Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:45 PM GMT

PDB ID	:	4MHI
Title	:	Crystal structure of a H5N1 influenza virus hemagglutinin from A/goose/Guangdong/1/96
Authors	:	Zhu, X.; Wilson, I.A.
Deposited on	:	2013-08-29
Resolution	:	2.60 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 (i) symbol.

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

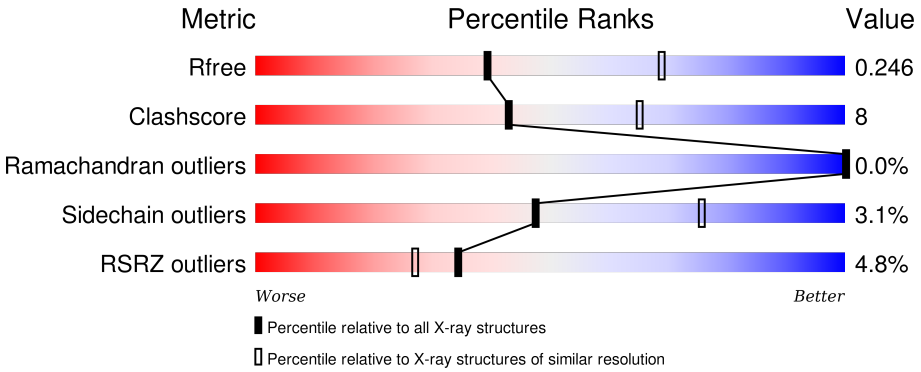
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	334	2% 77% 19%
1	C	334	8% 74% 19%
1	E	334	6% 72% 22%
1	G	334	2% 75% 20%
1	I	334	% 78% 18%

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Mol	Chain	Length	Quality of chain
1	K	334	5% 72% 23%
1	M	334	9% 75% 20%
1	O	334	5% 76% 20%
1	Q	334	% 78% 17%
2	B	182	2% 80% 15% 5%
2	D	182	3% 77% 18% 5%
2	F	182	13% 78% 17% 5%
2	H	182	9% 77% 17% 5%
2	J	182	2% 86% 9% 5%
2	L	182	9% 76% 18% 5%
2	N	182	4% 83% 12% 5%
2	P	182	3% 80% 15% 5%
2	R	182	% 82% 13% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36134 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	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	C	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	E	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	G	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	I	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	K	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	M	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	O	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			
1	Q	323	Total	C	N	O	S	0	0	0
			2551	1609	442	485	15			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
A	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
A	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
A	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
C	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
C	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
C	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
C	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
E	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
E	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
E	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6

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Chain	Residue	Modelled	Actual	Comment	Reference
E	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
G	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
G	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
G	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
G	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
I	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
I	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
I	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
I	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
K	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
K	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
K	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
K	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
M	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
M	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
M	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
M	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
O	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
O	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
O	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
O	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
Q	7	ALA	-	EXPRESSION TAG	UNP Q9Q0U6
Q	8	ASP	-	EXPRESSION TAG	UNP Q9Q0U6
Q	9	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
Q	10	GLY	-	EXPRESSION TAG	UNP Q9Q0U6

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	D	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	F	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	H	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	J	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	L	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	N	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			
2	R	173	Total	C	N	O	S	0	0	0
			1403	872	242	281	8			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
B	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
B	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
B	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
B	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
B	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
B	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
D	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
D	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
D	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
D	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
D	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
D	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
D	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
F	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
F	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
F	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
F	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
F	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
F	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
F	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
H	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
H	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
H	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
H	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
H	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
H	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
H	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
J	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
J	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
J	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
J	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
J	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
J	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6

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Chain	Residue	Modelled	Actual	Comment	Reference
J	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
L	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
L	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
L	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
L	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
L	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
L	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
L	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
N	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
N	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
N	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
N	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
N	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
N	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
N	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
P	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
P	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
P	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
P	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
P	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
P	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
P	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
R	176	SER	-	EXPRESSION TAG	UNP Q9Q0U6
R	177	GLY	-	EXPRESSION TAG	UNP Q9Q0U6
R	178	ARG	-	EXPRESSION TAG	UNP Q9Q0U6
R	179	LEU	-	EXPRESSION TAG	UNP Q9Q0U6
R	180	VAL	-	EXPRESSION TAG	UNP Q9Q0U6
R	181	PRO	-	EXPRESSION TAG	UNP Q9Q0U6
R	182	ARG	-	EXPRESSION TAG	UNP Q9Q0U6

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	I	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		

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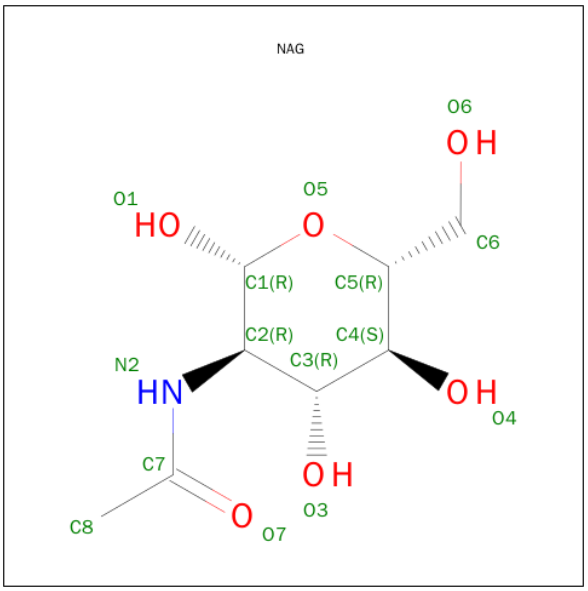
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	2	Total C N O 28 16 2 10	0	0
3	R	2	Total C N O 28 16 2 10	0	0

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	I	1	Total C N O 14 8 1 5	0	0
4	K	1	Total C N O 14 8 1 5	0	0
4	K	1	Total C N O 14 8 1 5	0	0

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

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Q	3	Total C N O 39 22 2 15	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	7	Total O 7 7	0	0
6	B	5	Total O 5 5	0	0
6	C	6	Total O 6 6	0	0
6	D	8	Total O 8 8	0	0
6	E	6	Total O 6 6	0	0
6	F	2	Total O 2 2	0	0
6	G	14	Total O 14 14	0	0
6	H	4	Total O 4 4	0	0
6	I	9	Total O 9 9	0	0
6	J	12	Total O 12 12	0	0
6	K	10	Total O 10 10	0	0

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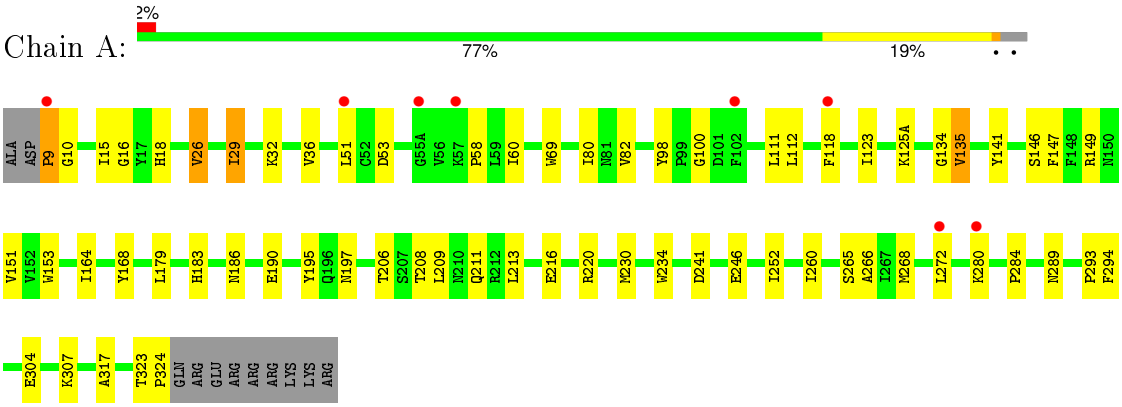
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	L	2	Total O 2 2	0	0
6	M	5	Total O 5 5	0	0
6	N	1	Total O 1 1	0	0
6	O	8	Total O 8 8	0	0
6	P	2	Total O 2 2	0	0
6	Q	8	Total O 8 8	0	0
6	R	8	Total O 8 8	0	0

3 Residue-property plots (i)

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.

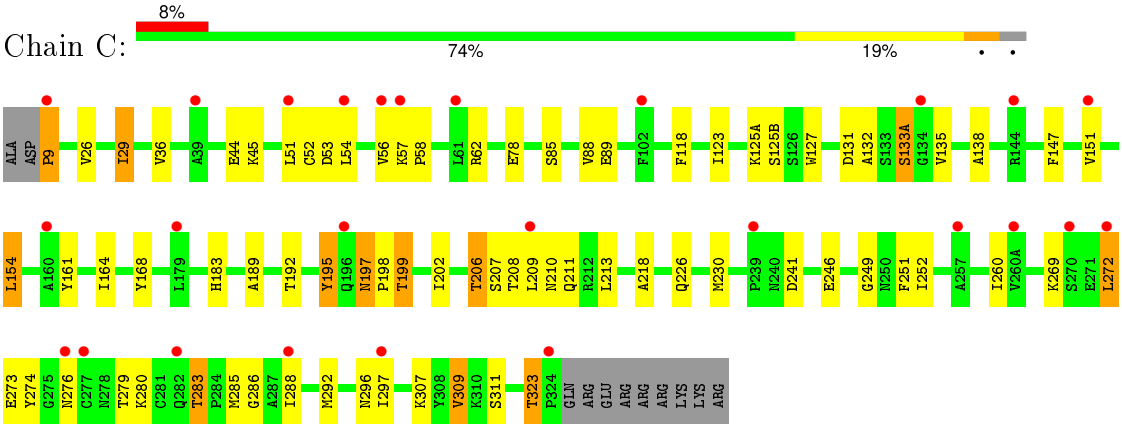
- Molecule 1: Hemagglutinin HA1 chain

Chain A:



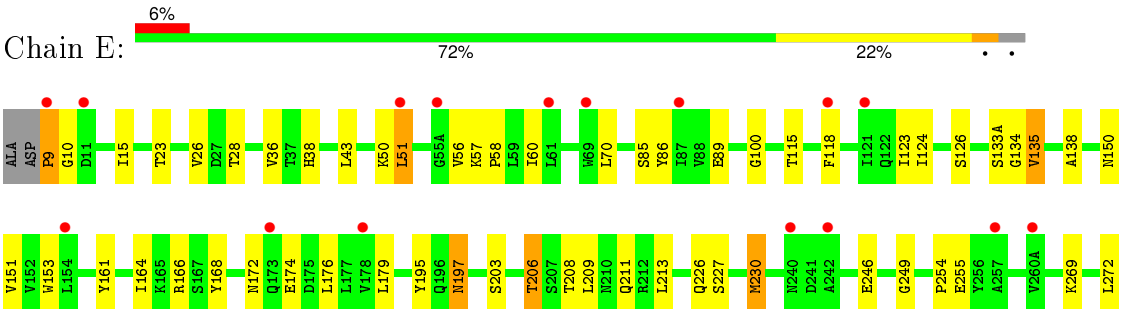
- Molecule 1: Hemagglutinin HA1 chain

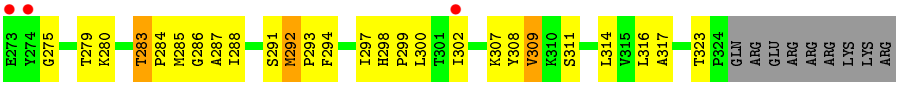
Chain C:



- Molecule 1: Hemagglutinin HA1 chain

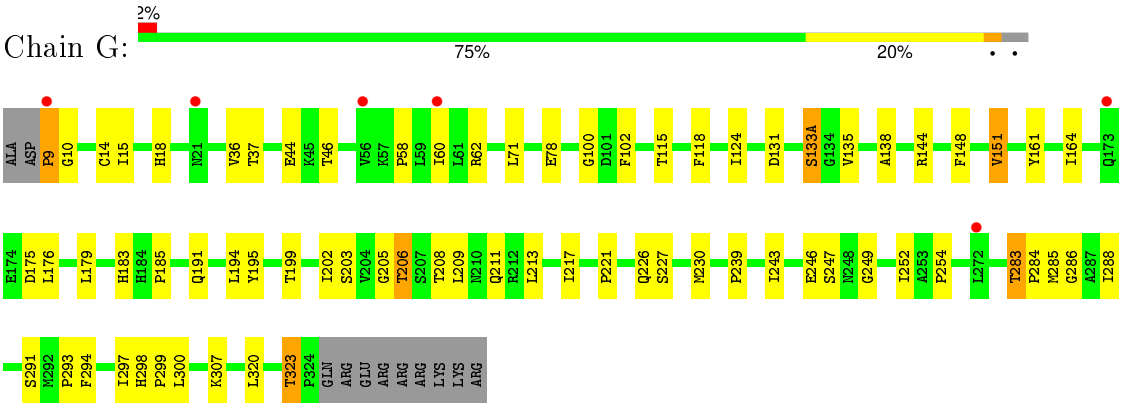
Chain E:





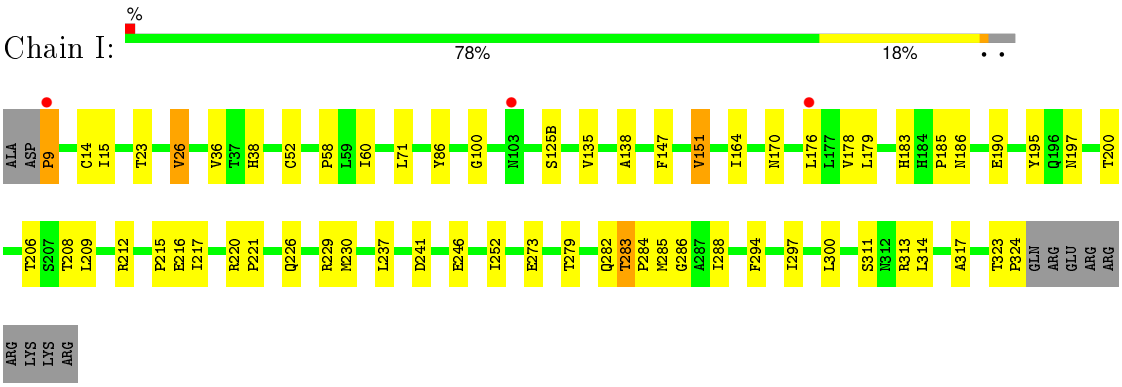
• Molecule 1: Hemagglutinin HA1 chain

Chain G:



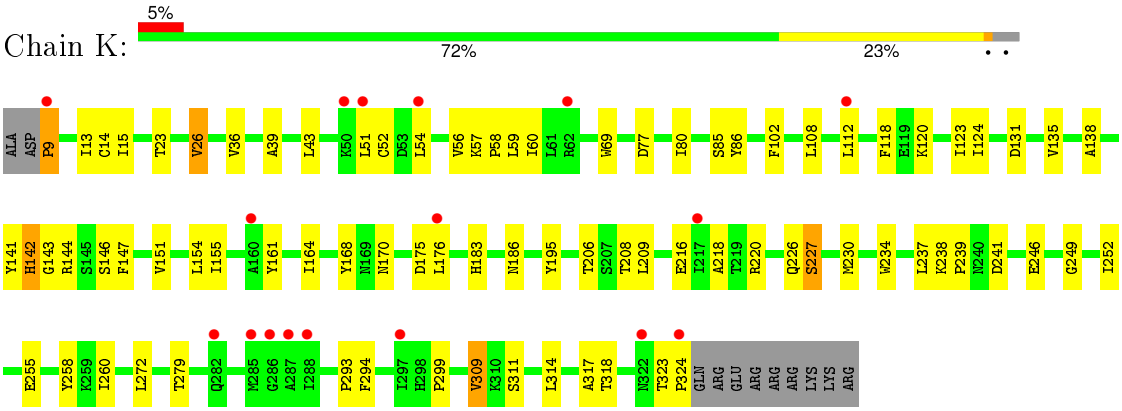
• Molecule 1: Hemagglutinin HA1 chain

Chain I:



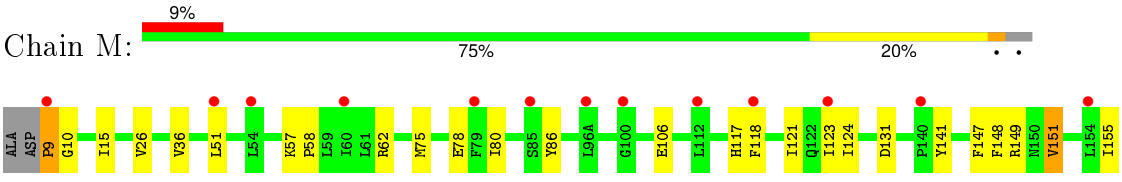
• Molecule 1: Hemagglutinin HA1 chain

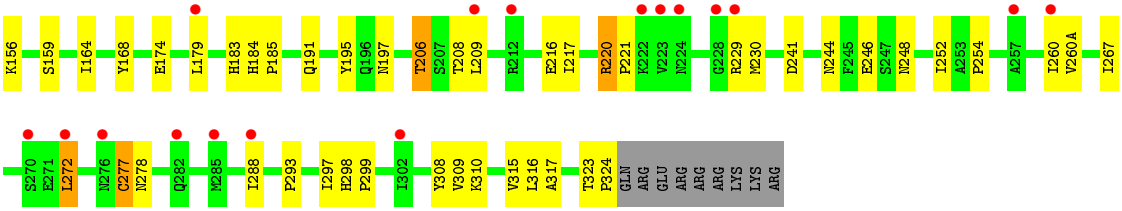
Chain K:



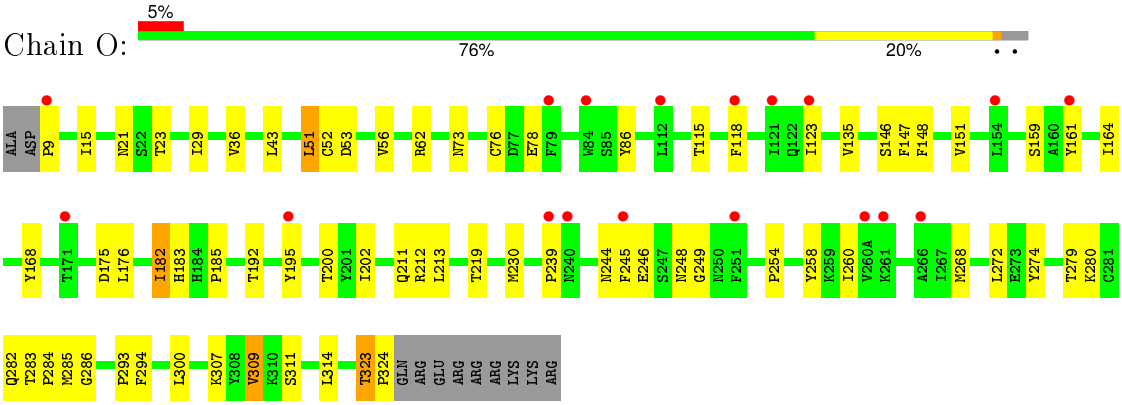
• Molecule 1: Hemagglutinin HA1 chain

Chain M:

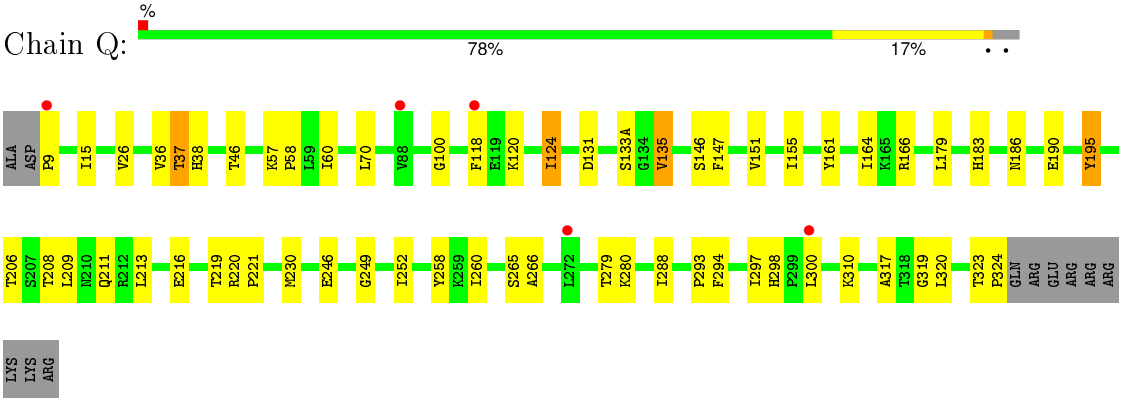




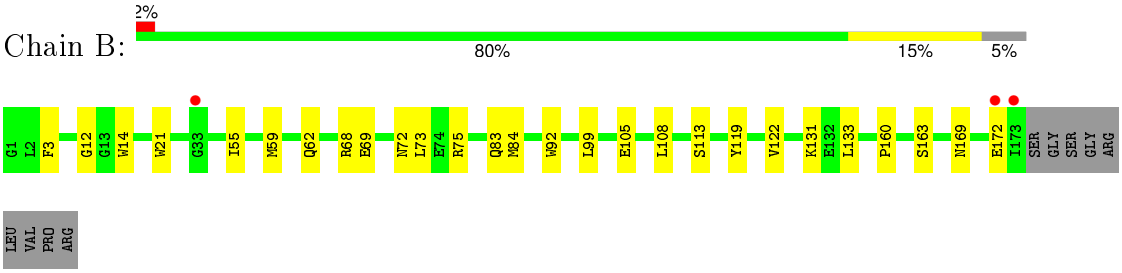
• Molecule 1: Hemagglutinin HA1 chain



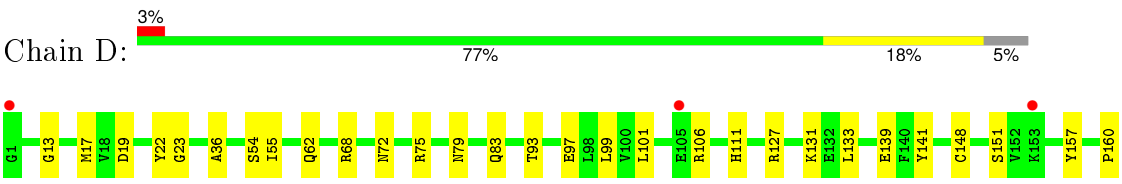
• Molecule 1: Hemagglutinin HA1 chain

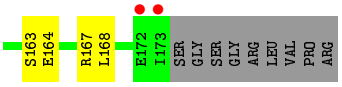


• Molecule 2: Hemagglutinin HA2 chain



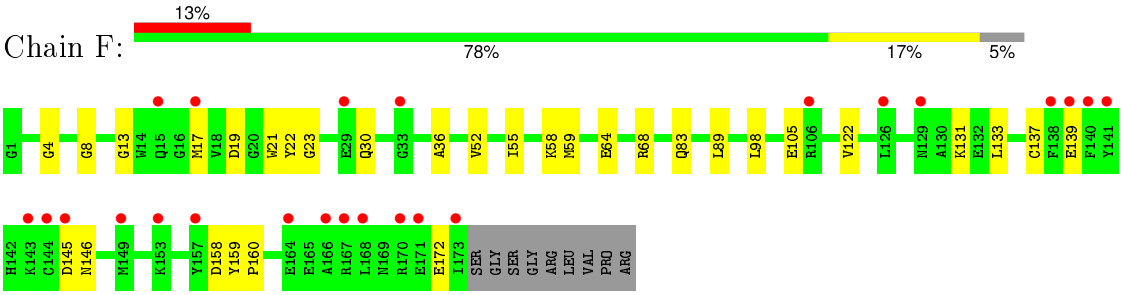
• Molecule 2: Hemagglutinin HA2 chain





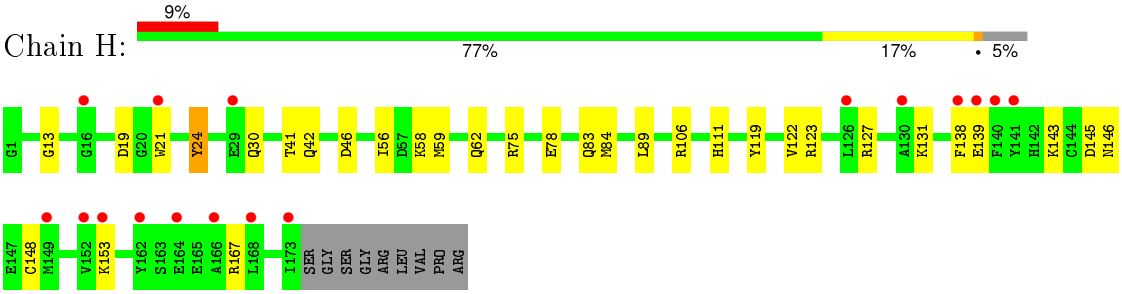
- Molecule 2: Hemagglutinin HA2 chain

Chain F:



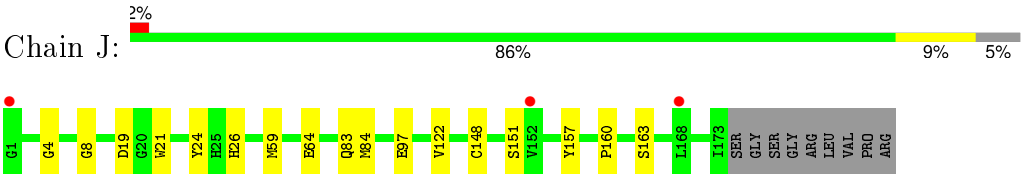
- Molecule 2: Hemagglutinin HA2 chain

Chain H:



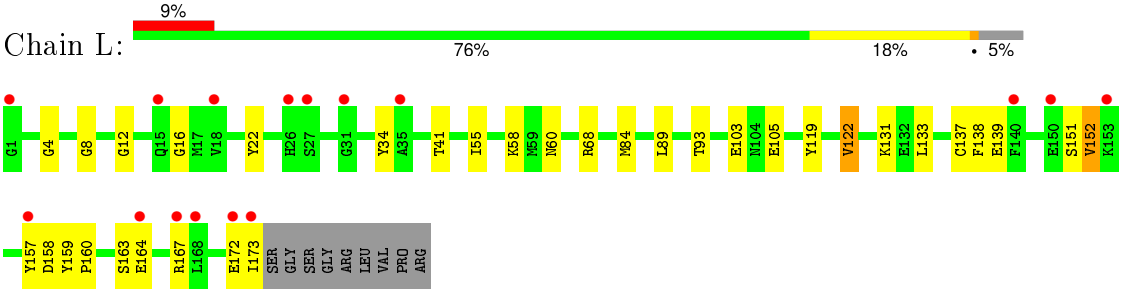
- Molecule 2: Hemagglutinin HA2 chain

Chain J:



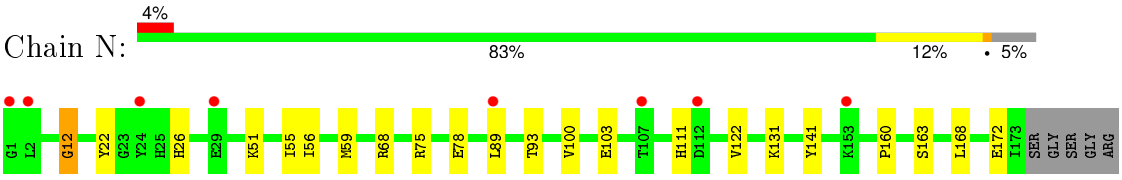
- Molecule 2: Hemagglutinin HA2 chain

Chain L:



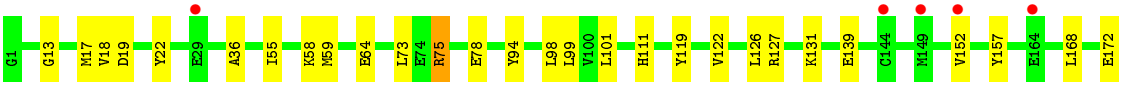
- Molecule 2: Hemagglutinin HA2 chain

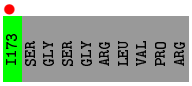
Chain N:



• Molecule 2: Hemagglutinin HA2 chain

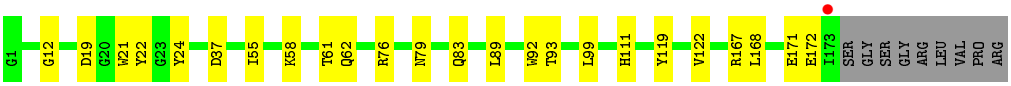
Chain P:





• Molecule 2: Hemagglutinin HA2 chain

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.48Å 225.73Å 211.63Å 90.00° 98.97° 90.00°	Depositor
Resolution (Å)	49.66 – 2.60 49.66 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.8 (49.66-2.60) 95.1 (49.66-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 2.58Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.189 , 0.243 0.196 , 0.246	Depositor DCC
R_{free} test set	9835 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	65.9	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 63.0	EDS
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	6 of 196437 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	36134	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.26 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.7239e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 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: 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	0.47	0/2616	0.67	1/3557 (0.0%)
1	C	0.44	0/2616	0.66	2/3557 (0.1%)
1	E	0.44	0/2616	0.65	2/3557 (0.1%)
1	G	0.46	0/2616	0.66	2/3557 (0.1%)
1	I	0.49	0/2616	0.70	1/3557 (0.0%)
1	K	0.44	0/2616	0.64	1/3557 (0.0%)
1	M	0.40	0/2616	0.62	2/3557 (0.1%)
1	O	0.42	0/2616	0.64	1/3557 (0.0%)
1	Q	0.46	0/2616	0.67	1/3557 (0.0%)
2	B	0.49	0/1430	0.65	0/1924
2	D	0.46	0/1430	0.58	0/1924
2	F	0.47	0/1430	0.60	0/1924
2	H	0.47	0/1430	0.60	0/1924
2	J	0.47	0/1430	0.61	0/1924
2	L	0.45	0/1430	0.55	0/1924
2	N	0.43	0/1430	0.59	0/1924
2	P	0.46	0/1430	0.60	0/1924
2	R	0.49	0/1430	0.62	0/1924
All	All	0.45	0/36414	0.64	13/49329 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	9	PRO	CA-N-CD	-8.94	98.98	111.50
1	C	9	PRO	CA-N-CD	-8.81	99.17	111.50
1	O	9	PRO	CA-N-CD	-8.72	99.29	111.50
1	G	9	PRO	CA-N-CD	-8.66	99.38	111.50
1	K	9	PRO	CA-N-CD	-8.51	99.59	111.50
1	A	9	PRO	CA-N-CD	-8.45	99.67	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	9	PRO	CA-N-CD	-8.45	99.67	111.50
1	E	9	PRO	CA-N-CD	-8.43	99.70	111.50
1	Q	9	PRO	CA-N-CD	-8.15	100.09	111.50
1	G	176	LEU	CA-CB-CG	5.97	129.03	115.30
1	E	176	LEU	CA-CB-CG	5.47	127.89	115.30
1	C	272	LEU	CA-CB-CG	5.02	126.85	115.30
1	M	272	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2551	0	2476	45	0
1	C	2551	0	2476	55	0
1	E	2551	0	2474	54	0
1	G	2551	0	2476	54	0
1	I	2551	0	2476	49	0
1	K	2551	0	2475	58	0
1	M	2551	0	2475	60	0
1	O	2551	0	2476	48	0
1	Q	2551	0	2476	43	0
2	B	1403	0	1302	22	0
2	D	1403	0	1302	24	0
2	F	1403	0	1302	24	0
2	H	1403	0	1302	31	0
2	J	1403	0	1302	13	0
2	L	1403	0	1302	24	0
2	N	1403	0	1302	21	0
2	P	1403	0	1302	22	0
2	R	1403	0	1301	23	0
3	A	28	0	25	0	0
3	C	28	0	25	0	0
3	E	28	0	25	3	0
3	I	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	28	0	25	1	0
3	M	28	0	25	1	0
3	R	28	0	25	0	0
4	A	14	0	13	0	0
4	C	14	0	13	0	0
4	E	28	0	26	0	0
4	G	28	0	26	0	0
4	I	14	0	13	0	0
4	K	28	0	26	3	0
4	M	28	0	26	0	0
4	O	28	0	26	0	0
4	Q	14	0	13	0	0
5	Q	39	0	34	0	0
6	A	7	0	0	1	0
6	B	5	0	0	0	0
6	C	6	0	0	0	0
6	D	8	0	0	0	0
6	E	6	0	0	0	0
6	F	2	0	0	0	0
6	G	14	0	0	0	0
6	H	4	0	0	0	0
6	I	9	0	0	0	0
6	J	12	0	0	0	0
6	K	10	0	0	3	0
6	L	2	0	0	0	0
6	M	5	0	0	0	0
6	N	1	0	0	0	0
6	O	8	0	0	1	0
6	P	2	0	0	0	0
6	Q	8	0	0	0	0
6	R	8	0	0	0	0
All	All	36134	0	34388	578	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 8.

