



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:57 PM GMT

PDB ID : 4JUL  
Title : Crystal structure of H5N1 influenza virus hemagglutinin, clade 2.3.4  
Authors : DuBois, R.M.; Zaraket, H.; Reddivari, M.; Coop, T.; Heath, R.J.; White, S.W.; Russell, C.J.  
Deposited on : 2013-03-25  
Resolution : 2.79 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](mailto: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.

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

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

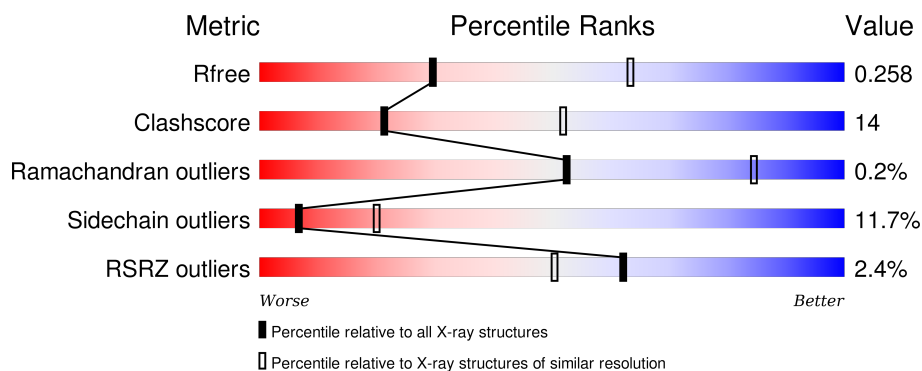
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.79 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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  $\geq 3$ , 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	329	 71% 24% . .
1	C	329	 64% 30% . .
1	E	329	 67% 27% . .
1	H	329	 67% 27% . .
1	J	329	 69% 26% . .

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Mol	Chain	Length	Quality of chain
1	L	329	
2	B	182	
2	D	182	
2	F	182	
2	I	182	
2	K	182	
2	M	182	

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	J	401	-	-	X	-
3	NAG	J	402	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23752 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2535	1601	436	485	13			
1	C	321	Total	C	N	O	S	0	0	0
			2535	1601	436	485	13			
1	E	322	Total	C	N	O	S	0	0	0
			2542	1606	437	486	13			
1	H	321	Total	C	N	O	S	0	0	0
			2535	1601	436	485	13			
1	J	321	Total	C	N	O	S	0	0	0
			2535	1601	436	485	13			
1	L	319	Total	C	N	O	S	0	0	0
			2523	1595	434	481	13			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLY	-	EXPRESSION TAG	UNP Q00G25
A	6	SER	-	EXPRESSION TAG	UNP Q00G25
A	7	ALA	-	EXPRESSION TAG	UNP Q00G25
A	8	ASP	-	EXPRESSION TAG	UNP Q00G25
A	9	PRO	-	EXPRESSION TAG	UNP Q00G25
A	10	GLY	-	EXPRESSION TAG	UNP Q00G25
C	5	GLY	-	EXPRESSION TAG	UNP Q00G25
C	6	SER	-	EXPRESSION TAG	UNP Q00G25
C	7	ALA	-	EXPRESSION TAG	UNP Q00G25
C	8	ASP	-	EXPRESSION TAG	UNP Q00G25
C	9	PRO	-	EXPRESSION TAG	UNP Q00G25
C	10	GLY	-	EXPRESSION TAG	UNP Q00G25
E	5	GLY	-	EXPRESSION TAG	UNP Q00G25
E	6	SER	-	EXPRESSION TAG	UNP Q00G25
E	7	ALA	-	EXPRESSION TAG	UNP Q00G25
E	8	ASP	-	EXPRESSION TAG	UNP Q00G25
E	9	PRO	-	EXPRESSION TAG	UNP Q00G25

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Chain	Residue	Modelled	Actual	Comment	Reference
E	10	GLY	-	EXPRESSION TAG	UNP Q00G25
H	5	GLY	-	EXPRESSION TAG	UNP Q00G25
H	6	SER	-	EXPRESSION TAG	UNP Q00G25
H	7	ALA	-	EXPRESSION TAG	UNP Q00G25
H	8	ASP	-	EXPRESSION TAG	UNP Q00G25
H	9	PRO	-	EXPRESSION TAG	UNP Q00G25
H	10	GLY	-	EXPRESSION TAG	UNP Q00G25
J	5	GLY	-	EXPRESSION TAG	UNP Q00G25
J	6	SER	-	EXPRESSION TAG	UNP Q00G25
J	7	ALA	-	EXPRESSION TAG	UNP Q00G25
J	8	ASP	-	EXPRESSION TAG	UNP Q00G25
J	9	PRO	-	EXPRESSION TAG	UNP Q00G25
J	10	GLY	-	EXPRESSION TAG	UNP Q00G25
L	5	GLY	-	EXPRESSION TAG	UNP Q00G25
L	6	SER	-	EXPRESSION TAG	UNP Q00G25
L	7	ALA	-	EXPRESSION TAG	UNP Q00G25
L	8	ASP	-	EXPRESSION TAG	UNP Q00G25
L	9	PRO	-	EXPRESSION TAG	UNP Q00G25
L	10	GLY	-	EXPRESSION TAG	UNP Q00G25

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	170	Total	C	N	O	S	0	0	0
			1380	859	241	272	8			
2	D	172	Total	C	N	O	S	0	0	0
			1398	869	243	278	8			
2	F	172	Total	C	N	O	S	0	0	0
			1398	869	243	278	8			
2	I	170	Total	C	N	O	S	0	0	0
			1380	859	241	272	8			
2	K	172	Total	C	N	O	S	0	0	0
			1398	869	243	278	8			
2	M	169	Total	C	N	O	S	0	0	0
			1369	853	237	271	8			

There are 36 discrepancies between the modelled and reference sequences:

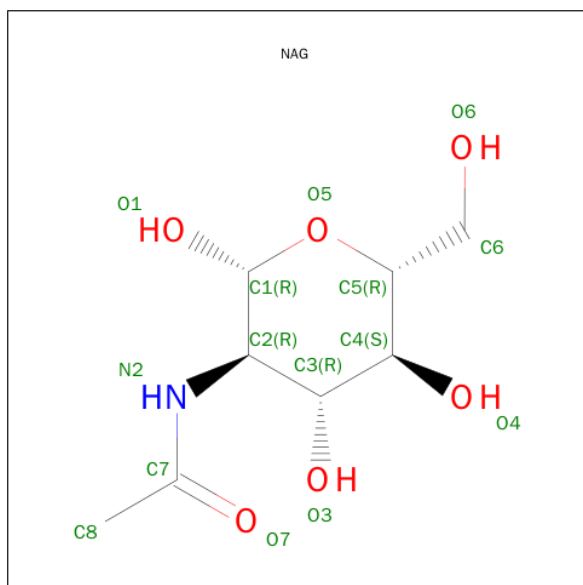
Chain	Residue	Modelled	Actual	Comment	Reference
B	177	ARG	-	EXPRESSION TAG	UNP Q00G25
B	178	SER	-	EXPRESSION TAG	UNP Q00G25
B	179	LEU	-	EXPRESSION TAG	UNP Q00G25

