324/334 (97%)	0.00	14 (4%) 39 23	33, 57, 143, 218	0
1	M	324/334 (97%)	-0.14	11 (3%) 49 32	26, 50, 152, 220	0
1	O	324/334 (97%)	-0.08	12 (3%) 45 28	25, 50, 140, 226	0
1	Q	324/334 (97%)	-0.06	23 (7%) 19 10	25, 49, 151, 212	0
1	S	324/334 (97%)	-0.03	13 (4%) 42 26	35, 64, 158, 195	0
1	U	324/334 (97%)	-0.01	19 (5%) 26 13	31, 64, 158, 214	0
1	W	324/334 (97%)	-0.06	13 (4%) 42 26	35, 64, 148, 211	0
1	Y	324/334 (97%)	0.31	24 (7%) 17 9	55, 91, 189, 248	0
1	a	324/334 (97%)	0.30	21 (6%) 22 11	55, 87, 184, 263	0
1	c	324/334 (97%)	0.36	22 (6%) 20 10	59, 90, 185, 253	0
2	B	177/181 (97%)	0.39	8 (4%) 37 21	26, 113, 153, 173	0
2	D	177/181 (97%)	0.85	29 (16%) 2 1	41, 155, 195, 210	0
2	F	177/181 (97%)	1.16	46 (25%) 1 0	42, 154, 196, 206	0
2	H	177/181 (97%)	0.34	10 (5%) 28 14	23, 113, 154, 174	0
2	J	177/181 (97%)	0.20	6 (3%) 49 32	27, 113, 153, 166	0
2	L	177/181 (97%)	1.11	35 (19%) 1 1	42, 148, 195, 206	0
2	N	177/181 (97%)	1.28	45 (25%) 1 0	38, 158, 213, 231	0
2	P	177/181 (97%)	1.44	54 (30%) 1 0	38, 163, 213, 231	0
2	R	177/181 (97%)	1.31	47 (26%) 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%)	1.13	46 (25%)	10	45, 153, 201, 209	0
2	V	177/181 (97%)	1.27	45 (25%)	10	49, 153, 213, 228	0
2	X	177/181 (97%)	1.11	38 (21%)	11	50, 155, 204, 220	0
2	Z	177/181 (97%)	2.11	78 (44%)	00	74, 191, 237, 256	0
2	b	177/181 (97%)	1.91	61 (34%)	00	73, 187, 239, 254	0
2	d	177/181 (97%)	2.15	73 (41%)	00	78, 194, 247, 269	0
All	All	7515/7725 (97%)	0.40	834 (11%)	73	19, 79, 201, 269	0

All (834) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	c	16	GLY	18.4
2	d	23	GLY	15.8
1	O	13	ILE	15.4
2	b	141	TYR	14.8
1	U	12	GLN	14.3
2	P	140	PHE	11.1
1	O	12	GLN	10.9
2	d	141	TYR	10.2
1	Q	16	GLY	10.0
1	a	16	GLY	9.9
2	P	27	SER	9.7
2	V	157	TYR	9.7
2	d	8	GLY	9.6
2	d	153	ARG	9.3
2	X	142	HIS	9.1
2	b	153	ARG	9.0
2	R	32	SER	9.0
1	c	23	THR	9.0
2	Z	22	TYR	8.9
2	P	32	SER	8.8
1	Y	12	GLN	8.8
2	P	33	GLY	8.6
1	Y	23	THR	8.4
2	Z	23	GLY	8.4
2	d	32	SER	8.4
2	Z	157	TYR	8.3
2	N	22	TYR	8.3
2	F	157	TYR	8.3
1	O	14	CYS	8.1

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Mol	Chain	Res	Type	RSRZ