All (578) 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:M:9:PRO:HD2	1:M:10:GLY:H	1.17	1.07
1:E:9:PRO:HD2	1:E:10:GLY:H	1.20	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:PRO:HD2	1:A:10:GLY:H	1.23	0.99
1:I:170:ASN:CG	1:I:176:LEU:HD23	1.85	0.97
1:I:170:ASN:ND2	1:I:176:LEU:HD23	1.81	0.96
1:I:206:THR:HG22	1:I:208:THR:H	1.31	0.91
1:M:9:PRO:HD2	1:M:10:GLY:N	1.86	0.90
1:K:206:THR:HG22	1:K:208:THR:H	1.38	0.89
1:E:9:PRO:HD2	1:E:10:GLY:N	1.88	0.86
1:Q:206:THR:HG22	1:Q:208:THR:H	1.40	0.84
1:A:9:PRO:HD2	1:A:10:GLY:N	1.91	0.84
2:N:131:LYS:NZ	2:P:127:ARG:HD2	1.93	0.84
1:G:323:THR:HG21	2:H:13:GLY:H	1.43	0.83
1:C:206:THR:HG22	1:C:209:LEU:H	1.44	0.83
1:M:206:THR:HG22	1:M:208:THR:H	1.44	0.82
1:O:323:THR:HG21	2:P:13:GLY:H	1.44	0.81
1:Q:206:THR:HB	1:Q:209:LEU:HB3	1.62	0.81
1:E:323:THR:HG21	2:F:13:GLY:H	1.43	0.81
1:M:323:THR:HG21	2:N:12:GLY:HA2	1.62	0.81
1:M:9:PRO:CD	1:M:10:GLY:H	1.94	0.80
1:C:56:VAL:HG23	1:C:85:SER:HB3	1.64	0.80
1:K:123:ILE:HD11	1:K:168:TYR:CE1	2.16	0.79
1:E:206:THR:HG22	1:E:209:LEU:H	1.48	0.79
1:O:283:THR:HG22	1:O:285:MET:H	1.49	0.78
1:A:206:THR:HB	1:A:209:LEU:HB3	1.66	0.78
1:M:310:LYS:H	2:N:93:THR:HG21	1.50	0.77
1:A:206:THR:HG22	1:A:208:THR:H	1.50	0.76
1:E:56:VAL:HG23	1:E:85:SER:HB3	1.66	0.76
1:E:51:LEU:HD13	1:E:272:LEU:HD11	1.66	0.76
1:K:56:VAL:HG23	1:K:85:SER:HB3	1.67	0.75
1:A:118:PHE:HE1	1:A:260:ILE:HD13	1.49	0.75
1:G:206:THR:HG22	1:G:208:THR:H	1.51	0.74
1:E:9:PRO:CD	1:E:10:GLY:H	1.98	0.74
1:M:147:PHE:HZ	1:M:230:MET:HE1	1.53	0.74
1:Q:310:LYS:H	2:R:93:THR:CG2	2.01	0.74
2:F:145:ASP:OD1	2:F:146:ASN:N	2.20	0.73
1:G:9:PRO:HD2	1:G:10:GLY:N	2.04	0.73
1:C:206:THR:HG22	1:C:208:THR:H	1.54	0.72
1:A:216:GLU:O	1:A:220:ARG:NH2	2.21	0.72
1:A:9:PRO:CD	1:A:10:GLY:H	2.02	0.72
1:Q:147:PHE:HZ	1:Q:230:MET:HE1	1.56	0.71
1:C:57:LYS:HD2	1:C:58:PRO:HD2	1.72	0.70
1:O:307:LYS:NZ	2:P:64:GLU:OE2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:9:PRO:CD	1:M:10:GLY:N	2.53	0.70
1:M:123:ILE:HD11	1:M:168:TYR:CZ	2.27	0.70
1:E:206:THR:HG22	1:E:208:THR:H	1.57	0.69
1:G:206:THR:HG22	1:G:209:LEU:H	1.58	0.68
1:A:307:LYS:HD3	2:B:59:MET:O	1.93	0.68
1:G:62:ARG:NH1	1:G:78:GLU:OE1	2.27	0.68
1:A:15:ILE:HD11	2:B:122:VAL:HG21	1.73	0.68
1:O:283:THR:HB	1:O:286:GLY:O	1.93	0.68
3:M:2001:NAG:H81	1:Q:221:PRO:HB3	1.76	0.68
1:A:118:PHE:CE1	1:A:260:ILE:HD13	2.28	0.68
1:G:283:THR:HG22	1:G:285:MET:H	1.57	0.68
1:Q:58:PRO:HG2	1:Q:60:ILE:HD11	1.75	0.67
2:D:164:GLU:OE2	2:D:167:ARG:NH2	2.21	0.67
1:Q:131:ASP:HB3	1:Q:155:ILE:HG13	1.74	0.67
2:N:131:LYS:HZ1	2:P:127:ARG:HD2	1.56	0.67
1:I:283:THR:HG22	1:I:285:MET:H	1.58	0.67
1:I:176:LEU:CD1	1:I:178:VAL:HG22	2.25	0.67
1:O:323:THR:HG21	2:P:13:GLY:N	2.09	0.66
2:L:164:GLU:OE2	2:L:167:ARG:NH2	2.22	0.66
1:E:9:PRO:CD	1:E:10:GLY:N	2.55	0.66
1:I:206:THR:HB	1:I:209:LEU:HB3	1.76	0.66
1:G:206:THR:HB	1:G:209:LEU:HB3	1.76	0.66
1:K:206:THR:HB	1:K:209:LEU:HB3	1.78	0.66
1:G:9:PRO:HD2	1:G:10:GLY:H	1.60	0.66
1:I:170:ASN:CG	1:I:176:LEU:CD2	2.63	0.66
1:Q:186:ASN:ND2	1:Q:190:GLU:OE1	2.23	0.65
1:G:115:THR:HG21	1:G:118:PHE:CE1	2.31	0.65
1:M:310:LYS:H	2:N:93:THR:CG2	2.10	0.65
1:Q:15:ILE:HD11	2:R:122:VAL:HG21	1.77	0.65
1:Q:310:LYS:H	2:R:93:THR:HG21	1.61	0.64
1:I:15:ILE:HD11	2:J:122:VAL:HG21	1.77	0.64
1:C:125(A):LYS:NZ	1:C:132:ALA:O	2.21	0.64
1:K:15:ILE:HD11	2:L:122:VAL:HG11	1.78	0.64
1:G:9:PRO:CD	2:H:139:GLU:OE2	2.46	0.64
1:I:230:MET:HE1	1:I:252:ILE:HG12	1.79	0.64
1:I:185:PRO:HD2	1:I:217:ILE:HD13	1.80	0.63
1:O:51:LEU:HD13	1:O:272:LEU:HD11	1.80	0.63
1:A:123:ILE:HD11	1:A:168:TYR:CZ	2.33	0.63
1:M:277:CYS:SG	1:M:278:ASN:N	2.72	0.63
1:E:307:LYS:NZ	2:F:64:GLU:OE2	2.32	0.63
1:A:9:PRO:CD	1:A:10:GLY:N	2.59	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:151:SER:OG	2:J:157:TYR:HA	1.99	0.62
1:K:43:LEU:HB2	1:K:314:LEU:HB2	1.81	0.62
2:D:17:MET:HE1	2:D:23:GLY:HA3	1.81	0.62
1:O:123:ILE:HD11	1:O:168:TYR:CZ	2.33	0.62
2:H:106:ARG:HH22	2:L:105:GLU:HG2	1.65	0.62
1:M:288:ILE:HD11	1:M:297:ILE:HD11	1.82	0.62
1:C:323:THR:HG21	2:D:13:GLY:H	1.65	0.61
1:E:57:LYS:HD2	1:E:58:PRO:HD2	1.82	0.61
1:K:123:ILE:HD11	1:K:168:TYR:CZ	2.35	0.61
1:K:147:PHE:HZ	1:K:230:MET:HE1	1.66	0.61
1:I:38:HIS:HD2	2:J:21:TRP:HE1	1.48	0.61
1:M:57:LYS:HD2	1:M:58:PRO:HD2	1.83	0.60
2:D:133:LEU:HD11	2:D:139:GLU:HB2	1.82	0.60
1:A:293:PRO:HG2	1:A:294:PHE:HD1	1.66	0.60
1:I:176:LEU:CD1	1:I:178:VAL:CG2	2.79	0.60
1:K:309:VAL:HG22	2:L:93:THR:HA	1.84	0.60
1:C:53:ASP:HA	1:C:58:PRO:HD3	1.84	0.59
1:Q:323:THR:HG21	2:R:12:GLY:HA2	1.84	0.59
1:E:50:LYS:HD3	1:E:275:GLY:HA3	1.84	0.59
1:E:58:PRO:HG2	1:E:60:ILE:HD11	1.84	0.59
1:M:220:ARG:HD2	1:M:229:ARG:HG2	1.85	0.59
1:I:186:ASN:ND2	1:I:190:GLU:OE1	2.28	0.59
1:G:71:LEU:HD23	1:G:179:LEU:HD13	1.84	0.59
2:B:83:GLN:OE1	2:D:68:ARG:NH2	2.27	0.59
1:K:9:PRO:HD2	1:K:9:PRO:O	2.02	0.59
2:L:151:SER:OG	2:L:157:TYR:HA	2.03	0.59
1:E:123:ILE:HD11	1:E:168:TYR:CZ	2.38	0.59
1:C:123:ILE:HD11	1:C:168:TYR:CZ	2.37	0.58
2:L:16:GLY:HA3	2:L:34:TYR:CE2	2.37	0.58
1:Q:216:GLU:O	1:Q:220:ARG:NH2	2.35	0.58
1:I:176:LEU:HD12	1:I:178:VAL:CG2	2.33	0.58
2:D:72:ASN:OD1	2:D:75:ARG:NH2	2.35	0.58
1:A:268:MET:HG3	1:A:284:PRO:HG3	1.84	0.58
1:Q:38:HIS:HD2	2:R:21:TRP:HE1	1.49	0.58
2:J:148:CYS:O	2:J:151:SER:HB3	2.04	0.58
2:R:168:LEU:O	2:R:172:GLU:HG2	2.04	0.58
1:M:206:THR:HB	1:M:209:LEU:HB3	1.85	0.58
1:Q:37:THR:HG22	1:Q:320:LEU:H	1.69	0.58
1:C:127:TRP:CD2	1:C:154:LEU:HD21	2.39	0.58
1:Q:183:HIS:HB2	1:Q:252:ILE:HD11	1.86	0.57
2:N:131:LYS:HZ3	2:P:127:ARG:HD2	1.65	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:15:ILE:HD11	2:P:122:VAL:HG21	1.87	0.57
2:B:131:LYS:NZ	2:D:127:ARG:HH21	2.02	0.57
1:C:206:THR:HB	1:C:209:LEU:HB3	1.85	0.57
1:G:131:ASP:OD2	1:G:133(A):SER:OG	2.23	0.57
1:Q:310:LYS:H	2:R:93:THR:HG22	1.70	0.57
2:H:167:ARG:NH1	2:L:173:ILE:O	2.38	0.57
1:K:118:PHE:HE1	1:K:260:ILE:HG12	1.70	0.57
1:C:118:PHE:CE1	1:C:260:ILE:HD13	2.40	0.57
1:C:151:VAL:HG22	1:C:252:ILE:HG22	1.87	0.57
1:I:9:PRO:O	1:I:9:PRO:HD2	2.04	0.57
1:M:221:PRO:HD3	1:O:244:ASN:ND2	2.19	0.57
1:G:9:PRO:CD	1:G:10:GLY:N	2.68	0.56
1:Q:288:ILE:HD11	1:Q:297:ILE:HG13	1.86	0.56
2:D:79:ASN:OD1	2:F:68:ARG:NH1	2.37	0.56
2:R:89:LEU:O	2:R:93:THR:HG23	2.06	0.56
2:H:131:LYS:HG2	2:H:139:GLU:HB3	1.86	0.56
1:Q:37:THR:CG2	1:Q:320:LEU:H	2.19	0.56
2:D:55:ILE:HG12	2:D:99:LEU:HD21	1.87	0.56
1:C:197:ASN:N	1:C:197:ASN:OD1	2.37	0.56
1:A:15:ILE:HG13	2:B:119:TYR:HA	1.88	0.56
1:I:183:HIS:HB2	1:I:252:ILE:HD11	1.86	0.56
1:M:164:ILE:O	1:M:246:GLU:HA	2.06	0.56
1:I:283:THR:CG2	1:I:285:MET:H	2.19	0.56
2:P:22:TYR:OH	2:P:111:HIS:ND1	2.31	0.56
1:M:117:HIS:HB3	1:M:260(A):VAL:HB	1.86	0.56
2:B:72:ASN:OD1	2:B:75:ARG:NH2	2.36	0.56
1:C:131:ASP:OD2	1:C:133(A):SER:OG	2.23	0.55
1:A:293:PRO:HG2	1:A:294:PHE:CD1	2.42	0.55
2:D:83:GLN:OE1	2:F:68:ARG:NH2	2.29	0.55
1:Q:293:PRO:HG2	1:Q:294:PHE:HD1	1.70	0.55
1:M:197:ASN:ND2	1:M:248:ASN:OD1	2.39	0.55
1:E:38:HIS:HD2	2:F:21:TRP:HE1	1.54	0.55
1:C:288:ILE:HD11	1:C:297:ILE:HD11	1.88	0.55
1:C:164:ILE:O	1:C:246:GLU:HA	2.07	0.55
1:A:100:GLY:HA3	1:A:230:MET:O	2.07	0.55
2:H:42:GLN:NE2	2:H:46:ASP:OD1	2.40	0.55
2:F:131:LYS:HG2	2:F:139:GLU:HB3	1.88	0.55
1:O:15:ILE:HG13	2:P:119:TYR:HA	1.88	0.55
2:N:68:ARG:NH1	2:R:79:ASN:OD1	2.39	0.55
1:Q:100:GLY:HA3	1:Q:230:MET:O	2.07	0.55
1:C:62:ARG:HG2	1:C:273:GLU:OE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:206:THR:HG23	1:M:241:ASP:OD2	2.07	0.54
1:I:283:THR:HB	1:I:286:GLY:O	2.07	0.54
1:Q:120:LYS:HD3	1:Q:258:TYR:CE1	2.41	0.54
2:H:30:GLN:OE1	2:H:146:ASN:N	2.39	0.54
1:M:185:PRO:HG2	1:M:191:GLN:OE1	2.07	0.54
1:M:183:HIS:HB2	1:M:252:ILE:HD11	1.89	0.54
2:F:17:MET:HE1	2:F:23:GLY:HA3	1.88	0.54
2:B:99:LEU:HD13	2:F:98:LEU:HD21	1.90	0.54
1:O:86:TYR:CZ	1:O:282:GLN:HG2	2.43	0.54
1:A:69:TRP:HZ3	1:A:112:LEU:HD21	1.73	0.54
1:I:221:PRO:HB3	3:K:2001:NAG:H81	1.90	0.54
1:G:15:ILE:HD11	2:H:122:VAL:HG21	1.89	0.54
1:A:186:ASN:ND2	1:A:190:GLU:OE1	2.33	0.53
1:E:206:THR:HB	1:E:209:LEU:HB3	1.90	0.53
1:I:52:CYS:HB2	1:I:279:THR:HG22	1.91	0.53
4:K:2004:NAG:C8	6:K:2110:HOH:O	2.55	0.53
1:M:156:LYS:HE3	1:M:159:SER:HA	1.91	0.53
1:K:216:GLU:O	1:K:220:ARG:NH2	2.42	0.53
1:K:230:MET:HE1	1:K:252:ILE:HG12	1.90	0.53
2:J:160:PRO:HA	2:J:163:SER:HB2	1.91	0.53
2:H:127:ARG:NH2	2:L:131:LYS:HE3	2.23	0.53
1:O:135:VAL:HG22	1:O:146:SER:HA	1.90	0.53
1:K:138:ALA:HB2	1:K:226:GLN:HG2	1.91	0.53
1:M:230:MET:CE	1:M:252:ILE:HG12	2.39	0.53
1:C:118:PHE:HE1	1:C:260:ILE:HD13	1.74	0.53
1:A:32:LYS:NZ	2:D:54:SER:OG	2.34	0.53
1:O:268:MET:HE3	1:O:284:PRO:HA	1.91	0.53
1:A:183:HIS:HB2	1:A:252:ILE:HD11	1.90	0.52
1:E:316:LEU:HD13	2:F:52:VAL:HG22	1.90	0.52
1:M:293:PRO:HB3	2:N:56:ILE:HG23	1.92	0.52
1:I:288:ILE:HD11	1:I:297:ILE:HG13	1.90	0.52
1:I:176:LEU:HG	1:I:237:LEU:HB3	1.92	0.52
1:C:51:LEU:HD13	1:C:88:VAL:HG21	1.90	0.52
2:H:145:ASP:OD1	2:H:148:CYS:N	2.39	0.52
1:K:69:TRP:HZ3	1:K:112:LEU:HD21	1.75	0.52
1:G:58:PRO:HG2	1:G:60:ILE:HD11	1.91	0.52
1:A:51:LEU:HD13	1:A:272:LEU:HB2	1.90	0.52
1:C:283:THR:HG23	1:C:285:MET:H	1.75	0.52
1:G:44:GLU:OE2	1:G:46:THR:HG22	2.10	0.52
1:O:294:PHE:HZ	2:P:59:MET:HG3	1.75	0.52
1:I:176:LEU:HD12	1:I:178:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:123:ILE:HD11	1:K:168:TYR:CD1	2.43	0.52
1:M:123:ILE:HD11	1:M:168:TYR:CE2	2.44	0.52
1:E:123:ILE:HG23	1:E:124:ILE:HG13	1.91	0.52
1:Q:298:HIS:HE1	1:Q:300:LEU:HD12	1.73	0.52
2:B:160:PRO:HA	2:B:163:SER:HB2	1.92	0.52
1:I:100:GLY:HA3	1:I:230:MET:O	2.10	0.52
1:A:26:VAL:HG11	1:A:317:ALA:HB2	1.91	0.52
1:K:309:VAL:HG13	1:K:311:SER:H	1.75	0.52
2:P:126:LEU:HD12	2:P:157:TYR:CE2	2.45	0.52
1:E:309:VAL:HG12	1:E:311:SER:H	1.75	0.52
1:K:176:LEU:HD11	1:K:237:LEU:HD23	1.91	0.52
1:K:293:PRO:HG2	1:K:294:PHE:HD1	1.74	0.51
1:O:21:ASN:ND2	6:O:2104:HOH:O	2.39	0.51
1:C:279:THR:OG1	1:C:280:LYS:N	2.43	0.51
1:K:170:ASN:CG	1:K:176:LEU:CD2	2.79	0.51
1:E:298:HIS:HE1	1:E:300:LEU:HD12	1.75	0.51
1:K:164:ILE:O	1:K:246:GLU:HA	2.11	0.51
2:P:17:MET:HE1	2:P:36:ALA:HA	1.93	0.51
2:D:17:MET:HE1	2:D:36:ALA:HA	1.91	0.51
2:N:22:TYR:OH	2:N:111:HIS:ND1	2.35	0.51
2:L:159:TYR:HB3	2:L:160:PRO:HD3	1.92	0.51
2:F:159:TYR:HB3	2:F:160:PRO:HD3	1.93	0.51
1:G:15:ILE:HG13	2:H:119:TYR:HA	1.92	0.51
1:O:182:ILE:HD12	1:O:202:ILE:HD12	1.93	0.50
1:Q:183:HIS:ND1	1:Q:195:TYR:OH	2.36	0.50
1:I:38:HIS:CD2	2:J:21:TRP:HE1	2.28	0.50
1:G:283:THR:HB	1:G:286:GLY:O	2.11	0.50
4:K:2004:NAG:H83	6:K:2110:HOH:O	2.12	0.50
1:M:118:PHE:CE1	1:M:260:ILE:HD13	2.47	0.50
1:E:209:LEU:HD21	1:E:211:GLN:HG2	1.92	0.50
2:P:19:ASP:OD1	2:P:19:ASP:N	2.39	0.50
2:P:122:VAL:HG13	2:P:152:VAL:HG21	1.94	0.50
1:G:294:PHE:HZ	2:H:59:MET:HG3	1.77	0.50
1:Q:15:ILE:HG13	2:R:119:TYR:HA	1.92	0.50
1:G:183:HIS:HB2	1:G:252:ILE:HD11	1.93	0.50
2:D:160:PRO:HA	2:D:163:SER:HB2	1.92	0.50
1:G:9:PRO:HD3	2:H:139:GLU:OE2	2.11	0.49
2:L:152:VAL:HG12	2:L:157:TYR:HD1	1.77	0.49
1:K:26:VAL:HG11	1:K:317:ALA:HB2	1.94	0.49
1:G:9:PRO:HD2	2:H:139:GLU:OE2	2.12	0.49
1:E:26:VAL:HG11	1:E:317:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:HIS:HB2	1:C:252:ILE:HD11	1.94	0.49
1:E:28:THR:HB	2:F:105:GLU:HB2	1.94	0.49
1:M:80:ILE:HD11	1:M:149:ARG:HD2	1.93	0.49
1:C:147:PHE:HZ	1:C:230:MET:HE1	1.77	0.49
1:G:307:LYS:HD2	2:H:62:GLN:HB3	1.94	0.49
2:R:62:GLN:HG3	2:R:92:TRP:CG	2.48	0.49
1:M:26:VAL:HG11	1:M:317:ALA:HB2	1.93	0.49
1:C:283:THR:HG22	1:C:286:GLY:H	1.77	0.49
1:A:323:THR:HG21	2:B:12:GLY:HA2	1.95	0.49
2:N:75:ARG:NH1	2:N:78:GLU:OE1	2.39	0.49
2:D:131:LYS:HG2	2:D:139:GLU:HB3	1.94	0.49
1:E:164:ILE:O	1:E:246:GLU:HA	2.13	0.49
1:M:151:VAL:HG22	1:M:252:ILE:HG22	1.95	0.49
1:A:98:TYR:CD1	1:A:230:MET:HG3	2.48	0.49
1:O:182:ILE:HD11	1:O:213:LEU:HD13	1.94	0.49
1:K:120:LYS:HD3	1:K:258:TYR:CE1	2.47	0.49
1:M:148:PHE:HB2	1:M:151:VAL:HG12	1.93	0.49
2:F:17:MET:HE1	2:F:36:ALA:HA	1.95	0.49
1:I:200:THR:OG1	1:I:215:PRO:HG3	2.13	0.49
1:K:13:ILE:HG22	2:L:138:PHE:HB2	1.95	0.49
1:Q:118:PHE:HE1	1:Q:260:ILE:HG12	1.78	0.49
1:I:206:THR:HG23	1:I:241:ASP:OD2	2.12	0.49
1:C:127:TRP:CE2	1:C:154:LEU:HD21	2.47	0.49
2:F:158:ASP:OD1	2:F:160:PRO:HD2	2.12	0.49
1:O:200:THR:HA	1:O:248:ASN:HD21	1.77	0.49
2:N:131:LYS:HD2	2:N:141:TYR:OH	2.13	0.49
1:I:147:PHE:HZ	1:I:230:MET:HE1	1.77	0.49
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.96	0.48
1:K:206:THR:HG23	1:K:241:ASP:OD2	2.13	0.48
1:O:283:THR:CG2	1:O:285:MET:H	2.24	0.48
2:D:131:LYS:HE2	2:D:141:TYR:CE1	2.47	0.48
1:I:216:GLU:O	1:I:220:ARG:NH2	2.46	0.48
1:G:164:ILE:O	1:G:246:GLU:HA	2.13	0.48
1:C:89:GLU:OE1	1:C:269:LYS:HE2	2.13	0.48
1:E:126:SER:OG	1:E:166:ARG:NH1	2.34	0.48
2:N:89:LEU:O	2:N:93:THR:HG23	2.12	0.48
1:G:9:PRO:CD	1:G:10:GLY:H	2.26	0.48
1:M:51:LEU:HG	1:M:272:LEU:HD11	1.94	0.48
1:A:289:ASN:ND2	6:A:2105:HOH:O	2.46	0.48
1:G:205:GLY:O	1:G:243:ILE:HA	2.12	0.48
1:O:43:LEU:HB2	1:O:314:LEU:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:58:PRO:HB3	1:M:86:TYR:CE1	2.48	0.48
1:E:283:THR:CG2	1:E:285:MET:H	2.27	0.48
1:K:323:THR:HG21	2:L:12:GLY:HA2	1.95	0.48
1:C:206:THR:CG2	1:C:208:THR:H	2.26	0.48
1:I:86:TYR:CZ	1:I:282:GLN:HG2	2.48	0.48
1:E:138:ALA:HB2	1:E:226:GLN:HG2	1.94	0.48
2:D:148:CYS:O	2:D:151:SER:HB3	2.13	0.48
1:K:15:ILE:HG13	2:L:119:TYR:HA	1.95	0.48
2:D:151:SER:OG	2:D:157:TYR:HA	2.13	0.48
2:J:4:GLY:O	2:J:8:GLY:HA3	2.14	0.48
2:F:172:GLU:OE1	2:F:172:GLU:N	2.46	0.48
1:O:182:ILE:HG23	1:O:202:ILE:HD12	1.96	0.48
1:E:172:ASN:HB3	1:E:174:GLU:OE1	2.14	0.48
1:I:176:LEU:HD11	1:I:178:VAL:CG2	2.43	0.48
2:P:131:LYS:HG2	2:P:139:GLU:HB3	1.95	0.48
1:O:164:ILE:O	1:O:246:GLU:HA	2.14	0.48
2:D:19:ASP:OD1	2:D:19:ASP:N	2.43	0.48
1:G:138:ALA:HB2	1:G:226:GLN:HG2	1.96	0.48
1:M:206:THR:HG22	1:M:209:LEU:H	1.79	0.48
1:O:118:PHE:CE1	1:O:260:ILE:HD13	2.49	0.48
1:O:123:ILE:HD11	1:O:168:TYR:CE2	2.49	0.47
1:M:51:LEU:HG	1:M:272:LEU:CD1	2.44	0.47