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Chain	Residue	Modelled	Actual	Comment	Reference
B	180	VAL	-	EXPRESSION TAG	UNP Q00G25
B	181	PRO	-	EXPRESSION TAG	UNP Q00G25
B	182	ARG	-	EXPRESSION TAG	UNP Q00G25
D	177	ARG	-	EXPRESSION TAG	UNP Q00G25
D	178	SER	-	EXPRESSION TAG	UNP Q00G25
D	179	LEU	-	EXPRESSION TAG	UNP Q00G25
D	180	VAL	-	EXPRESSION TAG	UNP Q00G25
D	181	PRO	-	EXPRESSION TAG	UNP Q00G25
D	182	ARG	-	EXPRESSION TAG	UNP Q00G25
F	177	ARG	-	EXPRESSION TAG	UNP Q00G25
F	178	SER	-	EXPRESSION TAG	UNP Q00G25
F	179	LEU	-	EXPRESSION TAG	UNP Q00G25
F	180	VAL	-	EXPRESSION TAG	UNP Q00G25
F	181	PRO	-	EXPRESSION TAG	UNP Q00G25
F	182	ARG	-	EXPRESSION TAG	UNP Q00G25
I	177	ARG	-	EXPRESSION TAG	UNP Q00G25
I	178	SER	-	EXPRESSION TAG	UNP Q00G25
I	179	LEU	-	EXPRESSION TAG	UNP Q00G25
I	180	VAL	-	EXPRESSION TAG	UNP Q00G25
I	181	PRO	-	EXPRESSION TAG	UNP Q00G25
I	182	ARG	-	EXPRESSION TAG	UNP Q00G25
K	177	ARG	-	EXPRESSION TAG	UNP Q00G25
K	178	SER	-	EXPRESSION TAG	UNP Q00G25
K	179	LEU	-	EXPRESSION TAG	UNP Q00G25
K	180	VAL	-	EXPRESSION TAG	UNP Q00G25
K	181	PRO	-	EXPRESSION TAG	UNP Q00G25
K	182	ARG	-	EXPRESSION TAG	UNP Q00G25
M	177	ARG	-	EXPRESSION TAG	UNP Q00G25
M	178	SER	-	EXPRESSION TAG	UNP Q00G25
M	179	LEU	-	EXPRESSION TAG	UNP Q00G25
M	180	VAL	-	EXPRESSION TAG	UNP Q00G25
M	181	PRO	-	EXPRESSION TAG	UNP Q00G25
M	182	ARG	-	EXPRESSION TAG	UNP Q00G25

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		
3	J	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		
3	J	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		

- 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		

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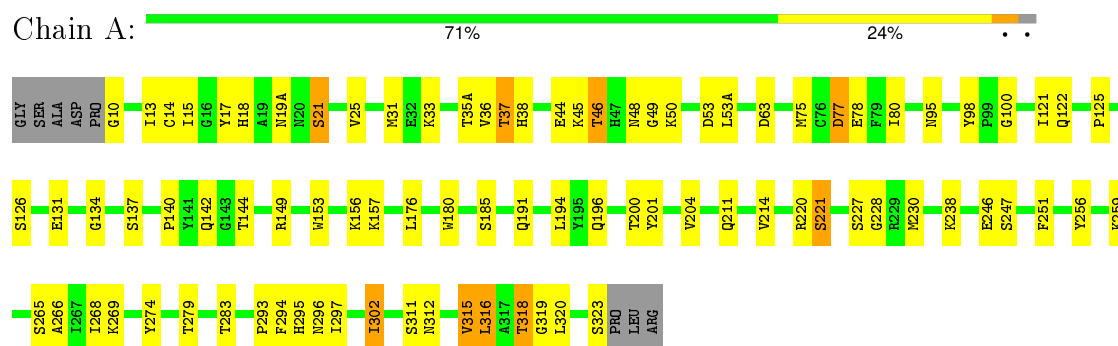
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	2	Total	C	N	O	0	0
			28	16	2	10		



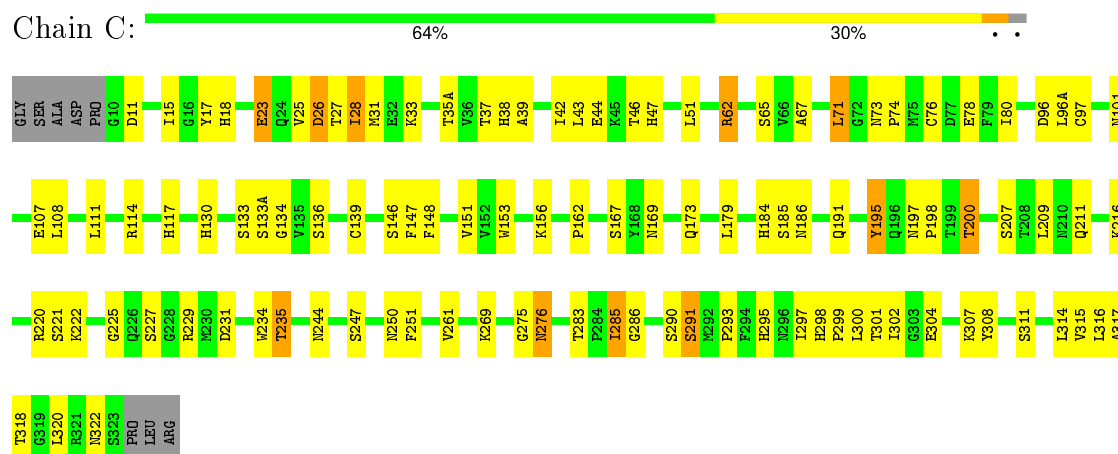
### 3 Residue-property plots

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.