1	Q	14	CYS	8.1
2	V	158	ASP	8.1
2	V	140	PHE	8.0
1	a	23	THR	8.0
2	X	27	SER	7.9
1	M	9	PRO	7.9
2	b	35	ALA	7.9
2	b	37	ASP	7.8
2	V	22	TYR	7.8
2	d	152	VAL	7.8
2	N	29	GLU	7.4
1	Q	13	ILE	7.4
2	R	22	TYR	7.4
1	S	12	GLN	7.4
1	W	12	GLN	7.4
2	X	140	PHE	7.3
1	K	12	GLN	7.3
2	F	1	GLY	7.3
2	P	26	HIS	7.3
2	Z	140	PHE	7.3
1	M	8	ASP	7.3
1	M	10	GLY	7.2
2	Z	37	ASP	7.1
2	b	142	HIS	7.1
2	Z	153	ARG	7.1
2	b	130	ALA	7.1
1	M	16	GLY	7.0
2	Z	152	VAL	7.0
2	Z	35	ALA	7.0
1	O	324	PRO	6.9
1	Q	12	GLN	6.9
2	b	24	TYR	6.9
1	c	15	ILE	6.8
1	M	14	CYS	6.8
2	Z	130	ALA	6.8
2	F	140	PHE	6.7
2	Z	38	LYS	6.7
2	T	140	PHE	6.7
2	Z	1	GLY	6.7
2	P	25	HIS	6.6
2	Z	159	TYR	6.6
2	N	160	PRO	6.6

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Mol	Chain	Res	Type	RSRZ
2	b	23	GLY	6.6
1	K	13	ILE	6.5
2	D	26	HIS	6.5
2	L	1	GLY	6.5
2	b	1	GLY	6.5
1	Y	14	CYS	6.5
1	Q	18	HIS	6.5
2	d	24	TYR	6.4
1	O	16	GLY	6.4
2	V	149	MET	6.4
2	R	27	SER	6.4
2	d	157	TYR	6.4
2	b	36	ALA	6.4
1	M	13	ILE	6.4
1	M	12	GLN	6.4
1	Y	13	ILE	6.3
1	K	16	GLY	6.3
2	b	129	ASN	6.3
2	d	37	ASP	6.2
2	X	143	LYS	6.2
2	P	31	GLY	6.2
2	N	140	PHE	6.2
2	P	22	TYR	6.2
2	V	143	LYS	6.2
2	Z	41	THR	6.2
2	b	26	HIS	6.2
1	I	324	PRO	6.2
2	b	140	PHE	6.2
2	L	142	HIS	6.1
2	Z	125	GLN	6.1
1	E	324	PRO	6.1
1	U	8	ASP	6.0
2	d	154	ASN	6.0
2	R	176	GLY	6.0
2	d	36	ALA	6.0
2	d	38	LYS	6.0
2	F	158	ASP	6.0
2	N	27	SER	5.9
2	b	157	TYR	5.9
1	Q	320	LEU	5.9
2	N	23	GLY	5.9
2	L	138	PHE	5.9

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Mol	Chain	Res	Type	RSRZ
2	X	22	TYR	5.9
1	Y	16	GLY	5.8
2	L	22	TYR	5.8
2	L	140	PHE	5.8
2	b	128	ASP	5.8
1	O	10	GLY	5.7
2	Z	24	TYR	5.7
2	L	144	CYS	5.7
2	b	143	LYS	5.6
1	U	13	ILE	5.6
2	X	157	TYR	5.5
2	X	26	HIS	5.5
2	V	27	SER	5.5
1	a	13	ILE	5.5
1	M	11	ASP	5.5
2	F	33	GLY	5.5
2	V	161	GLN	5.5
1	O	11	ASP	5.5
2	d	143	LYS	5.5
2	D	22	TYR	5.4
2	d	144	CYS	5.4
2	V	35	ALA	5.4
2	N	144	CYS	5.4
2	T	22	TYR	5.4
2	d	22	TYR	5.4
2	d	170	ARG	5.4
2	d	156	THR	5.4
2	V	144	CYS	5.3
2	L	134	GLY	5.3
1	c	14	CYS	5.3
1	G	324	PRO	5.3
2	T	157	TYR	5.3
2	b	32	SER	5.3
2	Z	148	CYS	5.3
2	Z	176	GLY	5.3
1	Y	21[A]	ASN	5.3
2	X	160	PRO	5.3