1:C:44:GLU:HB2	1:C:292:MET:HG3	1.96	0.47
1:E:89:GLU:OE1	1:E:269:LYS:HE2	2.14	0.47
1:E:288:ILE:HD11	1:E:297:ILE:HG13	1.95	0.47
1:E:43:LEU:HB2	1:E:314:LEU:HB2	1.96	0.47
2:J:83:GLN:OE1	2:L:68:ARG:NH2	2.42	0.47
1:I:311:SER:OG	2:J:97:GLU:OE2	2.29	0.47
2:L:160:PRO:HA	2:L:163:SER:HB2	1.95	0.47
1:K:141:TYR:O	1:K:143:GLY:N	2.40	0.47
1:A:18:HIS:N	2:B:21:TRP:O	2.39	0.47
1:K:142:HIS:C	1:K:144:ARG:H	2.17	0.47
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.96	0.47
1:Q:58:PRO:HG2	1:Q:60:ILE:CD1	2.42	0.47
1:C:147:PHE:HZ	1:C:230:MET:CE	2.28	0.47
3:E:2002:NAG:O3	3:E:2003:NAG:H2	2.15	0.47
1:C:283:THR:CG2	1:C:285:MET:H	2.28	0.47
1:M:118:PHE:HE1	1:M:260:ILE:HD13	1.77	0.47
1:E:283:THR:HG22	1:E:286:GLY:H	1.79	0.47
1:G:320:LEU:HB3	2:H:111:HIS:CG	2.49	0.47
1:G:185:PRO:HG2	1:G:191:GLN:OE1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:135:VAL:HG22	1:Q:146:SER:HA	1.95	0.47
1:I:58:PRO:HG2	1:I:60:ILE:HD11	1.95	0.47
1:G:323:THR:HG21	2:H:13:GLY:N	2.21	0.47
1:Q:37:THR:HG23	1:Q:319:GLY:HA3	1.96	0.47
1:Q:293:PRO:HG2	1:Q:294:PHE:CD1	2.49	0.47
1:C:45:LYS:HE3	1:C:296:ASN:HD21	1.79	0.47
2:N:168:LEU:O	2:N:172:GLU:HG2	2.14	0.47
1:C:189:ALA:O	1:C:192:THR:HG22	2.14	0.47
1:M:316:LEU:HD23	2:N:100:VAL:HG13	1.95	0.47
1:G:211:GLN:NE2	1:G:213:LEU:HD11	2.29	0.47
2:B:105:GLU:HG2	2:D:106:ARG:HH22	1.80	0.47
2:H:75:ARG:NH1	2:H:78:GLU:OE1	2.46	0.47
1:A:220:ARG:NE	1:C:210:ASN:OD1	2.45	0.46
1:M:217:ILE:HB	1:O:212:ARG:NH1	2.30	0.46
1:E:115:THR:HG21	1:E:118:PHE:CE1	2.50	0.46
1:G:283:THR:CG2	1:G:285:MET:H	2.24	0.46
2:N:68:ARG:NH2	2:R:83:GLN:OE1	2.44	0.46
2:D:22:TYR:OH	2:D:111:HIS:ND1	2.36	0.46
1:Q:211:GLN:OE1	1:Q:213:LEU:HD11	2.15	0.46
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.97	0.46
1:Q:38:HIS:CD2	2:R:21:TRP:HE1	2.32	0.46
1:K:118:PHE:CE1	1:K:260:ILE:HG12	2.49	0.46
1:G:299:PRO:HB3	2:H:89:LEU:HD21	1.96	0.46
1:M:174:GLU:N	1:M:174:GLU:OE1	2.48	0.46
1:E:279:THR:HG21	1:E:287:ALA:HB1	1.97	0.46
1:M:147:PHE:HZ	1:M:230:MET:CE	2.26	0.46
1:K:52:CYS:HB2	1:K:279:THR:HG22	1.97	0.46
2:P:55:ILE:HG23	2:P:99:LEU:HD23	1.97	0.46
1:M:184:HIS:CE1	1:M:216:GLU:H	2.34	0.46
1:M:62:ARG:NH1	1:M:78:GLU:OE1	2.49	0.46
2:H:127:ARG:HH21	2:L:131:LYS:HE3	1.80	0.46
1:E:284:PRO:HD3	1:E:300:LEU:O	2.16	0.46
1:G:284:PRO:HG2	1:G:298:HIS:CE1	2.50	0.46
1:M:131:ASP:HB3	1:M:155:ILE:HG13	1.97	0.46
1:Q:161:TYR:CZ	1:Q:249:GLY:HA2	2.50	0.46
1:M:308:TYR:HD2	2:N:89:LEU:HD22	1.79	0.46
1:A:147:PHE:HZ	1:A:230:MET:HE1	1.81	0.46
1:K:77:ASP:O	1:K:80:ILE:HG12	2.15	0.46
1:G:175:ASP:OD1	1:G:239:PRO:HD3	2.16	0.46
1:M:230:MET:HE1	1:M:252:ILE:HG12	1.98	0.46
1:C:161:TYR:CZ	1:C:249:GLY:HA2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:123:ILE:HG23	1:M:124:ILE:HG23	1.98	0.46
1:K:170:ASN:CG	1:K:176:LEU:HD21	2.37	0.46
1:K:135:VAL:HG22	1:K:146:SER:HA	1.98	0.46
1:M:179:LEU:O	1:M:254:PRO:HB3	2.16	0.45
1:C:309:VAL:HG13	1:C:311:SER:H	1.82	0.45
1:K:131:ASP:HB3	1:K:155:ILE:HB	1.97	0.45
1:K:142:HIS:HB2	1:K:144:ARG:HG2	1.97	0.45
1:C:309:VAL:HG22	2:D:93:THR:HA	1.99	0.45
2:N:160:PRO:HA	2:N:163:SER:HB2	1.98	0.45
1:K:14:CYS:HA	2:L:137:CYS:HA	1.97	0.45
1:O:211:GLN:OE1	1:O:213:LEU:HD11	2.17	0.45
1:Q:26:VAL:HG11	1:Q:317:ALA:HB2	1.98	0.45
1:M:15:ILE:HD11	2:N:122:VAL:HG21	1.97	0.45
2:F:4:GLY:O	2:F:8:GLY:HA3	2.16	0.45
2:L:133:LEU:HD21	2:L:139:GLU:HB2	1.98	0.45
1:O:175:ASP:OD1	1:O:239:PRO:HD3	2.17	0.45
2:F:30:GLN:OE1	2:F:30:GLN:N	2.41	0.45
1:E:197:ASN:N	1:E:197:ASN:OD1	2.47	0.45
1:O:52:CYS:HB2	1:O:279:THR:HG22	1.97	0.45
1:K:323:THR:HA	1:K:324:PRO:HD3	1.84	0.45
1:A:53:ASP:HA	1:A:58:PRO:HD3	1.99	0.45
1:M:298:HIS:HA	1:M:299:PRO:HD3	1.77	0.45
1:O:29:ILE:HD12	2:P:101:LEU:HB3	1.98	0.45
1:K:123:ILE:HD12	1:K:123:ILE:HA	1.52	0.45
1:A:147:PHE:CZ	1:A:230:MET:HE1	2.52	0.45
1:E:284:PRO:HG2	1:E:298:HIS:CE1	2.51	0.45
2:B:68:ARG:NH2	2:F:83:GLN:OE1	2.39	0.45
2:P:98:LEU:HD21	2:R:99:LEU:HD13	1.98	0.45
2:R:167:ARG:NH1	2:R:171:GLU:OE1	2.50	0.45
1:M:220:ARG:HD2	1:M:229:ARG:CG	2.45	0.44
1:C:52:CYS:HB2	1:C:279:THR:HG22	1.99	0.44
1:A:323:THR:HA	1:A:324:PRO:HD3	1.77	0.44
1:A:141:TYR:CZ	1:A:149:ARG:NH2	2.84	0.44
1:C:230:MET:CE	1:C:252:ILE:HG12	2.48	0.44
1:K:39:ALA:HA	1:K:318:THR:HG22	1.98	0.44
2:N:55:ILE:O	2:N:59:MET:HG2	2.18	0.44
2:R:19:ASP:OD1	2:R:19:ASP:N	2.34	0.44
1:O:279:THR:OG1	1:O:280:LYS:N	2.50	0.44
2:R:58:LYS:HA	2:R:58:LYS:HD3	1.85	0.44
1:C:123:ILE:HD11	1:C:168:TYR:CE2	2.53	0.44
1:M:183:HIS:O	1:M:185:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:217:ILE:O	1:I:212:ARG:HD2	2.17	0.44
2:R:24:TYR:CE1	2:R:37:ASP:HB2	2.52	0.44
2:H:24:TYR:HB2	2:H:153:LYS:HE2	2.00	0.44
1:K:299:PRO:HB3	2:L:89:LEU:HD11	1.98	0.44
1:E:161:TYR:CZ	1:E:249:GLY:HA2	2.52	0.44
1:I:151:VAL:HG13	1:I:252:ILE:CG2	2.48	0.44
1:Q:323:THR:HA	1:Q:324:PRO:HD3	1.79	0.44
2:R:55:ILE:HG12	2:R:99:LEU:HD21	2.00	0.44
1:I:26:VAL:HG11	1:I:317:ALA:HB2	1.99	0.44
1:I:176:LEU:HD12	1:I:178:VAL:HG23	2.00	0.44
1:K:206:THR:HG22	1:K:209:LEU:H	1.82	0.44
2:D:97:GLU:HB3	2:F:58:LYS:HE3	1.99	0.44
1:C:51:LEU:HG	1:C:272:LEU:CD1	2.47	0.44
1:M:141:TYR:CZ	1:M:149:ARG:NH2	2.84	0.44
1:O:62:ARG:NH1	1:O:78:GLU:OE1	2.51	0.44
2:L:4:GLY:O	2:L:8:GLY:HA3	2.18	0.44
1:E:299:PRO:HG3	1:E:308:TYR:CE2	2.53	0.44
1:C:211:GLN:OE1	1:C:213:LEU:HD11	2.18	0.43
1:A:135:VAL:HG22	1:A:146:SER:HA	2.00	0.43
1:E:293:PRO:HG2	1:E:294:PHE:HD2	1.84	0.43
2:F:133:LEU:HD12	2:F:137:CYS:HB2	2.00	0.43
1:I:71:LEU:HA	1:I:71:LEU:HD23	1.80	0.43
1:C:230:MET:HE1	1:C:252:ILE:HG12	2.00	0.43
1:G:298:HIS:HA	1:G:299:PRO:HD3	1.86	0.43
1:I:323:THR:HA	1:I:324:PRO:HD3	1.84	0.43
1:C:202:ILE:HD11	1:C:251:PHE:HA	2.00	0.43
1:C:9:PRO:HD2	1:C:9:PRO:O	2.18	0.43
2:F:55:ILE:O	2:F:59:MET:HG2	2.18	0.43
1:I:284:PRO:HD3	1:I:300:LEU:O	2.18	0.43
1:K:170:ASN:CG	1:K:176:LEU:HD23	2.38	0.43
1:A:58:PRO:HG2	1:A:60:ILE:HD11	2.00	0.43
1:I:294:PHE:HZ	2:J:59:MET:HG3	1.83	0.43
1:C:218:ALA:HB2	1:E:203:SER:OG	2.18	0.43
1:O:245:PHE:CE2	1:O:254:PRO:HG2	2.54	0.43
1:I:230:MET:CE	1:I:252:ILE:HG12	2.46	0.43
1:G:203:SER:HB2	1:K:218:ALA:HB2	2.00	0.43
1:I:313:ARG:O	1:I:314:LEU:HD23	2.18	0.43
1:O:183:HIS:O	1:O:185:PRO:HD3	2.18	0.43
1:O:115:THR:HG21	1:O:118:PHE:CE1	2.53	0.43
1:Q:279:THR:OG1	1:Q:280:LYS:N	2.52	0.43
2:J:19:ASP:OD1	2:J:19:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:CYS:O	2:J:24:TYR:HA	2.18	0.43
1:K:238:LYS:HA	1:K:239:PRO:HD3	1.88	0.43
1:O:118:PHE:HE1	1:O:260:ILE:HD13	1.83	0.43
2:H:123:ARG:HB2	2:H:138:PHE:CZ	2.53	0.43
1:C:183:HIS:ND1	1:C:195:TYR:OH	2.41	0.43
1:O:293:PRO:HG2	1:O:294:PHE:HD1	1.84	0.43
1:G:124:ILE:HD12	1:G:254:PRO:HG2	2.00	0.43
1:A:206:THR:HG23	1:A:241:ASP:OD2	2.19	0.43
1:G:161:TYR:CZ	1:G:249:GLY:HA2	2.54	0.43
1:C:62:ARG:NH1	1:C:78:GLU:OE2	2.52	0.42
2:P:94:TYR:CZ	2:P:98:LEU:HD22	2.54	0.42
1:K:175:ASP:OD1	1:K:239:PRO:HD3	2.19	0.42
1:O:309:VAL:HG12	1:O:311:SER:H	1.84	0.42
1:M:106:GLU:HB3	2:R:76:ARG:HD3	2.00	0.42
2:P:58:LYS:HA	2:P:58:LYS:HD3	1.81	0.42
1:K:9:PRO:CD	1:K:9:PRO:O	2.66	0.42
1:C:307:LYS:HB3	2:D:62:GLN:NE2	2.34	0.42
1:K:161:TYR:CZ	1:K:249:GLY:HA2	2.55	0.42
1:Q:230:MET:HE1	1:Q:252:ILE:HG12	2.01	0.42
1:O:148:PHE:HB2	1:O:151:VAL:HG12	2.01	0.42
2:F:89:LEU:HD23	2:F:89:LEU:HA	1.87	0.42
1:O:314:LEU:HD23	1:O:314:LEU:HA	1.84	0.42
1:C:29:ILE:HD12	2:D:101:LEU:HB3	2.00	0.42
1:C:274:TYR:CZ	1:C:276:ASN:HA	2.54	0.42
1:E:15:ILE:HD11	2:F:122:VAL:HG21	2.01	0.42
1:Q:57:LYS:HG3	1:Q:58:PRO:HD2	2.01	0.42
1:E:124:ILE:O	1:E:255:GLU:HG3	2.20	0.42
1:G:288:ILE:HD11	1:G:297:ILE:HD12	2.02	0.42
1:K:58:PRO:HB3	1:K:86:TYR:CE1	2.54	0.42
1:G:293:PRO:HB3	2:H:56:ILE:HG23	2.01	0.42
1:M:299:PRO:HG3	1:M:308:TYR:CE2	2.55	0.42
1:O:284:PRO:HD3	1:O:300:LEU:O	2.20	0.42
1:I:220:ARG:HD3	1:I:229:ARG:HG2	2.02	0.42
1:G:203:SER:OG	1:G:246:GLU:HB3	2.19	0.42
1:C:138:ALA:HB2	1:C:226:GLN:HG2	2.01	0.42
2:P:168:LEU:O	2:P:172:GLU:HG2	2.20	0.42
2:B:133:LEU:HA	2:B:133:LEU:HD23	1.77	0.42
1:G:100:GLY:HA3	1:G:230:MET:O	2.20	0.42
1:E:51:LEU:HD12	1:E:51:LEU:HA	1.77	0.42
1:G:284:PRO:HD3	1:G:300:LEU:O	2.19	0.42
1:Q:124:ILE:HG22	1:Q:166:ARG:NH2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:PHE:CE2	2:B:113:SER:HB2	2.55	0.42
1:G:37:THR:HG23	1:G:320:LEU:O	2.20	0.42
1:G:202:ILE:HG12	1:G:247:SER:OG	2.20	0.42
1:E:100:GLY:HA3	1:E:230:MET:O	2.20	0.42
1:I:164:ILE:O	1:I:246:GLU:HA	2.20	0.42
1:Q:265:SER:OG	1:Q:266:ALA:N	2.53	0.42
1:I:283:THR:HG22	1:I:286:GLY:H	1.85	0.42
1:E:283:THR:HG23	1:E:285:MET:H	1.85	0.42
1:G:221:PRO:HB3	3:I:2001:NAG:H81	2.02	0.42
1:A:80:ILE:HA	1:A:80:ILE:HD13	1.92	0.42
2:L:152:VAL:HG12	2:L:157:TYR:CD1	2.53	0.42
1:O:161:TYR:CZ	1:O:249:GLY:HA2	2.55	0.42
2:P:75:ARG:HH21	2:P:78:GLU:CD	2.23	0.41
1:E:58:PRO:HB3	1:E:86:TYR:CE1	2.55	0.41
1:E:292:MET:HG3	1:E:293:PRO:HD2	2.00	0.41
1:Q:164:ILE:O	1:Q:246:GLU:HA	2.19	0.41
2:H:58:LYS:HA	2:H:58:LYS:HD2	1.83	0.41
1:Q:70:LEU:HB3	1:Q:179:LEU:HD11	2.02	0.41
1:O:323:THR:HA	1:O:324:PRO:HD3	1.84	0.41
1:C:54:LEU:O	1:C:56:VAL:HG22	2.19	0.41
1:M:309:VAL:HB	2:N:93:THR:HG22	2.01	0.41
1:E:86:TYR:HB3	1:E:302:ILE:HD13	2.01	0.41
4:K:2004:NAG:H82	6:K:2110:HOH:O	2.20	0.41
1:C:274:TYR:CE2	1:C:276:ASN:HA	2.55	0.41
1:A:16:GLY:HA3	2:B:14:TRP:CH2	2.56	0.41
1:C:198:PRO:HG2	1:C:199:THR:HG22	2.02	0.41
2:B:169:ASN:O	2:B:172:GLU:OE1	2.37	0.41
1:Q:310:LYS:HB2	2:R:93:THR:HG21	2.02	0.41
1:A:280:LYS:HE3	1:A:304:GLU:CG	2.50	0.41
1:O:176:LEU:HD12	1:O:258:TYR:C	2.40	0.41
2:B:73:LEU:HA	2:B:73:LEU:HD23	1.90	0.41
2:H:83:GLN:NE2	2:J:64:GLU:O	2.53	0.41
1:G:62:ARG:HH12	1:G:78:GLU:CD	2.23	0.41
2:H:19:ASP:OD1	2:H:19:ASP:N	2.42	0.41
1:M:183:HIS:HD2	1:M:230:MET:HG3	1.85	0.41
1:A:164:ILE:O	1:A:246:GLU:HA	2.20	0.41
1:I:138:ALA:HB2	1:I:226:GLN:HG2	2.03	0.41
1:G:18:HIS:N	2:H:21:TRP:O	2.49	0.41
1:E:133(A):SER:O	1:E:135:VAL:N	2.53	0.41
1:K:183:HIS:HB2	1:K:252:ILE:HD11	2.03	0.41
3:E:2002:NAG:H4	3:E:2003:NAG:H2	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:57:LYS:HG3	1:K:58:PRO:HD2	2.01	0.41
1:O:147:PHE:HZ	1:O:230:MET:CE	2.33	0.41
1:K:124:ILE:O	1:K:255:GLU:HG3	2.21	0.41
2:B:62:GLN:HG3	2:B:92:TRP:CD2	2.55	0.41
1:M:244:ASN:ND2	1:Q:221:PRO:HD3	2.36	0.41
2:N:51:LYS:HD3	2:N:103:GLU:HB3	2.03	0.41
2:H:84:MET:HB3	2:H:84:MET:HE2	1.88	0.41
1:K:54:LEU:O	1:K:56:VAL:HG22	2.20	0.41
1:O:182:ILE:CD1	1:O:202:ILE:HD12	2.51	0.41
1:E:279:THR:OG1	1:E:280:LYS:N	2.54	0.41
1:G:148:PHE:HB2	1:G:151:VAL:HG12	2.02	0.41
1:C:207:SER:OG	1:C:241:ASP:OD1	2.32	0.41
1:M:221:PRO:HD3	1:O:244:ASN:HD21	1.86	0.41
2:L:158:ASP:OD1	2:L:160:PRO:HD2	2.21	0.41
1:G:14:CYS:O	2:H:24:TYR:HA	2.21	0.41
1:K:58:PRO:HG2	1:K:60:ILE:HD11	2.03	0.41
1:K:108:LEU:HB2	1:K:234:TRP:CE2	2.56	0.41
1:I:9:PRO:O	1:I:9:PRO:CD	2.69	0.40
1:G:320:LEU:HB3	2:H:111:HIS:CD2	2.56	0.40
1:A:211:GLN:NE2	1:A:213:LEU:HD11	2.36	0.40
2:F:19:ASP:OD1	2:F:19:ASP:N	2.42	0.40
1:M:297:ILE:HD13	1:M:297:ILE:HG21	1.85	0.40
1:K:230:MET:CE	1:K:252:ILE:HG12	2.50	0.40
1:A:265:SER:OG	1:A:266:ALA:N	2.53	0.40
1:G:144:ARG:HD2	1:G:144:ARG:HA	1.89	0.40
1:A:29:ILE:H	1:A:29:ILE:HG13	1.58	0.40
1:O:53:ASP:OD1	1:O:274:TYR:OH	2.25	0.40
1:E:179:LEU:O	1:E:254:PRO:HB3	2.21	0.40
1:K:186:ASN:OD1	1:K:227:SER:HB3	2.21	0.40
3:E:2002:NAG:C3	3:E:2003:NAG:H2	2.49	0.40
2:R:22:TYR:OH	2:R:111:HIS:ND1	2.39	0.40
2:B:108:LEU:HD23	2:B:108:LEU:HA	1.90	0.40
2:H:143:LYS:O	2:H:143:LYS:HG3	2.21	0.40
1:M:323:THR:HA	1:M:324:PRO:HD3	1.81	0.40
2:B:75:ARG:HD3	2:B:75:ARG:HA	1.92	0.40
1:O:73:ASN:HB3	1:O:76:CYS:SG	2.61	0.40
2:L:55:ILE:HD11	2:L:103:GLU:HG3	2.03	0.40
1:E:70:LEU:O	1:E:150:ASN:ND2	2.46	0.40
2:B:84:MET:HB3	2:B:84:MET:HE2	2.00	0.40
2:L:58:LYS:HA	2:L:58:LYS:HD2	1.88	0.40
1:K:51:LEU:HD13	1:K:272:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:ILE:HG23	2:B:99:LEU:HD23	2.03	0.40
2:R:62:GLN:HG3	2:R:92:TRP:CD2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	321/334 (96%)	312 (97%)	9 (3%)	0	100	100
1	C	321/334 (96%)	309 (96%)	12 (4%)	0	100	100
1	E	321/334 (96%)	311 (97%)	10 (3%)	0	100	100
1	G	321/334 (96%)	311 (97%)	10 (3%)	0	100	100
1	I	321/334 (96%)	310 (97%)	11 (3%)	0	100	100
1	K	321/334 (96%)	311 (97%)	9 (3%)	1 (0%)	46	72
1	M	321/334 (96%)	309 (96%)	12 (4%)	0	100	100
1	O	321/334 (96%)	314 (98%)	7 (2%)	0	100	100
1	Q	321/334 (96%)	311 (97%)	10 (3%)	0	100	100
2	B	171/182 (94%)	167 (98%)	4 (2%)	0	100	100
2	D	171/182 (94%)	167 (98%)	4 (2%)	0	100	100
2	F	171/182 (94%)	166 (97%)	5 (3%)	0	100	100
2	H	171/182 (94%)	168 (98%)	3 (2%)	0	100	100
2	J	171/182 (94%)	168 (98%)	3 (2%)	0	100	100
2	L	171/182 (94%)	166 (97%)	5 (3%)	0	100	100
2	N	171/182 (94%)	167 (98%)	3 (2%)	1 (1%)	30	56
2	P	171/182 (94%)	167 (98%)	4 (2%)	0	100	100
2	R	171/182 (94%)	167 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4428/4644 (95%)	4301 (97%)	125 (3%)	2 (0%)	100 100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	142	HIS
2	N	12	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	287/297 (97%)	277 (96%)	10 (4%)	43 71
1	C	287/297 (97%)	273 (95%)	14 (5%)	31 57
1	E	287/297 (97%)	272 (95%)	15 (5%)	29 54
1	G	287/297 (97%)	274 (96%)	13 (4%)	34 62
1	I	287/297 (97%)	276 (96%)	11 (4%)	40 68
1	K	287/297 (97%)	277 (96%)	10 (4%)	43 71
1	M	287/297 (97%)	277 (96%)	10 (4%)	43 71
1	O	287/297 (97%)	276 (96%)	11 (4%)	40 68
1	Q	287/297 (97%)	278 (97%)	9 (3%)	47 76
2	B	148/155 (96%)	147 (99%)	1 (1%)	88 96
2	D	148/155 (96%)	147 (99%)	1 (1%)	88 96
2	F	148/155 (96%)	147 (99%)	1 (1%)	88 96
2	H	148/155 (96%)	146 (99%)	2 (1%)	74 90
2	J	148/155 (96%)	146 (99%)	2 (1%)	74 90
2	L	148/155 (96%)	141 (95%)	7 (5%)	32 59
2	N	148/155 (96%)	147 (99%)	1 (1%)	88 96
2	P	148/155 (96%)	145 (98%)	3 (2%)	63 85
2	R	148/155 (96%)	147 (99%)	1 (1%)	88 96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3915/4068 (96%)	3793 (97%)	122 (3%)	47 76