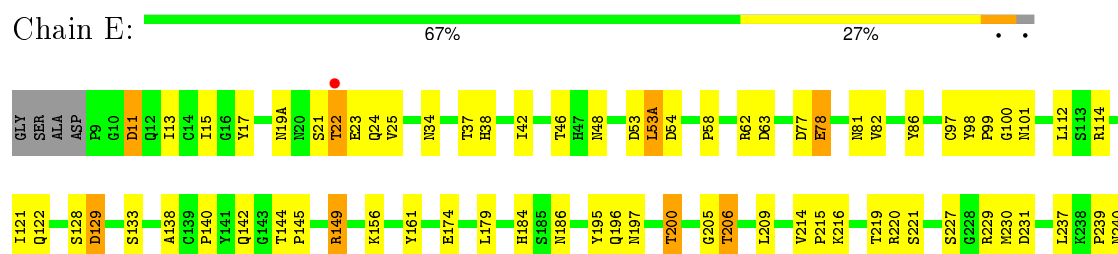
#### • Molecule 1: Hemagglutinin HA1



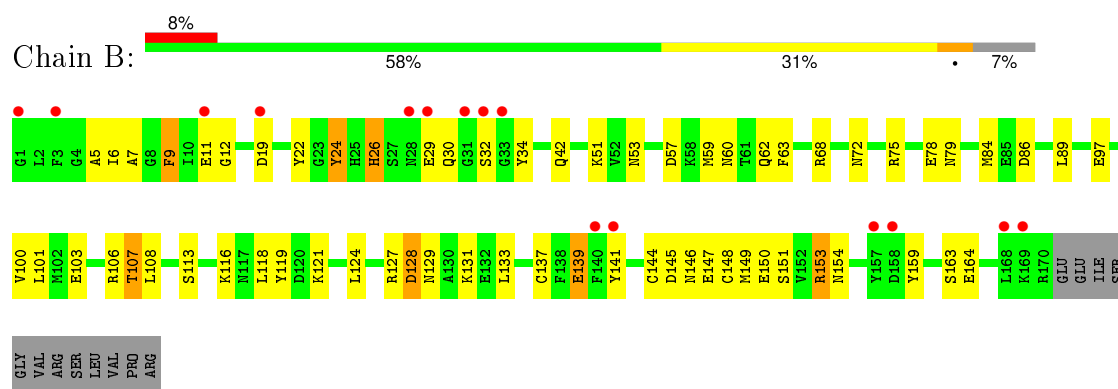
#### • Molecule 1: Hemagglutinin HA1



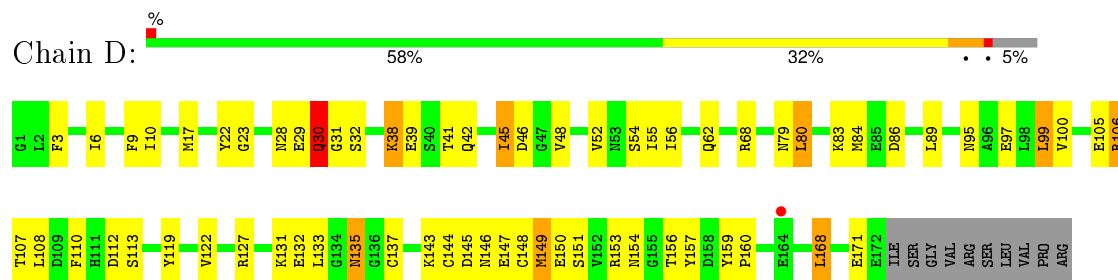
#### • Molecule 1: Hemagglutinin HA1



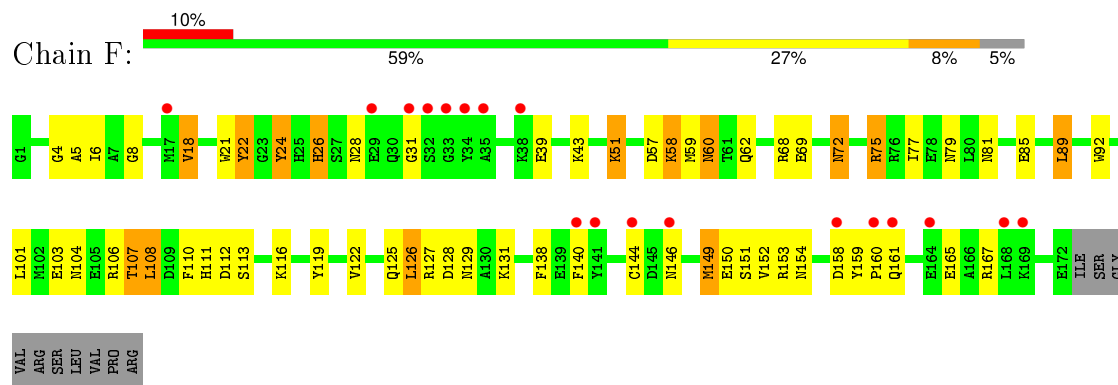




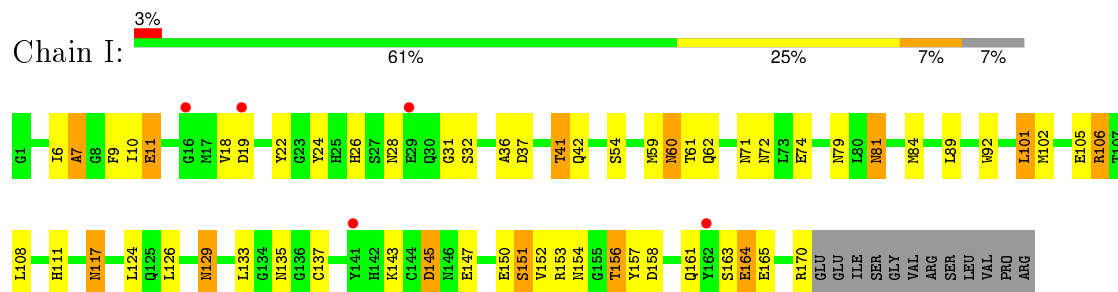
• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2

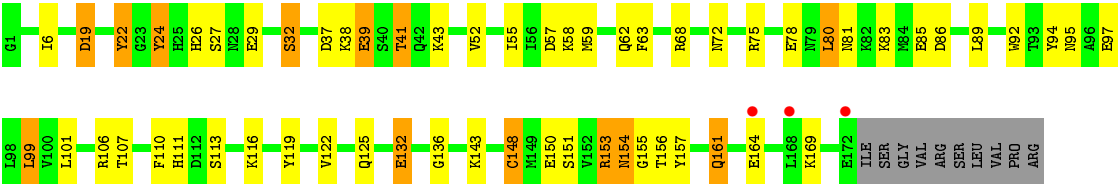


• Molecule 2: Hemagglutinin HA2

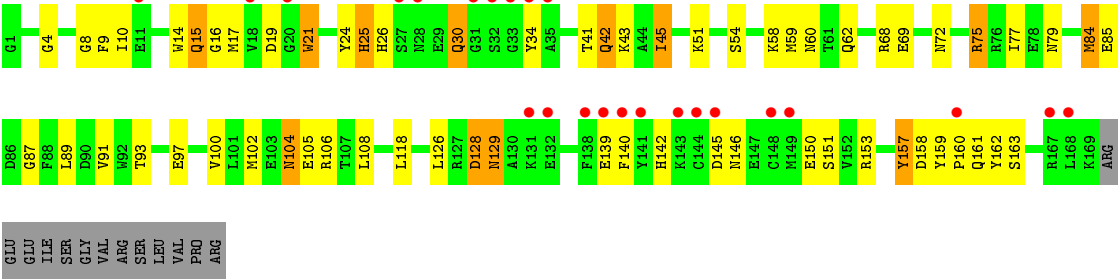


• Molecule 2: Hemagglutinin HA2





● Molecule 2: Hemagglutinin HA2



GLU  
GLU  
ILE  
SER  
GLY  
VAL  
ARG  
SER  
SER  
VAL  
PRO  
ARG

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.58Å 71.56Å 247.05Å 83.94° 85.46° 60.68°	Depositor
Resolution (Å)	48.87 – 2.79 48.87 – 2.79	Depositor EDS
% Data completeness (in resolution range)	81.4 (48.87-2.79) 79.3 (48.87-2.79)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.196 , 0.254 0.204 , 0.258	Depositor DCC
$R_{free}$ test set	4355 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.5	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.0	EDS
Estimated twinning fraction	0.018 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 85847 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	23752	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.52	0/2596	0.68	0/3529
1	C	0.59	0/2596	0.69	0/3529
1	E	0.52	0/2604	0.69	0/3540
1	H	0.53	1/2596 (0.0%)	0.66	0/3529
1	J	0.55	0/2596	0.69	0/3529
1	L	0.51	0/2584	0.69	0/3513
2	B	0.51	0/1407	0.66	1/1891 (0.1%)
2	D	0.51	0/1425	0.68	1/1915 (0.1%)
2	F	0.49	0/1425	0.63	0/1915
2	I	0.52	0/1407	0.71	1/1891 (0.1%)
2	K	0.49	0/1425	0.62	0/1915
2	M	0.48	0/1396	0.65	0/1877
All	All	0.52	1/24057 (0.0%)	0.67	3/32573 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	125	PRO	N-CD	-5.58	1.40	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	30	GLN	N-CA-C	-5.55	96.02	111.00
2	B	153	ARG	NE-CZ-NH2	5.17	122.89	120.30
2	I	7	ALA	N-CA-C	-5.03	97.42	111.00

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	2535	0	2468	66	0
1	C	2535	0	2469	73	0
1	E	2542	0	2478	81	0
1	H	2535	0	2469	67	0
1	J	2535	0	2469	52	0
1	L	2523	0	2462	74	0
2	B	1380	0	1291	54	0
2	D	1398	0	1303	64	0
2	F	1398	0	1303	57	0
2	I	1380	0	1291	47	0
2	K	1398	0	1303	42	0
2	M	1369	0	1278	63	0
3	A	14	0	13	2	0
3	C	28	0	26	0	0
3	E	14	0	13	5	0
3	H	14	0	13	1	0
3	J	28	0	26	8	0
3	L	42	0	39	4	0
4	A	28	0	25	2	0
4	E	28	0	25	5	0
4	H	28	0	25	2	0
All	All	23752	0	22789	658	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 14.