2	D	140	PHE	5.2
2	d	16	GLY	5.2
2	T	35	ALA	5.2
1	Q	10	GLY	5.2
2	Z	42	GLN	5.2

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Mol	Chain	Res	Type	RSRZ
2	d	155	GLY	5.1
1	c	13	ILE	5.1
2	D	1	GLY	5.1
2	b	152	VAL	5.1
2	X	23	GLY	5.0
1	a	11	ASP	5.0
2	V	24	TYR	5.0
2	P	23	GLY	5.0
1	C	12	GLN	5.0
2	N	157	TYR	5.0
2	d	132	GLU	5.0
2	P	160	PRO	5.0
2	P	10	ILE	4.9
2	d	158	ASP	4.9
2	d	163	SER	4.9
2	R	33	GLY	4.9
2	V	141	TYR	4.9
2	P	29	GLU	4.9
2	T	158	ASP	4.9
2	R	138	PHE	4.9
2	D	144	CYS	4.9
2	Z	36	ALA	4.9
2	T	141	TYR	4.9
2	d	35	ALA	4.9
2	T	143	LYS	4.9
2	b	38	LYS	4.9
1	Q	319	GLY	4.9
2	R	171	GLU	4.9
2	P	144	CYS	4.8
2	P	148	CYS	4.8
2	V	148	CYS	4.8
1	K	15	ILE	4.8
2	F	141	TYR	4.8
1	U	14	CYS	4.8
1	C	13	ILE	4.8
1	a	22	SER	4.8
2	H	175	SER	4.8
2	Z	16	GLY	4.8
2	X	149	MET	4.8
2	b	160	PRO	4.8
2	N	32	SER	4.8
2	N	24	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
2	R	31	GLY	4.7
2	T	24	TYR	4.7
2	N	159	TYR	4.7
2	Z	4	GLY	4.7
2	R	160	PRO	4.7
2	X	24	TYR	4.7
2	N	21	TRP	4.7
2	F	142	HIS	4.7
2	T	21	TRP	4.7
2	d	31	GLY	4.7
2	R	25	HIS	4.6
1	Y	15	ILE	4.6
1	S	13	ILE	4.6
2	X	32	SER	4.6
2	T	38	LYS	4.6
2	b	7	ALA	4.6
2	N	176	GLY	4.6
2	X	158	ASP	4.6
2	L	133	LEU	4.6
1	c	22	SER	4.6
2	b	144	CYS	4.6
2	b	22	TYR	4.5
2	V	156	THR	4.5
2	Z	136	GLY	4.5
2	b	149	MET	4.5
1	E	322	ASN	4.5
2	d	164	GLU	4.5
2	P	7	ALA	4.5
2	b	148	CYS	4.5
2	L	132	GLU	4.4
2	Z	26	HIS	4.4
2	d	148	CYS	4.4
1	c	320	LEU	4.4
2	X	141	TYR	4.4
2	F	32	SER	4.4
2	Z	126	LEU	4.4
2	T	144	CYS	4.4
1	Y	323	SER	4.4
2	Z	32	SER	4.4
2	L	145	ASP	4.4
1	Y	22	SER	4.3
2	T	149	MET	4.3

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Mol	Chain	Res	Type	RSRZ
2	P	139	GLU	4.3
2	d	168	LEU	4.3
2	b	27	SER	4.3
1	O	9	PRO	4.3
2	D	134	GLY	4.3
2	b	31	GLY	4.3
1	S	8	ASP	4.3
2	H	177	ARG	4.3
2	Z	29	GLU	4.3
2	R	157	TYR	4.3
2	d	26	HIS	4.3
2	R	175	SER	4.2
2	F	126	LEU	4.2
2	F	22	TYR	4.2
1	C	24	GLU	4.2
1	I	8	ASP	4.2
2	V	21	TRP	4.2
1	C	324	PRO	4.2
2	b	34	TYR	4.2
1	c	21[A]	ASN	4.2
2	P	138	PHE	4.2
2	d	9	PHE	4.2
2	P	157	TYR	4.2
2	N	46	ASP	4.1
2	Z	128	ASP	4.1
2	b	138	PHE	4.1
2	b	168	LEU	4.1
2	H	176	GLY	4.1
2	R	177	ARG	4.1