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	29	ILE
1	A	36	VAL
1	A	82	VAL
1	A	111	LEU
1	A	125(A)	LYS
1	A	135	VAL
1	A	151	VAL
1	A	195	TYR
1	A	197	ASN
2	B	69	GLU
1	C	26	VAL
1	C	29	ILE
1	C	36	VAL
1	C	125(B)	SER
1	C	133(A)	SER
1	C	135	VAL
1	C	154	LEU
1	C	195	TYR
1	C	197	ASN
1	C	199	THR
1	C	206	THR
1	C	283	THR
1	C	309	VAL
1	C	323	THR
2	D	168	LEU
1	E	23	THR
1	E	36	VAL
1	E	51	LEU
1	E	135	VAL
1	E	151	VAL
1	E	195	TYR
1	E	197	ASN
1	E	206	THR
1	E	213	LEU
1	E	227	SER
1	E	230	MET

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Mol	Chain	Res	Type
1	E	283	THR
1	E	291	SER
1	E	292	MET
1	E	309	VAL
2	F	22	TYR
1	G	36	VAL
1	G	102	PHE
1	G	133(A)	SER
1	G	135	VAL
1	G	151	VAL
1	G	194	LEU
1	G	195	TYR
1	G	199	THR
1	G	206	THR
1	G	227	SER
1	G	283	THR
1	G	291	SER
1	G	323	THR
2	H	24	TYR
2	H	41	THR
1	I	23	THR
1	I	26	VAL
1	I	36	VAL
1	I	125(B)	SER
1	I	135	VAL
1	I	151	VAL
1	I	179	LEU
1	I	195	TYR
1	I	197	ASN
1	I	273	GLU
1	I	283	THR
2	J	26	HIS
2	J	84	MET
1	K	23	THR
1	K	26	VAL
1	K	36	VAL
1	K	59	LEU
1	K	102	PHE
1	K	151	VAL
1	K	154	LEU
1	K	195	TYR
1	K	227	SER