All (658) 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:H:34:ASN:HD21	3:H:401:NAG:C1	1.04	1.59
1:E:34:ASN:HD21	3:E:401:NAG:C1	0.95	1.58
1:J:34:ASN:HD21	3:J:401:NAG:C1	1.14	1.57
1:E:53(A):LEU:HD23	1:E:53(A):LEU:O	1.44	1.15
2:M:158:ASP:O	2:M:161:GLN:HB3	1.51	1.10
1:E:242:ALA:HB3	4:E:402:NAG:H82	1.24	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:157:TYR:C	2:M:157:TYR:CD2	2.29	1.02
1:E:34:ASN:HD21	3:E:401:NAG:C2	1.72	1.02
1:A:142:GLN:NE2	1:A:142:GLN:HA	1.76	0.98
2:M:161:GLN:HG3	2:M:162:TYR:CD2	2.01	0.95
1:A:142:GLN:HE21	1:A:142:GLN:HA	1.31	0.95
1:A:49:GLY:O	1:A:50:LYS:HD3	1.69	0.93
1:J:33:LYS:HB2	3:J:401:NAG:H82	1.51	0.92
1:C:27:THR:HG22	1:C:31:MET:H	1.31	0.92
1:A:17:TYR:CZ	2:B:6:ILE:HG23	2.06	0.91
1:E:242:ALA:CB	4:E:402:NAG:H82	2.03	0.89
2:M:157:TYR:C	2:M:157:TYR:HD2	1.75	0.88
2:M:161:GLN:HG3	2:M:162:TYR:HD2	1.34	0.88
2:M:157:TYR:O	2:M:157:TYR:HD2	1.57	0.88
1:C:275:GLY:O	1:C:276:ASN:HB2	1.73	0.86
2:K:27:SER:CB	2:K:32:SER:OG	2.24	0.86
2:F:26:HIS:O	2:F:26:HIS:HD2	1.56	0.85
2:D:68:ARG:HE	2:F:79:ASN:HD22	1.22	0.85
2:F:26:HIS:O	2:F:26:HIS:CD2	2.30	0.85
2:D:9:PHE:CE1	2:D:10:ILE:HG13	2.12	0.84
2:M:26:HIS:O	2:M:26:HIS:CD2	2.30	0.84
2:B:26:HIS:O	2:B:26:HIS:CD2	2.30	0.84
1:E:206:THR:HG23	1:E:209:LEU:HB3	1.60	0.84
1:H:295:HIS:HD2	1:H:297:ILE:H	1.25	0.82
1:H:57:LYS:HG2	1:H:58:PRO:HD2	1.61	0.82
1:C:18:HIS:CD2	2:D:17:MET:O	2.33	0.82
1:A:75:MET:HB2	1:A:95:ASN:ND2	1.96	0.81
2:F:126:LEU:HD12	2:F:126:LEU:N	1.94	0.81
2:F:122:VAL:O	2:F:126:LEU:HD13	1.79	0.81
2:I:7:ALA:HB1	2:I:11:GLU:O	1.79	0.81
3:L:401:NAG:C1	3:L:403:NAG:C4	2.59	0.80
1:E:15:ILE:HD13	2:F:119:TYR:HA	1.63	0.80
1:H:242:ALA:H	4:H:402:NAG:H82	1.47	0.80
1:A:98:TYR:CE2	1:A:230:MET:HG3	2.16	0.80
1:E:53(A):LEU:CD2	1:E:53(A):LEU:O	2.30	0.79
2:I:7:ALA:HB1	2:I:11:GLU:HA	1.65	0.78
2:D:145:ASP:O	2:D:148:CYS:HB3	1.84	0.78
1:E:317:ALA:H	2:F:104:ASN:ND2	1.82	0.78
1:J:34:ASN:HD22	3:J:401:NAG:C1	1.98	0.77
2:B:26:HIS:HD2	2:B:26:HIS:O	1.67	0.75
2:D:127:ARG:HH12	2:F:131:LYS:HE2	1.51	0.75
1:H:98:TYR:CD2	1:H:230:MET:HG3	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:LYS:O	1:C:220:ARG:NH2	2.20	0.75
2:F:4:GLY:O	2:F:8:GLY:HA3	1.85	0.75
1:J:25:VAL:HG21	1:J:317:ALA:HB2	1.69	0.75
2:M:26:HIS:ND1	2:M:153:ARG:NH2	2.34	0.74
2:F:28:ASN:ND2	2:F:146:ASN:OD1	2.21	0.74
1:A:295:HIS:HD2	1:A:297:ILE:H	1.35	0.74
2:I:18:VAL:O	2:I:18:VAL:HG12	1.87	0.74
1:H:25:VAL:HG21	1:H:317:ALA:HB2	1.68	0.74
1:J:275:GLY:O	1:J:276:ASN:HB2	1.87	0.74
1:H:283:THR:HG22	1:H:301:THR:HG22	1.68	0.73
1:E:34:ASN:CG	3:E:401:NAG:C1	2.57	0.73
1:C:311:SER:HB3	2:D:97:GLU:OE2	1.89	0.73
1:C:283:THR:HG22	1:C:285:ILE:H	1.52	0.73
2:F:126:LEU:N	2:F:126:LEU:CD1	2.52	0.72
1:J:33:LYS:CB	3:J:401:NAG:H82	2.20	0.72
2:M:142:HIS:CE1	2:M:162:TYR:CD1	2.78	0.72
1:E:11:ASP:O	2:F:140:PHE:HB2	1.90	0.72
1:L:159:ASN:O	1:L:196:GLN:NE2	2.21	0.72
1:E:295:HIS:HD2	1:E:297:ILE:H	1.37	0.72
1:E:317:ALA:H	2:F:104:ASN:HD21	1.36	0.72
2:D:80:LEU:C	2:D:80:LEU:HD12	2.11	0.71
2:B:147:GLU:O	2:B:151:SER:HB3	1.90	0.71
1:H:307:LYS:HE2	2:I:60:ASN:HA	1.72	0.71
1:C:51:LEU:O	1:C:275:GLY:N	2.22	0.71
1:C:191:GLN:NE2	1:C:197:ASN:O	2.23	0.71
2:D:9:PHE:CE1	2:D:10:ILE:CG1	2.74	0.70
2:M:128:ASP:OD1	2:M:128:ASP:C	2.29	0.70
1:H:295:HIS:CD2	1:H:297:ILE:H	2.09	0.70
1:C:18:HIS:HD2	2:D:17:MET:O	1.74	0.70
2:B:150:GLU:O	2:B:154:ASN:ND2	2.24	0.70
1:C:96:ASP:OD2	1:C:96(A):LEU:HD13	1.91	0.70
1:E:34:ASN:ND2	3:E:401:NAG:C2	2.42	0.70
2:M:159:TYR:HB3	2:M:160:PRO:CD	2.21	0.70
1:H:294:PHE:HZ	2:I:59:MET:HG3	1.57	0.70
2:M:159:TYR:C	2:M:161:GLN:H	1.96	0.70
2:B:150:GLU:OE2	2:B:153:ARG:CZ	2.41	0.69
2:M:26:HIS:O	2:M:26:HIS:HD2	1.75	0.69