1	E	25	GLN	4.1
1	Y	317	ALA	4.1
2	d	27	SER	4.1
2	V	152	VAL	4.1
2	Z	154	ASN	4.1
2	P	142	HIS	4.1
2	N	33	GLY	4.1
1	Y	30	MET	4.0
1	K	319	GLY	4.0
2	N	35	ALA	4.0
1	K	17	TYR	4.0
2	F	177	ARG	4.0
2	d	121	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
2	Z	143	LYS	4.0
2	Z	151	SER	4.0
1	Q	24	GLU	4.0
2	T	156	THR	4.0
2	V	23	GLY	4.0
2	Z	40	SER	4.0
2	d	15	GLN	4.0
2	V	153	ARG	4.0
2	b	33	GLY	4.0
2	L	141	TYR	4.0
2	T	172	GLU	4.0
1	G	9	PRO	3.9
2	d	18	VAL	3.9
2	d	25	HIS	3.9
1	Y	11	ASP	3.9
2	Z	46	ASP	3.9
2	d	172	GLU	3.9
1	S	324	PRO	3.9
1	K	324	PRO	3.9
2	N	148	CYS	3.9
2	D	27	SER	3.9
2	X	16	GLY	3.9
1	Q	324	PRO	3.9
2	d	1	GLY	3.9
1	K	14	CYS	3.9
2	X	156	THR	3.9
1	A	8	ASP	3.9
2	Z	39	GLU	3.9
2	N	143	LYS	3.9
2	P	5	ALA	3.9
1	c	20	ASN	3.9
2	L	24	TYR	3.9
2	Z	25	HIS	3.9
2	Z	141	TYR	3.9
2	d	142	HIS	3.9
2	N	142	HIS	3.9
1	Q	11	ASP	3.8
2	F	38	LYS	3.8
1	E	24	GLU	3.8
2	R	140	PHE	3.8
2	V	126	LEU	3.8
1	a	15	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
2	V	139	GLU	3.8
2	B	176	GLY	3.8
2	R	134	GLY	3.8
2	B	175	SER	3.8
2	b	177	ARG	3.8
1	c	37	THR	3.8
2	d	136	GLY	3.8
2	D	157	TYR	3.8
2	X	7	ALA	3.8
2	R	26	HIS	3.8
2	D	139	GLU	3.8
2	N	25	HIS	3.8
2	V	151	SER	3.8
2	N	158	ASP	3.8
2	V	162	TYR	3.7
2	X	25	HIS	3.7
2	D	33	GLY	3.7
2	X	151	SER	3.7
2	P	158	ASP	3.7
1	W	8	ASP	3.7
2	R	19	ASP	3.7
2	X	161	GLN	3.7
2	T	26	HIS	3.7
2	b	170	ARG	3.7
2	P	162	TYR	3.7
1	E	23	THR	3.7
2	V	25	HIS	3.7
2	d	166	ALA	3.7
1	c	11	ASP	3.7
2	P	6	ILE	3.7
2	P	4	GLY	3.7
2	F	35	ALA	3.7
2	R	158	ASP	3.6
2	d	171	GLU	3.6
2	R	137	CYS	3.6
2	R	1	GLY	3.6
2	F	21	TRP	3.6
2	d	140	PHE	3.6
2	Z	160	PRO	3.6
2	N	30	GLN	3.6
1	U	11	ASP	3.6
2	d	149	MET	3.6

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Mol	Chain	Res	Type	RSRZ
1	a	323	SER	3.6
2	T	27	SER	3.6
1	A	324	PRO	3.6
1	W	288	ILE	3.6
2	L	146	ASN	3.6
2	R	18	VAL	3.6
2	X	35	ALA	3.6
2	V	155	GLY	3.6
2	Z	47	GLY	3.6
2	Z	127	ARG	3.6
1	Y	9	PRO	3.6
2	b	158	ASP	3.6
1	U	9	PRO	3.6
2	V	147	GLU	3.5
2	R	159	TYR	3.5
2	F	156	THR	3.5
2	d	106	ARG	3.5
1	Q	8	ASP	3.5
1	W	11	ASP	3.5
2	b	9	PHE	3.5
2	F	138	PHE	3.5
2	b	156	THR	3.5
2	N	26	HIS	3.5
2	X	153	ARG	3.5