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Mol	Chain	Res	Type
1	K	309	VAL
2	L	22	TYR
2	L	41	THR
2	L	60	ASN
2	L	84	MET
2	L	122	VAL
2	L	152	VAL
2	L	172	GLU
1	M	36	VAL
1	M	75	MET
1	M	121	ILE
1	M	151	VAL
1	M	195	TYR
1	M	206	THR
1	M	220	ARG
1	M	267	ILE
1	M	277	CYS
1	M	315	VAL
2	N	26	HIS
1	O	23	THR
1	O	36	VAL
1	O	51	LEU
1	O	56	VAL
1	O	159	SER
1	O	182	ILE
1	O	192	THR
1	O	195	TYR
1	O	219	THR
1	O	309	VAL
1	O	323	THR
2	P	18	VAL
2	P	73	LEU
2	P	75	ARG
1	Q	36	VAL
1	Q	37	THR
1	Q	46	THR
1	Q	124	ILE
1	Q	133(A)	SER
1	Q	135	VAL
1	Q	151	VAL
1	Q	195	TYR
1	Q	219	THR

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Mol	Chain	Res	Type
2	R	61	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	GLN
1	C	172	ASN
1	E	38	HIS
1	E	211	GLN
2	F	129	ASN
1	G	211	GLN
1	I	38	HIS
1	M	197	ASN
1	M	211	GLN
2	N	83	GLN
2	P	26	HIS
1	Q	38	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

17 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	0.46	0	15,19,21	1.26	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	A	2002	3	14,14,15	0.49	0	15,19,21	1.00	1 (6%)
3	NAG	C	2001	1,3	14,14,15	0.44	0	15,19,21	1.06	1 (6%)
3	NAG	C	2002	3	14,14,15	0.40	0	15,19,21	0.93	1 (6%)
3	NAG	E	2002	1,3	14,14,15	0.52	0	15,19,21	1.75	4 (26%)
3	NAG	E	2003	3	14,14,15	0.51	0	15,19,21	1.50	1 (6%)
3	NAG	I	2001	1,3	14,14,15	0.58	0	15,19,21	1.70	2 (13%)
3	NAG	I	2002	3	14,14,15	0.52	0	15,19,21	0.96	1 (6%)
3	NAG	K	2001	1,3	14,14,15	0.48	0	15,19,21	1.66	2 (13%)
3	NAG	K	2002	3	14,14,15	0.51	0	15,19,21	0.69	0
3	NAG	M	2001	1,3	14,14,15	0.52	0	15,19,21	1.79	3 (20%)
3	NAG	M	2002	3	14,14,15	0.54	0	15,19,21	1.25	1 (6%)
5	NAG	Q	2001	1,5	14,14,15	0.44	0	15,19,21	1.11	0
5	NAG	Q	2002	5	14,14,15	0.46	0	15,19,21	0.99	1 (6%)
5	MAN	Q	2003	5	11,11,12	0.50	0	14,15,17	1.62	2 (14%)
3	NAG	R	2001	3,2	14,14,15	0.60	0	15,19,21	1.59	2 (13%)
3	NAG	R	2002	3	14,14,15	0.50	0	15,19,21	1.67	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
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	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	NAG	E	2002	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2003	3	-	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	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	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
5	NAG	Q	2001	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Q	2002	5	-	0/6/23/26	0/1/1/1
5	MAN	Q	2003	5	-	0/2/19/22	0/1/1/1
3	NAG	R	2001	3,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	R	2002	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	2001	NAG	O4-C4-C3	-3.15	103.25	110.34
3	K	2001	NAG	C2-N2-C7	-2.95	119.25	123.04
3	I	2001	NAG	O4-C4-C3	-2.85	103.91	110.34
3	M	2001	NAG	C2-N2-C7	-2.72	119.55	123.04
5	Q	2002	NAG	C2-N2-C7	-2.54	119.78	123.04
3	E	2002	NAG	O4-C4-C5	-2.49	102.64	109.24
3	A	2002	NAG	C2-N2-C7	-2.02	120.45	123.04
3	C	2002	NAG	C1-O5-C5	2.23	115.08	112.25
3	C	2001	NAG	C1-O5-C5	2.53	115.46	112.25
3	I	2002	NAG	C4-C3-C2	2.54	115.18	111.23
3	E	2002	NAG	C1-O5-C5	2.66	115.62	112.25
3	M	2002	NAG	C4-C3-C2	2.76	115.52	111.23
3	R	2002	NAG	C3-C4-C5	3.00	115.42	110.20
5	Q	2003	MAN	C3-C4-C5	3.06	115.53	110.20
3	R	2001	NAG	C2-N2-C7	3.15	127.08	123.04
3	E	2002	NAG	C4-C3-C2	3.15	116.13	111.23
3	A	2001	NAG	C1-O5-C5	3.89	117.18	112.25
3	E	2002	NAG	C3-C4-C5	4.18	117.48	110.20
3	K	2001	NAG	C1-O5-C5	4.20	117.58	112.25
5	Q	2003	MAN	C1-O5-C5	4.26	117.65	112.25
3	R	2001	NAG	C1-O5-C5	4.29	117.69	112.25
3	E	2003	NAG	C1-O5-C5	4.41	117.85	112.25
3	M	2001	NAG	C1-O5-C5	4.69	118.20	112.25
3	R	2002	NAG	C1-O5-C5	4.88	118.44	112.25
3	I	2001	NAG	C1-O5-C5	4.88	118.44	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2002	NAG	3	0
3	E	2003	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	2001	NAG	1	0
3	K	2001	NAG	1	0
3	M	2001	NAG	1	0