1:C:169:ASN:OD1	1:C:169:ASN:C	2.30	0.69
2:F:146:ASN:O	2:F:150:GLU:HG2	1.93	0.68
2:M:151:SER:OG	2:M:157:TYR:HB2	1.93	0.68
2:I:26:HIS:HD2	2:I:153:ARG:HH12	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:28:ASN:O	2:I:31:GLY:N	2.25	0.68
1:J:294:PHE:HZ	2:K:59:MET:HG3	1.59	0.68
2:F:125:GLN:C	2:F:126:LEU:HD12	2.13	0.68
2:I:151:SER:HA	2:I:154:ASN:HB2	1.77	0.67
1:H:137:SER:O	1:H:140:PRO:HD3	1.94	0.67
1:H:70:LEU:O	1:H:150:ASN:ND2	2.28	0.67
1:A:18:HIS:HE1	1:A:19(A):ASN:HB3	1.60	0.67
1:L:203:SER:HB3	1:L:212:ARG:HD2	1.76	0.67
1:L:49:GLY:HA2	1:L:286:GLY:HA2	1.77	0.67
2:D:9:PHE:CD1	2:D:10:ILE:HG13	2.29	0.67
2:M:159:TYR:HB3	2:M:160:PRO:HD3	1.76	0.67
2:M:157:TYR:CD2	2:M:158:ASP:N	2.63	0.67
1:L:283:THR:HG22	1:L:285:ILE:H	1.60	0.67
1:H:77:ASP:OD1	1:H:149:ARG:HD2	1.94	0.66
1:C:275:GLY:O	1:C:276:ASN:CB	2.42	0.66
1:A:37:THR:HG22	1:A:319:GLY:HA3	1.75	0.66
1:H:125:PRO:HB2	1:H:126:SER:OG	1.95	0.66
1:H:100:GLY:HA3	1:H:230:MET:O	1.94	0.66
1:J:50:LYS:HD3	1:J:275:GLY:HA3	1.77	0.66
2:B:9:PHE:O	2:B:9:PHE:HD1	1.79	0.66
1:A:311:SER:HB3	2:B:97:GLU:OE2	1.96	0.66
2:K:27:SER:HB2	2:K:32:SER:OG	1.95	0.66
1:J:106:GLU:N	1:J:106:GLU:OE1	2.29	0.66
1:C:15:ILE:HD11	2:D:122:VAL:HG21	1.77	0.66
1:E:62:ARG:NH1	1:E:78:GLU:OE1	2.25	0.65
1:A:137:SER:O	1:A:140:PRO:HD3	1.97	0.65
1:A:316:LEU:HD13	2:B:100:VAL:HG22	1.78	0.65
2:B:106:ARG:NH2	2:D:106:ARG:HD2	2.12	0.65
2:B:30:GLN:N	2:B:30:GLN:OE1	2.30	0.65
1:J:15:ILE:HD11	2:K:122:VAL:HG21	1.79	0.65
1:J:186:ASN:N	1:J:186:ASN:OD1	2.28	0.64
1:C:27:THR:HG23	2:D:105:GLU:HB2	1.78	0.64
2:I:28:ASN:O	2:I:31:GLY:HA2	1.96	0.64
2:I:26:HIS:O	2:I:26:HIS:ND1	2.30	0.64
2:B:150:GLU:OE2	2:B:153:ARG:NE	2.29	0.64
2:D:80:LEU:HD12	2:D:80:LEU:O	1.97	0.64
1:H:197:ASN:OD1	1:H:197:ASN:N	2.27	0.64
1:H:17:TYR:CZ	2:I:6:ILE:HG23	2.33	0.64
1:C:316:LEU:HD13	2:D:100:VAL:HG22	1.80	0.64
1:L:206:THR:OG1	1:L:209:LEU:HB3	1.98	0.63
1:A:15:ILE:HD12	2:B:119:TYR:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:42:GLN:HA	2:M:42:GLN:HE21	1.63	0.63
2:B:24:TYR:CE2	2:B:153:ARG:HG2	2.34	0.63
1:L:294:PHE:HZ	2:M:59:MET:HG3	1.64	0.63
2:M:77:ILE:HD12	2:M:77:ILE:H	1.63	0.63
2:K:22:TYR:OH	2:K:111:HIS:ND1	2.28	0.63
1:L:177:LEU:HB3	1:L:258:TYR:HB2	1.81	0.63
1:A:17:TYR:CE2	2:B:6:ILE:HG23	2.33	0.63
2:I:18:VAL:O	2:I:18:VAL:CG1	2.46	0.63
1:L:156:LYS:HD2	1:L:159:ASN:HA	1.81	0.62
1:H:242:ALA:N	4:H:402:NAG:H82	2.14	0.62
1:J:179:LEU:HD23	1:J:234:TRP:HB3	1.81	0.62
2:I:106:ARG:HH21	2:K:106:ARG:HH11	1.46	0.62
1:H:220:ARG:NH1	1:H:227:SER:O	2.30	0.62
1:E:24:GLN:NE2	1:E:34:ASN:HB3	2.14	0.62
2:B:9:PHE:CD1	2:B:9:PHE:C	2.73	0.62
2:D:68:ARG:HE	2:F:79:ASN:ND2	1.97	0.61
1:C:200:THR:HG21	1:C:250:ASN:OD1	2.00	0.61
1:A:75:MET:CB	1:A:95:ASN:ND2	2.62	0.61
2:I:7:ALA:CB	2:I:11:GLU:O	2.46	0.61
1:A:37:THR:HG23	1:A:38:HIS:ND1	2.15	0.61
1:J:33:LYS:HG3	3:J:401:NAG:H82	1.82	0.61
2:D:55:ILE:HG12	2:D:99:LEU:HD11	1.82	0.61
1:L:124:ILE:HB	1:L:254:PRO:O	2.00	0.61
1:L:131:GLU:OE2	1:L:131:GLU:HA	2.00	0.61
2:K:119:TYR:HE1	2:K:136:GLY:HA2	1.66	0.61
2:B:68:ARG:HH11	2:D:79:ASN:ND2	1.98	0.61
2:K:119:TYR:CE1	2:K:136:GLY:HA2	2.36	0.60
1:A:142:GLN:NE2	1:A:142:GLN:CA	2.55	0.60
2:M:129:ASN:O	2:M:129:ASN:ND2	2.30	0.60
1:J:295:HIS:HD2	1:J:297:ILE:H	1.48	0.60
2:B:127:ARG:HH12	2:D:131:LYS:HG2	1.66	0.60
1:E:205:GLY:O	1:E:206:THR:HG22	2.02	0.60
2:F:128:ASP:OD1	2:F:129:ASN:N	2.35	0.60
2:B:26:HIS:O	2:B:32:SER:HA	2.02	0.60
1:J:216:LYS:O	1:J:220:ARG:NH2	2.35	0.60
2:D:28:ASN:OD1	2:D:28:ASN:C	2.39	0.60
1:A:294:PHE:HZ	2:B:59:MET:HG3	1.65	0.59
1:C:283:THR:HB	1:C:286:GLY:O	2.01	0.59
2:K:26:HIS:HD2	2:K:153:ARG:HH12	1.50	0.59
1:A:125:PRO:HG2	1:A:126:SER:HB3	1.84	0.59