2	Z	175	SER	3.5
1	a	20	ASN	3.5
2	X	162	TYR	3.5
2	V	150	GLU	3.5
2	d	17	MET	3.5
1	Y	322	ASN	3.5
1	a	63	ASP	3.5
2	B	140	PHE	3.5
2	N	19	ASP	3.5
1	S	9	PRO	3.4
2	D	25	HIS	3.4
2	L	177	ARG	3.4
2	Z	144	CYS	3.4
2	d	151	SER	3.4
2	d	29	GLU	3.4
2	F	26	HIS	3.4
1	E	13	ILE	3.4
2	D	158	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
2	Z	156	THR	3.4
2	Z	45	ILE	3.4
1	O	34	VAL	3.4
2	F	145	ASP	3.4
2	R	29	GLU	3.4
2	Z	171	GLU	3.4
2	P	137	CYS	3.4
2	Z	131	LYS	3.4
2	Z	13	GLY	3.4
2	X	144	CYS	3.4
1	c	63	ASP	3.4
2	N	161	GLN	3.4
2	P	132	GLU	3.4
1	O	323	SER	3.4
2	T	23	GLY	3.4
1	Q	20	ASN	3.4
2	b	132	GLU	3.4
2	X	21	TRP	3.4
1	Y	34	VAL	3.3
2	F	24	TYR	3.3
2	P	156	THR	3.3
2	V	26	HIS	3.3
2	Z	149	MET	3.3
2	F	171	GLU	3.3
2	R	141	TYR	3.3
2	N	36	ALA	3.3
1	c	312	ASN	3.3
2	X	31	GLY	3.3
1	c	24	GLU	3.3
2	T	18	VAL	3.3
2	b	109	ASP	3.3
2	Z	34	TYR	3.3
1	E	16	GLY	3.3
1	W	16	GLY	3.3
2	L	148	CYS	3.3
1	G	12	GLN	3.3
2	F	166	ALA	3.3
1	W	13	ILE	3.3
2	X	29	GLU	3.3
2	P	145	ASP	3.3
2	D	145	ASP	3.3
2	V	16	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	b	163	SER	3.3
2	V	29	GLU	3.2
2	Z	33	GLY	3.2
2	B	156	THR	3.2
2	F	176	GLY	3.2
2	R	21	TRP	3.2
2	b	155	GLY	3.2
2	V	118	LEU	3.2
2	d	135	ASN	3.2
2	N	42	GLN	3.2
2	N	177	ARG	3.2
2	F	31	GLY	3.2
2	b	2	LEU	3.2
1	G	8	ASP	3.2
1	O	8	ASP	3.2
2	P	154	ASN	3.2
1	K	24	GLU	3.2
2	R	132	GLU	3.2
2	Z	147	GLU	3.2
1	Q	17	TYR	3.2
2	N	146	ASN	3.2
2	T	161	GLN	3.2
2	V	125	GLN	3.2
1	A	9	PRO	3.2
1	I	9	PRO	3.2
1	Q	9	PRO	3.2
2	L	23	GLY	3.2
2	D	153	ARG	3.2
2	T	19	ASP	3.1
2	P	131	LYS	3.1
2	N	175	SER	3.1
2	b	159	TYR	3.1
2	d	130	ALA	3.1
1	U	21[A]	ASN	3.1
1	W	324	PRO	3.1
1	c	17	TYR	3.1
2	D	32	SER	3.1
2	R	168	LEU	3.1
2	F	144	CYS	3.1
2	L	168	LEU	3.1
2	P	155	GLY	3.1
2	P	161	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
2	N	31	GLY	3.1
2	P	28	ASN	3.1
2	D	177	ARG	3.1
2	N	44	ALA	3.1
2	J	38	LYS	3.1
2	Z	18	VAL	3.1
2	B	177	ARG	3.1
2	d	33	GLY	3.1
2	Z	132	GLU	3.1
2	L	175	SER	3.1
1	E	12	GLN	3.1
2	X	33	GLY	3.0
1	U	322	ASN	3.0
2	L	158	ASP	3.0
1	U	22	SER	3.0
2	F	175	SER	3.0
2	T	160	PRO	3.0
1	S	21[A]	ASN	3.0
2	L	126	LEU	3.0
2	V	38	LYS	3.0
2	Z	158	ASP	3.0