5.6 Ligand geometry (i)

14 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	$\#\|Z\| > 2$
4	NAG	A	2003	1	14,14,15	0.57	0	15,19,21	1.63	3 (20%)
4	NAG	C	2003	1	14,14,15	0.55	0	15,19,21	1.58	3 (20%)
4	NAG	E	2001	1	14,14,15	0.45	0	15,19,21	1.08	1 (6%)
4	NAG	E	2004	1	14,14,15	0.37	0	15,19,21	0.72	0
4	NAG	G	2001	1	14,14,15	0.43	0	15,19,21	1.46	1 (6%)
4	NAG	G	2002	1	14,14,15	0.45	0	15,19,21	1.88	1 (6%)
4	NAG	I	2003	1	14,14,15	0.44	0	15,19,21	1.26	1 (6%)
4	NAG	K	2003	1	14,14,15	0.58	0	15,19,21	1.52	3 (20%)
4	NAG	K	2004	1	14,14,15	0.41	0	15,19,21	1.38	2 (13%)
4	NAG	M	2003	1	14,14,15	0.43	0	15,19,21	0.86	0
4	NAG	M	2004	1	14,14,15	0.50	0	15,19,21	0.80	0
4	NAG	O	2001	1	14,14,15	0.45	0	15,19,21	1.57	1 (6%)
4	NAG	O	2002	1	14,14,15	0.37	0	15,19,21	1.50	1 (6%)
4	NAG	Q	2004	1	14,14,15	0.52	0	15,19,21	1.33	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	2003	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	2003	1	-	0/6/23/26	0/1/1/1
4	NAG	E	2001	1	-	0/6/23/26	0/1/1/1
4	NAG	E	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	G	2001	1	-	0/6/23/26	0/1/1/1
4	NAG	G	2002	1	-	0/6/23/26	0/1/1/1
4	NAG	I	2003	1	-	0/6/23/26	0/1/1/1
4	NAG	K	2003	1	-	0/6/23/26	0/1/1/1
4	NAG	K	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	M	2003	1	-	0/6/23/26	0/1/1/1
4	NAG	M	2004	1	-	0/6/23/26	0/1/1/1
4	NAG	O	2001	1	-	0/6/23/26	0/1/1/1
4	NAG	O	2002	1	-	0/6/23/26	0/1/1/1
4	NAG	Q	2004	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	2003	NAG	O4-C4-C5	-3.78	99.22	109.24
4	K	2004	NAG	C2-N2-C7	-3.09	119.07	123.04
4	A	2003	NAG	O3-C3-C2	-2.26	104.64	109.11
4	K	2003	NAG	O3-C3-C2	-2.18	104.80	109.11
4	C	2003	NAG	C4-C3-C2	2.38	114.93	111.23
4	K	2003	NAG	C3-C4-C5	2.39	114.37	110.20
4	E	2001	NAG	C1-O5-C5	2.61	115.56	112.25
4	C	2003	NAG	C1-O5-C5	2.80	115.80	112.25
4	A	2003	NAG	C3-C4-C5	2.96	115.35	110.20
4	K	2004	NAG	C1-O5-C5	3.52	116.71	112.25
4	O	2002	NAG	C1-O5-C5	3.74	116.99	112.25
4	C	2003	NAG	C3-C4-C5	3.86	116.92	110.20
4	A	2003	NAG	C4-C3-C2	3.86	117.23	111.23
4	Q	2004	NAG	C1-O5-C5	4.00	117.33	112.25
4	I	2003	NAG	C1-O5-C5	4.03	117.37	112.25
4	G	2001	NAG	C1-O5-C5	4.69	118.20	112.25
4	O	2001	NAG	C1-O5-C5	5.05	118.65	112.25
4	G	2002	NAG	C1-O5-C5	6.61	120.64	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	K	2004	NAG	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	323/334 (96%)	0.21	8 (2%) 61 54	62, 86, 117, 157	0
1	C	323/334 (96%)	0.48	26 (8%) 15 10	69, 102, 130, 161	0
1	E	323/334 (96%)	0.33	19 (5%) 26 19	67, 94, 121, 167	0
1	G	323/334 (96%)	0.27	6 (1%) 70 64	63, 85, 112, 148	0
1	I	323/334 (96%)	0.13	3 (0%) 85 83	46, 80, 100, 138	0
1	K	323/334 (96%)	0.37	17 (5%) 30 23	52, 93, 121, 164	0
1	M	323/334 (96%)	0.57	30 (9%) 11 7	79, 112, 143, 176	0
1	O	323/334 (96%)	0.35	18 (5%) 28 21	65, 102, 130, 154	0
1	Q	323/334 (96%)	0.13	5 (1%) 76 71	61, 82, 107, 135	0
2	B	173/182 (95%)	0.33	3 (1%) 73 68	54, 83, 115, 159	0
2	D	173/182 (95%)	0.39	5 (2%) 55 48	62, 91, 124, 171	0
2	F	173/182 (95%)	1.00	24 (13%) 4 2	57, 104, 165, 216	0
2	H	173/182 (95%)	0.83	17 (9%) 10 6	62, 101, 155, 194	0
2	J	173/182 (95%)	0.26	3 (1%) 73 68	58, 84, 120, 167	0
2	L	173/182 (95%)	0.70	16 (9%) 11 7	64, 101, 153, 167	0
2	N	173/182 (95%)	0.53	8 (4%) 36 29	69, 97, 135, 155	0
2	P	173/182 (95%)	0.63	6 (3%) 48 40	63, 91, 126, 181	0
2	R	173/182 (95%)	0.26	1 (0%) 90 88	61, 79, 106, 147	0
All	All	4464/4644 (96%)	0.40	215 (4%) 34 27	46, 91, 134, 216	0

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	9	PRO	10.6
2	P	173	ILE	8.9
2	F	140	PHE	8.2

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Mol	Chain	Res	Type	RSRZ
1	E	9	PRO	7.3
2	H	173	ILE	7.0
2	F	164	GLU	6.4
2	H	140	PHE	6.3
2	L	150	GLU	6.2
2	F	149	MET	5.7
1	K	176	LEU	5.5
1	C	9	PRO	5.2
1	K	9	PRO	5.1
1	E	173	GLN	5.0
1	O	9	PRO	4.9
2	F	141	TYR	4.7
1	M	270	SER	4.6
1	M	9	PRO	4.6
1	M	100	GLY	4.5
1	M	228	GLY	4.5
2	H	153	LYS	4.4
2	F	29	GLU	4.2
2	F	168	LEU	4.2
1	I	9	PRO	4.2
2	H	149	MET	4.2
1	C	257	ALA	4.1
1	C	276	ASN	4.0
2	F	33	GLY	4.0
1	M	272	LEU	4.0
1	C	51	LEU	4.0
1	E	240	ASN	3.9
2	N	153	LYS	3.9
2	H	139	GLU	3.9
1	Q	118	PHE	3.9
1	A	9	PRO	3.8
1	Q	9	PRO	3.7
2	P	152	VAL	3.7
1	O	251	PHE	3.7
1	C	151	VAL	3.7
1	C	134	GLY	3.7
1	O	123	ILE	3.7
1	O	240	ASN	3.6
2	N	1	GLY	3.5
2	F	144	CYS	3.5
2	H	164	GLU	3.5
1	E	11	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	M	179	LEU	3.5
1	A	55(A)	GLY	3.4
2	F	173	ILE	3.4
2	F	126	LEU	3.4
1	M	222	LYS	3.4
1	M	118	PHE	3.3
1	C	260(A)	VAL	3.3
2	D	172	GLU	3.3
1	C	61	LEU	3.3
1	O	121	ILE	3.3
2	L	157	TYR	3.3
2	L	153	LYS	3.3
1	K	51	LEU	3.3
1	E	260(A)	VAL	3.3
1	K	160	ALA	3.3
2	H	168	LEU	3.2
2	L	167	ARG	3.2
1	C	160	ALA	3.2
2	D	173	ILE	3.2
2	H	166	ALA	3.2
1	E	87	ILE	3.2
1	M	212	ARG	3.2
2	P	149	MET	3.2
2	B	172	GLU	3.1
2	H	138	PHE	3.1
1	I	176	LEU	3.1
1	K	112	LEU	3.1
1	O	239	PRO	3.0
2	P	29	GLU	3.0
2	F	171	GLU	3.0
1	M	123	ILE	3.0
1	E	51	LEU	3.0
2	J	1	GLY	3.0
1	M	302	ILE	2.9
2	P	164	GLU	2.9
1	C	288	ILE	2.9
1	M	223	VAL	2.9
1	C	179	LEU	2.9
1	A	118	PHE	2.9
1	E	302	ILE	2.9
1	A	272	LEU	2.9
1	Q	272	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	167	ARG	2.8
2	N	24	TYR	2.8
2	F	145	ASP	2.8
1	E	121	ILE	2.8
1	C	39	ALA	2.8
2	F	139	GLU	2.8
2	H	141	TYR	2.7
1	E	257	ALA	2.7
2	L	164	GLU	2.7
2	H	21	TRP	2.7
1	C	144	ARG	2.7
2	H	126	LEU	2.7
1	O	161	TYR	2.7
1	E	61	LEU	2.7
1	C	270	SER	2.7
2	N	29	GLU	2.6
1	E	118	PHE	2.6
1	E	69	TRP	2.6
1	M	276	ASN	2.6
1	K	54	LEU	2.6
2	B	33	GLY	2.6
1	A	51	LEU	2.6
1	K	324	PRO	2.6
1	M	51	LEU	2.6
1	C	282	GLN	2.6
1	I	103	ASN	2.6
2	F	106	ARG	2.6
2	B	173	ILE	2.5
2	H	29	GLU	2.5
2	F	129	ASN	2.5
2	D	153	LYS	2.5
1	O	195	TYR	2.5
2	L	31	GLY	2.5
1	M	79	PHE	2.5
1	M	154	LEU	2.5
2	L	140	PHE	2.5
2	J	152	VAL	2.5
1	Q	300	LEU	2.5
1	C	56	VAL	2.4
2	L	26	HIS	2.4
1	M	140	PRO	2.4
1	C	272	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
2	L	27	SER	2.4
2	H	130	ALA	2.4
1	K	50	LYS	2.4
1	O	171	THR	2.4
1	C	102	PHE	2.4
1	E	242	ALA	2.4
1	O	266	ALA	2.4
2	D	105	GLU	2.4
1	E	178	VAL	2.4
1	M	229	ARG	2.4
1	M	288	ILE	2.4
1	K	286	GLY	2.3
1	M	282	GLN	2.3
2	L	173	ILE	2.3
2	R	173	ILE	2.3
1	O	118	PHE	2.3
1	M	54	LEU	2.3
1	M	209	LEU	2.3
2	H	162	TYR	2.3
1	G	60	ILE	2.3
1	O	245	PHE	2.3
1	O	84	TRP	2.3
1	G	272	LEU	2.3
1	M	85	SER	2.3
1	C	297	ILE	2.2
1	K	217	ILE	2.2
1	O	79	PHE	2.2
2	P	144	CYS	2.2
1	E	274	TYR	2.2
1	K	285	MET	2.2
1	K	288	ILE	2.2
1	M	60	ILE	2.2
1	K	282	GLN	2.2
1	C	277	CYS	2.2
2	F	15	GLN	2.2
1	M	224	ASN	2.2
2	L	172	GLU	2.2
2	F	170	ARG	2.2
1	A	280	LYS	2.2
1	O	260(A)	VAL	2.2
1	O	261	LYS	2.2
1	Q	88	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	260	ILE	2.2
1	K	62	ARG	2.2
2	N	112	ASP	2.2
1	A	57	LYS	2.1
1	M	112	LEU	2.1
1	C	324	PRO	2.1
1	C	196	GLN	2.1
2	L	1	GLY	2.1
1	O	112	LEU	2.1
2	L	18	VAL	2.1
2	F	157	TYR	2.1
1	C	54	LEU	2.1
1	O	154	LEU	2.1
2	N	2	LEU	2.1
1	E	55(A)	GLY	2.1
2	H	16	GLY	2.1
2	F	166	ALA	2.1
1	C	57	LYS	2.1
2	L	15	GLN	2.1
1	E	154	LEU	2.1
1	C	239	PRO	2.1
2	H	152	VAL	2.1
1	K	322	ASN	2.1
1	M	96(A)	LEU	2.1
1	G	56	VAL	2.1
1	G	173	GLN	2.1
1	E	273	GLU	2.1
2	F	138	PHE	2.1
2	J	168	LEU	2.1
2	L	35	ALA	2.0
2	F	17	MET	2.0
2	D	1	GLY	2.0
1	A	102	PHE	2.0
1	C	209	LEU	2.0
2	L	168	LEU	2.0
1	G	21	ASN	2.0
2	F	153	LYS	2.0
1	M	285	MET	2.0
2	N	107	THR	2.0
1	K	287	ALA	2.0
1	M	257	ALA	2.0
1	K	297	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	N	89	LEU	2.0
2	F	143	LYS	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	2001	14/15	0.96	0.12	-0.52	85,105,126,131	0
5	NAG	Q	2001	14/15	0.95	0.12	-0.72	86,104,121,126	0
3	NAG	K	2001	14/15	0.96	0.08	-0.79	74,93,106,109	0
3	NAG	I	2001	14/15	0.93	0.12	-1.73	68,84,96,98	0
3	NAG	M	2001	14/15	0.93	0.10	-1.83	91,109,123,143	0
3	NAG	C	2001	14/15	0.92	0.12	-1.95	82,103,115,116	0
3	NAG	E	2003	14/15	0.80	0.35	-	135,145,154,158	0
3	NAG	R	2002	14/15	0.91	0.21	-	119,142,154,163	0
3	NAG	R	2001	14/15	0.88	0.31	-	96,115,120,135	0
3	NAG	I	2002	14/15	0.89	0.20	-	111,122,137,152	0
3	NAG	C	2002	14/15	0.87	0.24	-	109,132,145,152	0
3	NAG	M	2002	14/15	0.82	0.19	-	144,161,171,177	0
5	MAN	Q	2003	11/12	0.84	0.32	-	143,164,169,173	0
3	NAG	A	2002	14/15	0.81	0.24	-	121,139,156,167	0
5	NAG	Q	2002	14/15	0.87	0.20	-	122,141,155,162	0
3	NAG	K	2002	14/15	0.90	0.17	-	123,135,150,165	0
3	NAG	E	2002	14/15	0.86	0.16	-	92,126,137,139	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, 95^{th} percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	E	2001	14/15	0.84	0.30	0.64	103,118,138,158	0
4	NAG	G	2001	14/15	0.91	0.14	0.14	86,106,114,116	0
4	NAG	O	2001	14/15	0.86	0.18	-0.58	75,105,120,122	0
4	NAG	I	2003	14/15	0.91	0.18	-	102,115,121,121	0
4	NAG	G	2002	14/15	0.91	0.14	-	107,124,130,133	0
4	NAG	K	2003	14/15	0.82	0.19	-	103,125,134,148	0
4	NAG	M	2003	14/15	0.90	0.16	-	112,129,135,138	0
4	NAG	M	2004	14/15	0.85	0.33	-	112,151,162,166	0
4	NAG	O	2002	14/15	0.91	0.13	-	92,112,118,125	0
4	NAG	C	2003	14/15	0.88	0.31	-	115,124,136,149	0
4	NAG	E	2004	14/15	0.81	0.22	-	119,136,150,151	0
4	NAG	Q	2004	14/15	0.85	0.20	-	115,127,133,135	0
4	NAG	K	2004	14/15	0.74	0.23	-	133,149,159,163	0
4	NAG	A	2003	14/15	0.86	0.20	-	102,127,143,157	0

6.5 Other polymers

There are no such residues in this entry.