2:I:22:TYR:OH	2:I:111:HIS:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:134:GLY:HA3	1:J:153:TRP:HB3	1.84	0.59
1:J:33:LYS:CG	3:J:401:NAG:H82	2.33	0.59
2:B:68:ARG:HD3	2:D:79:ASN:HD22	1.68	0.59
1:H:97:CYS:O	1:H:138:ALA:HB1	2.03	0.59
1:L:200:THR:HG23	1:L:215:PRO:HG2	1.84	0.59
1:C:37:THR:HG23	1:C:320:LEU:O	2.03	0.59
1:C:295:HIS:HD2	1:C:297:ILE:H	1.49	0.59
2:B:131:LYS:HG2	2:F:127:ARG:NH2	2.18	0.59
2:M:126:LEU:O	2:M:129:ASN:HB3	2.03	0.58
1:L:100:GLY:HA3	1:L:230:MET:O	2.03	0.58
2:F:158:ASP:HB3	2:F:161:GLN:HB2	1.85	0.58
1:L:311:SER:HB3	2:M:97:GLU:OE2	2.03	0.58
2:K:68:ARG:HH21	2:M:79:ASN:ND2	2.01	0.58
2:F:26:HIS:CD2	2:F:26:HIS:C	2.76	0.58
1:J:200:THR:HG21	1:J:250:ASN:OD1	2.02	0.58
1:L:295:HIS:HD2	1:L:297:ILE:H	1.50	0.58
1:H:52:CYS:HB2	1:H:279:THR:HG22	1.84	0.58
2:K:27:SER:HB3	2:K:32:SER:OG	2.02	0.58
1:H:123:ILE:C	1:H:124:ILE:HD12	2.24	0.58
2:I:79:ASN:HD22	2:M:68:ARG:HE	1.52	0.58
1:E:295:HIS:CD2	1:E:297:ILE:H	2.18	0.57
1:J:138:ALA:C	1:J:140:PRO:HD3	2.24	0.57
1:L:49:GLY:HA2	1:L:286:GLY:CA	2.33	0.57
1:C:27:THR:HG22	1:C:31:MET:N	2.13	0.57
1:H:23:GLU:HG2	1:H:39:ALA:HB3	1.86	0.57
1:L:314:LEU:HD22	2:M:100:VAL:HG21	1.85	0.57
1:A:201:TYR:OH	1:A:246:GLU:OE1	2.23	0.57
2:D:17:MET:HE1	2:D:23:GLY:HA3	1.87	0.57
1:A:17:TYR:OH	2:B:6:ILE:HG23	2.04	0.56
1:J:311:SER:HB3	2:K:97:GLU:OE2	2.03	0.56
1:A:142:GLN:HE21	1:A:142:GLN:CA	2.06	0.56
2:M:21:TRP:HB2	2:M:41:THR:HG23	1.87	0.56
2:F:6:ILE:HD12	2:F:112:ASP:HA	1.86	0.56
1:E:42:ILE:HD13	1:E:316:LEU:HD22	1.85	0.56
2:D:41:THR:HG22	2:D:45:ILE:HD11	1.87	0.56
1:E:37:THR:HG22	1:E:322:ASN:HB3	1.87	0.56
2:D:6:ILE:HG13	2:D:112:ASP:HA	1.88	0.56
1:A:131:GLU:OE2	1:A:157:LYS:HE3	2.05	0.56
1:J:77:ASP:O	1:J:80:ILE:HG12	2.05	0.56
1:E:265:SER:OG	1:E:266:ALA:N	2.35	0.56
2:M:129:ASN:HD22	2:M:129:ASN:C	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:HIS:C	2:B:26:HIS:CD2	2.79	0.56
1:E:25:VAL:HG21	1:E:317:ALA:HB2	1.88	0.56
2:B:68:ARG:HH11	2:D:79:ASN:HD21	1.53	0.56
2:I:28:ASN:O	2:I:31:GLY:CA	2.53	0.56
2:D:150:GLU:OE1	2:D:154:ASN:ND2	2.39	0.56
1:L:183:HIS:ND1	1:L:195:TYR:OH	2.31	0.56
1:A:53(A):LEU:HD22	1:A:302:ILE:HD11	1.87	0.56
2:D:29:GLU:O	2:D:30:GLN:C	2.42	0.56
2:K:125:GLN:HE22	2:K:155:GLY:C	2.09	0.55
1:C:299:PRO:HB3	2:D:89:LEU:HD11	1.88	0.55
1:H:25:VAL:HG12	1:H:315:VAL:HG22	1.88	0.55
1:L:317:ALA:H	2:M:104:ASN:HD21	1.53	0.55
1:A:49:GLY:C	1:A:50:LYS:HD3	2.25	0.55
1:J:100:GLY:HA3	1:J:230:MET:O	2.06	0.55
1:A:185:SER:OG	1:A:191:GLN:OE1	2.22	0.55
1:H:169:ASN:OD1	1:H:169:ASN:C	2.44	0.55
1:L:179:LEU:HD23	1:L:234:TRP:HB3	1.88	0.55
1:L:134:GLY:HA3	1:L:153:TRP:HB3	1.87	0.55
1:H:45:LYS:HA	1:H:296:ASN:HD21	1.72	0.55
1:A:98:TYR:OH	1:A:228:GLY:HA3	2.07	0.55
1:E:307:LYS:HE3	2:F:62:GLN:HG2	1.88	0.55
2:I:7:ALA:HB1	2:I:11:GLU:CA	2.35	0.55
2:F:24:TYR:CD2	2:F:153:ARG:HD3	2.42	0.55
1:L:124:ILE:HD12	1:L:254:PRO:HG2	1.88	0.55
1:L:317:ALA:H	2:M:104:ASN:ND2	2.05	0.55
1:H:62:ARG:NH2	1:H:78:GLU:OE2	2.38	0.54
2:I:81:ASN:HB2	2:K:80:LEU:HD22	1.90	0.54
1:C:184:HIS:HB2	1:C:229:ARG:HB2	1.88	0.54
1:E:77:ASP:OD2	1:E:149:ARG:HD2	2.08	0.54
2:I:59:MET:O	2:I:62:GLN:HB2	2.08	0.54
1:J:27:THR:HG22	1:J:32:GLU:H	1.73	0.54
1:C:67:ALA:O	1:C:71:LEU:HB2	2.07	0.54
1:H:220:ARG:HH12	1:H:228:GLY:HA2	1.73	0.54
3:J:402:NAG:C8	1:L:221:SER:HB3	2.38	0.54
2:B:145:ASP:O	2:B:148:CYS:HB3	2.08	0.54
1:J:316:LEU:HD23	2:K:52:VAL:HG22	1.89	0.53
1:J:44:GLU:OE1	1:J:46:THR:HG22	2.08	0.53
2:B:150:GLU:OE2	2:B:153:ARG:NH2	2.39	0.53
1:C:73:ASN:ND2	1:C:97:CYS:HB3	2.23	0.53
2:B:72:ASN:OD1	2:B:75:ARG:NH1	2.42	0.53
1:J:61:LEU:HA	1:J:79:PHE:CZ	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:28:ASN:OD1	2:F:31:GLY:O	2.26	0.53