2	L	21	TRP	3.0
1	C	21[A]	ASN	3.0
2	D	149	MET	3.0
2	Z	14	TRP	3.0
2	L	31	GLY	3.0
2	P	177	ARG	3.0
1	K	10	GLY	3.0
2	X	147	GLU	3.0
2	L	38	LYS	3.0
2	d	111	HIS	3.0
2	P	143	LYS	3.0
2	R	139	GLU	3.0
2	V	160	PRO	3.0
2	P	146	ASN	3.0
2	L	157	TYR	3.0
2	P	34	TYR	3.0
2	F	127	ARG	3.0
2	P	46	ASP	2.9
2	R	142	HIS	2.9
2	L	143	LYS	2.9
2	B	16	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
2	T	173	ILE	2.9
2	d	34	TYR	2.9
2	L	139	GLU	2.9
2	V	145	ASP	2.9
2	Z	142	HIS	2.9
2	R	164	GLU	2.9
2	R	166	ALA	2.9
2	T	16	GLY	2.9
1	G	13	ILE	2.9
2	d	131	LYS	2.9
2	d	134	GLY	2.9
2	D	126	LEU	2.9
2	T	25	HIS	2.9
1	U	34	VAL	2.9
1	Y	324	PRO	2.9
1	c	12	GLN	2.9
1	K	31	GLU	2.9
1	W	21[A]	ASN	2.9
2	T	142	HIS	2.9
2	b	8	GLY	2.9
1	K	23	THR	2.9
2	R	144	CYS	2.9
1	S	323	SER	2.9
2	D	31	GLY	2.9
1	C	23	THR	2.9
2	T	33	GLY	2.9
2	V	154	ASN	2.8
2	T	168	LEU	2.8
2	N	34	TYR	2.8
2	P	153	ARG	2.8
2	b	25	HIS	2.8
1	a	317	ALA	2.8
2	J	177	ARG	2.8
1	Y	20	ASN	2.8
2	L	27	SER	2.8
2	L	166	ALA	2.8
1	a	21[A]	ASN	2.8
2	R	4	GLY	2.8
2	T	171	GLU	2.8
2	V	142	HIS	2.8
1	Q	322	ASN	2.8
1	a	17	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
2	P	47	GLY	2.8
2	T	29	GLU	2.8
1	G	85	SER	2.8
2	b	164	GLU	2.8
2	D	143	LYS	2.8
2	F	19	ASP	2.8
2	N	145	ASP	2.8
2	Z	137	CYS	2.8
2	b	145	ASP	2.8
2	H	22	TYR	2.8
1	Q	36	VAL	2.8
2	P	35	ALA	2.8
2	T	42	GLN	2.8
2	L	152	VAL	2.7
2	d	28	ASN	2.7
2	N	1	GLY	2.7
2	R	34	TYR	2.7
2	X	148	CYS	2.7
1	U	294	PHE	2.7
2	V	177	ARG	2.7
2	P	44	ALA	2.7
2	P	130	ALA	2.7
2	F	173	ILE	2.7
2	P	134	GLY	2.7
2	P	159	TYR	2.7
1	c	19	ALA	2.7
2	Z	170	ARG	2.7
2	d	14	TRP	2.7
2	L	131	LYS	2.7
2	Z	48	VAL	2.7
1	W	318	THR	2.7
2	b	124	LEU	2.7
1	Q	22	SER	2.7
1	C	15	ILE	2.7
2	R	170	ARG	2.7
2	Z	49	THR	2.7
2	T	153	ARG	2.7
2	X	145	ASP	2.7
2	b	126	LEU	2.6
1	E	320	LEU	2.6
2	R	135	ASN	2.6
2	T	36	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	N	28	ASN	2.6
2	P	30	GLN	2.6
2	N	17	MET	2.6
2	T	165	GLU	2.6
2	T	34	TYR	2.6
2	B	38	LYS	2.6
2	T	166	ALA	2.6
2	D	21	TRP	2.6
2	P	1	GLY	2.6
2	X	1	GLY	2.6
1	Y	63	ASP	2.6
2	T	9	PHE	2.6
1	E	323	SER	2.6
1	Q	323	SER	2.6
2	T	162	TYR	2.6
2	F	120	ASP	2.6
2	F	146	ASN	2.6
2	d	42	GLN	2.6
2	b	29	GLU	2.6
2	d	160	PRO	2.6
1	O	320	LEU	2.5
2	F	37	ASP	2.5
1	Y	17	TYR	2.5
2	F	168	LEU	2.5
2	T	146	ASN	2.5
2	Z	174	SER	2.5
2	D	148	CYS	2.5
2	B	142	HIS	2.5
2	V	146	ASN	2.5
2	F	152	VAL	2.5
2	P	24	TYR	2.5
2	J	140	PHE	2.5
2	d	10	ILE	2.5
2	P	19	ASP	2.5
2	L	149	MET	2.5
1	A	12	GLN	2.5
2	F	162	TYR	2.5
1	Y	35	THR	2.5
1	W	20	ASN	2.5
2	F	153	ARG	2.5
2	R	156	THR	2.5
1	E	51	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	R	42	GLN	2.5
2	Z	8	GLY	2.5
1	Y	31	GLU	2.5
2	Z	106	ARG	2.5
2	F	169	LYS	2.4
2	N	16	GLY	2.4
2	d	162	TYR	2.4
1	U	23	THR	2.4
2	d	41	THR	2.4
2	L	33	GLY	2.4
2	d	139	GLU	2.4
2	T	44	ALA	2.4
2	R	23	GLY	2.4
2	R	155	GLY	2.4
1	a	324	PRO	2.4
1	c	95	ASN	2.4
2	F	139	GLU	2.4
1	Q	25	GLN	2.4
2	d	173	ILE	2.4
1	K	320	LEU	2.4
2	Z	122	VAL	2.4
1	C	14	CYS	2.4
2	Z	27	SER	2.4
1	c	39	ALA	2.4
2	Z	164	GLU	2.4
2	F	18	VAL	2.4
2	Z	163	SER	2.4
1	M	21[A]	ASN	2.4
2	b	167	ARG	2.4
1	I	12	GLN	2.4
2	T	148	CYS	2.4
2	T	152	VAL	2.4
1	c	311	SER	2.4
2	Z	21	TRP	2.4
1	S	25	GLN	2.4
1	a	280	LYS	2.3
1	E	22	SER	2.3
2	D	35	ALA	2.3
2	H	140	PHE	2.3
2	P	21	TRP	2.3
2	d	45	ILE	2.3
1	S	50	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	T	151	SER	2.3
2	Z	7	ALA	2.3
1	E	18	HIS	2.3
2	F	34	TYR	2.3
2	b	125	GLN	2.3
2	N	168	LEU	2.3
2	d	6	ILE	2.3
1	Q	21[A]	ASN	2.3
2	H	142	HIS	2.3
2	V	30	GLN	2.3
1	C	16	GLY	2.3
2	D	23	GLY	2.3
2	T	20	GLY	2.3
1	C	22	SER	2.3
2	V	163	SER	2.3
2	D	113	SER	2.3
2	R	8	GLY	2.3
2	Z	50	ASN	2.3
2	X	19	ASP	2.3
1	U	307	LYS	2.3
2	L	32	SER	2.3
2	Z	161	GLN	2.3
2	d	133	LEU	2.3
1	W	18	HIS	2.3
2	N	14	TRP	2.3
1	Y	95	ASN	2.3
2	N	126	LEU	2.3
2	R	126	LEU	2.3
1	E	17	TYR	2.2
2	F	109	ASP	2.2
2	L	120	ASP	2.2
1	a	32	LYS	2.2
2	D	36	ALA	2.2
1	a	312	ASN	2.2
2	b	135	ASN	2.2
2	D	24	TYR	2.2
1	C	36	VAL	2.2
1	U	25	GLN	2.2
2	H	174	SER	2.2
2	X	146	ASN	2.2
2	b	162	TYR	2.2
1	K	25	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	26	HIS	2.2
2	D	132	GLU	2.2
2	b	171	GLU	2.2
2	R	153	ARG	2.2
2	X	20	GLY	2.2
2	b	176	GLY	2.2
2	F	112	ASP	2.2
2	d	57	ASP	2.2
2	b	131	LYS	2.2
1	c	48	ASN	2.2
2	P	18	VAL	2.2
2	T	147	GLU	2.2
2	b	121	LYS	2.2
2	N	149	MET	2.2