1:E:37:THR:OG1	1:E:38:HIS:HD2	1.91	0.53
1:E:77:ASP:OD1	1:E:149:ARG:NH1	2.41	0.53
1:A:33:LYS:HG2	3:A:401:NAG:H82	1.90	0.53
1:L:156:LYS:HE2	1:L:193:LYS:O	2.08	0.53
1:L:294:PHE:CZ	2:M:59:MET:HG3	2.43	0.53
2:D:133:LEU:HD12	2:D:137:CYS:CB	2.38	0.53
1:E:216:LYS:O	1:E:220:ARG:NH2	2.42	0.53
2:M:21:TRP:CZ3	2:M:45:ILE:HG13	2.43	0.53
2:I:7:ALA:HB1	2:I:11:GLU:C	2.27	0.53
2:F:58:LYS:HE3	2:F:58:LYS:HA	1.90	0.53
1:H:14:CYS:O	2:I:24:TYR:HA	2.09	0.53
1:J:101:ASN:HB2	1:J:231:ASP:OD1	2.09	0.53
1:H:161:TYR:CD1	1:H:195:TYR:HB3	2.44	0.53
1:E:13:ILE:HG22	2:F:138:PHE:HB2	1.91	0.53
1:J:295:HIS:CD2	1:J:297:ILE:H	2.27	0.52
1:E:174:GLU:N	1:E:174:GLU:OE1	2.41	0.52
2:K:75:ARG:NH2	2:K:78:GLU:OE1	2.37	0.52
1:A:134:GLY:HA3	1:A:153:TRP:HB3	1.89	0.52
1:L:121:ILE:HD11	1:L:176:LEU:HD11	1.92	0.52
2:M:159:TYR:C	2:M:161:GLN:N	2.62	0.52
1:A:98:TYR:CD2	1:A:230:MET:HG3	2.43	0.52
2:F:150:GLU:O	2:F:154:ASN:HB2	2.09	0.52
2:D:133:LEU:HD12	2:D:137:CYS:HB3	1.90	0.52
2:I:19:ASP:HB3	2:I:36:ALA:HB2	1.90	0.52
1:H:47:HIS:ND1	1:H:48:ASN:O	2.43	0.52
1:C:26:ASP:HB3	1:C:33:LYS:HD3	1.90	0.52
1:A:75:MET:HB2	1:A:95:ASN:HD22	1.73	0.52
2:F:22:TYR:OH	2:F:111:HIS:HD2	1.93	0.52
1:A:45:LYS:HG2	1:A:296:ASN:HD22	1.75	0.52
1:E:100:GLY:HA3	1:E:230:MET:O	2.10	0.52
2:B:62:GLN:HG2	2:B:63:PHE:H	1.75	0.52
2:B:103:GLU:O	2:B:107:THR:OG1	2.25	0.52
1:L:27:THR:HB	2:M:105:GLU:HB2	1.92	0.52
1:L:309:VAL:HG13	2:M:93:THR:HA	1.91	0.52
2:I:135:ASN:OD1	2:I:137:CYS:HB2	2.09	0.52
1:A:33:LYS:CB	3:A:401:NAG:H82	2.40	0.51
1:H:37:THR:HB	1:H:319:GLY:HA3	1.92	0.51
2:M:150:GLU:OE2	2:M:153:ARG:NH1	2.42	0.51
2:B:131:LYS:HE3	2:F:127:ARG:HH22	1.75	0.51
1:L:60:ILE:HD13	1:L:274:TYR:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:44:GLU:OE2	1:H:46:THR:HG22	2.09	0.51
2:K:68:ARG:HE	2:M:79:ASN:HD22	1.58	0.51
2:K:27:SER:CA	2:K:32:SER:OG	2.59	0.51
1:E:98:TYR:CD2	1:E:230:MET:HG3	2.46	0.51
2:I:154:ASN:HB3	2:I:156:THR:HG23	1.91	0.51
2:K:132:GLU:HG2	2:K:132:GLU:O	2.09	0.51
1:L:205:GLY:O	1:L:206:THR:HG23	2.10	0.51
2:M:30:GLN:HE22	2:M:146:ASN:ND2	2.09	0.51
2:M:159:TYR:N	2:M:160:PRO:HD2	2.26	0.51
2:B:106:ARG:HH21	2:D:106:ARG:HD2	1.76	0.51
2:K:58:LYS:HE3	2:M:97:GLU:HB3	1.93	0.51
1:E:220:ARG:O	1:E:227:SER:HB2	2.11	0.51
1:H:124:ILE:HG22	1:H:124:ILE:O	2.11	0.51
2:M:84:MET:HG3	2:M:85:GLU:N	2.25	0.51
1:J:38:HIS:HB2	1:J:318:THR:HG23	1.92	0.51
2:I:9:PHE:O	2:I:135:ASN:HA	2.11	0.50
1:C:23:GLU:HG2	1:C:39:ALA:HB3	1.92	0.50
2:I:129:ASN:HD21	2:I:163:SER:HA	1.76	0.50
1:H:158:ASN:O	1:H:160:THR:HG23	2.11	0.50
2:D:151:SER:OG	2:D:157:TYR:HA	2.11	0.50
1:L:130:HIS:CE1	1:L:162:PRO:HD2	2.46	0.50
2:I:158:ASP:HB3	2:I:161:GLN:HB3	1.93	0.50
1:J:283:THR:HG22	1:J:285:ILE:H	1.76	0.50
1:L:34:ASN:ND2	3:L:402:NAG:O7	2.45	0.50
1:A:14:CYS:HA	2:B:137:CYS:HA	1.93	0.50
1:E:48:ASN:OD1	1:E:48:ASN:O	2.29	0.50
2:F:151:SER:HA	2:F:154:ASN:HB2	1.93	0.50
2:K:55:ILE:O	2:K:59:MET:HG2	2.12	0.50
2:F:128:ASP:C	2:F:128:ASP:OD1	2.50	0.50
1:E:174:GLU:OE2	1:E:259:LYS:HE2	2.11	0.50
2:I:9:PHE:CD1	2:I:10:ILE:HG13	2.45	0.50
2:D:119:TYR:OH	2:D:132:GLU:OE2	2.25	0.50
2:K:125:GLN:HG2	2:K:157:TYR:HB3	1.94	0.50
2:B:144:CYS:SG	2:B:149:MET:HG3	2.52	0.50
1:E:101:ASN:HB2	1:E:231:ASP:OD1	2.12	0.49
1:E:53(A):LEU:HD23	1:E:53(A):LEU:C	2.25	0.49
1:E:279:THR:OG1	1:E:280:LYS:N	2.44	0.49
1:C:25:VAL:HG11	1:C:317:ALA:HB2	1.94	0.49
1:L:307:LYS:HB3	2:M:62:GLN:NE2	2.27	0.49
2:I:150:GLU:O	2:I:154:ASN:HB2	2.12	0.49
2:F:62:GLN:HB2	2:F:92:TRP:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:119:GLU:OE1	1:H:259:LYS:NZ	2.34	0.49
2:M:30:GLN:NE2	2:M:146:ASN:ND2	2.60	0.49
1:H:126:SER:HB3	1:H:166:ARG:NH2	2.27	0.49