1	Q	19	ALA	2.2
1	U	319	GLY	2.2
2	Z	44	ALA	2.2
2	N	37	ASP	2.2
2	R	37	ASP	2.2
1	a	14	CYS	2.2
1	U	15	ILE	2.2
2	d	109	ASP	2.2
1	U	323	SER	2.2
2	N	163	SER	2.2
2	b	28	ASN	2.2
2	d	39	GLU	2.1
1	U	10	GLY	2.1
1	W	281	CYS	2.1
2	J	149	MET	2.1
1	W	319	GLY	2.1
2	T	30	GLN	2.1
2	Z	31	GLY	2.1
2	T	154	ASN	2.1
2	F	172	GLU	2.1
1	M	17	TYR	2.1
2	P	149	MET	2.1
1	S	10	GLY	2.1
2	F	148	CYS	2.1
2	P	11	GLU	2.1
2	L	45	ILE	2.1
1	I	23	THR	2.1
2	D	38	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	126	LEU	2.1
2	Z	116	LYS	2.1
1	Y	85	SER	2.1
2	b	4	GLY	2.1
2	b	120	ASP	2.1
1	E	34	VAL	2.1
2	d	21	TRP	2.1
2	H	144	CYS	2.1
2	X	9	PHE	2.1
2	F	111	HIS	2.1
2	X	17	MET	2.1
1	a	281	CYS	2.1
1	a	30	MET	2.1
1	S	34	VAL	2.1
2	X	18	VAL	2.1
1	U	40	GLN	2.1
2	Z	150	GLU	2.1
1	Q	318	THR	2.1
2	N	153	ARG	2.1
1	c	97	CYS	2.0
2	V	175	SER	2.0
2	J	176	GLY	2.0
1	M	324	PRO	2.0
2	Z	115	VAL	2.0
1	Y	8	ASP	2.0
2	J	175	SER	2.0
2	d	169	LYS	2.0
1	a	35	THR	2.0
2	P	8	GLY	2.0
2	V	33	GLY	2.0
1	a	36	VAL	2.0
2	V	44	ALA	2.0
2	d	7	ALA	2.0
2	R	30	GLN	2.0
2	V	138	PHE	2.0
2	F	113	SER	2.0
2	Z	15	GLN	2.0
2	Z	138	PHE	2.0
2	d	138	PHE	2.0
2	F	132	GLU	2.0
2	Z	57	ASP	2.0
2	Z	134	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	b	134	GLY	2.0
2	d	113	SER	2.0
2	R	146	ASN	2.0
2	V	129	ASN	2.0
1	S	14	CYS	2.0
1	S	272	LEU	2.0
2	R	46	ASP	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	2.96	56,75,85,89	0
3	NAG	O	2001	14/15	0.95	0.28	1.60	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	0.89	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	0.47	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	0.04	64,71,80,92	0
3	NAG	G	2001	14/15	0.95	0.18	-0.18	54,63,66,66	0
3	BMA	K	2003	11/12	0.78	0.21	-0.19	32,49,59,61	0
4	NAG	S	2001	14/15	0.90	0.18	-0.19	50,69,87,102	0
4	NAG	Y	2001	14/15	0.90	0.19	-1.36	95,100,108,119	0
4	NAG	Y	2002	14/15	0.79	0.24	-	115,131,144,145	0
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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(Å 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	0.67	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.