2:B:9:PHE:CD1	2:B:9:PHE:O	2.64	0.49
1:A:48:ASN:OD1	1:A:48:ASN:O	2.30	0.49
1:C:220:ARG:O	1:C:227:SER:HB2	2.13	0.49
1:L:317:ALA:N	2:M:104:ASN:HD21	2.11	0.49
1:H:294:PHE:CZ	2:I:59:MET:HG3	2.43	0.49
1:E:294:PHE:HZ	2:F:59:MET:HG3	1.78	0.49
2:I:150:GLU:HA	2:I:153:ARG:HE	1.78	0.49
1:L:131:GLU:OE1	1:L:133(A):SER:OG	2.30	0.49
1:H:121:ILE:HG21	1:H:259:LYS:HD3	1.94	0.49
1:J:107:GLU:OE2	2:M:75:ARG:HB2	2.12	0.49
2:D:154:ASN:HB3	2:D:156:THR:HG23	1.95	0.49
2:M:25:HIS:HB2	2:M:34:TYR:CD1	2.48	0.49
1:J:105:TYR:CE2	1:J:109:LYS:HE3	2.48	0.48
2:D:52:VAL:O	2:D:56:ILE:HG12	2.13	0.48
2:K:148:CYS:O	2:K:151:SER:HB3	2.12	0.48
1:E:128:SER:HB2	1:E:129:ASP:OD2	2.12	0.48
1:C:207:SER:HA	1:E:229:ARG:NH2	2.27	0.48
1:C:44:GLU:HG3	1:C:290:SER:CB	2.43	0.48
2:F:158:ASP:OD2	2:F:161:GLN:OE1	2.30	0.48
2:B:103:GLU:OE1	1:C:28:ILE:HD12	2.12	0.48
2:D:145:ASP:O	2:D:148:CYS:CB	2.55	0.48
2:B:51:LYS:NZ	2:B:107:THR:OG1	2.47	0.48
1:A:156:LYS:HD2	1:A:196:GLN:HB2	1.95	0.48
1:C:222:LYS:HD3	1:C:225:GLY:O	2.12	0.48
1:J:128:SER:O	1:J:157:LYS:HE3	2.14	0.48
2:F:5:ALA:HB2	2:F:116:LYS:HB2	1.94	0.48
2:I:62:GLN:HG3	2:I:92:TRP:CD2	2.47	0.48
1:J:117:HIS:O	1:J:261:VAL:HG12	2.14	0.48
1:A:265:SER:OG	1:A:266:ALA:N	2.46	0.48
2:I:145:ASP:N	2:I:145:ASP:OD2	2.40	0.48
1:A:221:SER:HB3	4:E:402:NAG:H81	1.94	0.48
1:C:134:GLY:HA2	1:C:153:TRP:HB3	1.96	0.48
1:L:77:ASP:O	1:L:80:ILE:HG12	2.13	0.48
2:B:24:TYR:CZ	2:B:153:ARG:HG2	2.48	0.48
1:H:125:PRO:O	1:H:126:SER:HB2	2.13	0.48
1:L:60:ILE:CD1	1:L:274:TYR:HB2	2.44	0.48
2:D:127:ARG:HH12	2:F:131:LYS:CE	2.24	0.48
1:C:42:ILE:O	1:C:293:PRO:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLU:OE2	1:A:46:THR:HB	2.13	0.47
1:E:239:PRO:O	1:E:240:ASN:CB	2.62	0.47
2:F:51:LYS:HE3	2:F:103:GLU:HB3	1.97	0.47
1:H:124:ILE:HD12	1:H:124:ILE:N	2.29	0.47
1:E:186:ASN:ND2	1:E:227:SER:OG	2.47	0.47
1:A:31:MET:HB3	1:A:31:MET:HE3	1.65	0.47
2:F:68:ARG:NH1	2:F:81:ASN:OD1	2.44	0.47
1:L:197:ASN:N	1:L:197:ASN:HD22	2.11	0.47
1:C:107:GLU:OE2	2:F:75:ARG:HB2	2.14	0.47
2:F:24:TYR:CE2	2:F:153:ARG:HD3	2.49	0.47
1:E:129:ASP:OD2	1:E:129:ASP:N	2.47	0.47
1:C:139:CYS:HB2	1:C:146:SER:O	2.14	0.47
1:A:220:ARG:NH1	1:A:227:SER:O	2.46	0.47
2:B:6:ILE:HA	2:B:7:ALA:HA	1.68	0.47
1:C:314:LEU:HD22	2:D:100:VAL:HG21	1.96	0.47
2:D:45:ILE:HG13	2:D:45:ILE:H	1.49	0.47
2:K:151:SER:OG	2:K:157:TYR:HA	2.14	0.47
1:J:283:THR:HB	1:J:286:GLY:O	2.14	0.47
1:H:32:GLU:OE1	1:H:321:ARG:NH2	2.37	0.47
1:C:130:HIS:NE2	1:C:162:PRO:HD2	2.30	0.47
1:J:89:GLU:OE1	1:J:269:LYS:NZ	2.47	0.47
2:M:161:GLN:C	2:M:161:GLN:CD	2.72	0.47
2:I:126:LEU:O	2:I:129:ASN:HB2	2.15	0.47
1:E:239:PRO:O	1:E:240:ASN:HB2	2.14	0.47
2:K:62:GLN:HG3	2:K:92:TRP:CD2	2.50	0.47
1:E:200:THR:HA	1:E:248:ASN:OD1	2.14	0.47
1:L:220:ARG:O	1:L:227:SER:HB2	2.15	0.47
1:H:174:GLU:OE1	1:H:259:LYS:HE3	2.14	0.47
1:J:204:VAL:HG22	1:J:245:PHE:CD2	2.50	0.47
2:K:68:ARG:NH1	2:K:81:ASN:OD1	2.48	0.47
2:I:26:HIS:CD2	2:I:153:ARG:HH12	2.28	0.47
1:L:205:GLY:O	1:L:206:THR:CG2	2.63	0.47
1:L:127:TRP:HB2	1:L:132:ALA:HB2	1.97	0.47
2:K:150:GLU:O	2:K:154:ASN:HB2	2.15	0.47
2:F:51:LYS:HE2	2:F:107:THR:OG1	2.15	0.47
1:C:44:GLU:HG3	1:C:290:SER:HB2	1.96	0.47
2:M:142:HIS:ND1	2:M:162:TYR:CD1	2.83	0.46
1:C:38:HIS:CB	1:C:318:THR:HG23	2.46	0.46
1:H:21:SER:OG	1:H:22:THR:N	2.47	0.46
2:M:26:HIS:CD2	2:M:26:HIS:C	2.89	0.46
1:H:307:LYS:HD2	2:I:62:GLN:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:200:THR:HG21	1:L:250:ASN:OD1	2.15	0.46
1:C:133(A):SER:N	1:C:134:GLY:HA3	2.30	0.46
1:A:200:THR:O	1:A:214:VAL:HG13	2.16	0.46
1:E:156:LYS:HD2	1:E:196:GLN:HG2	1.97	0.46
1:C:117:HIS:HB3	1:C:261:VAL:HG23	1.97	0.46
1:C:62:ARG:NH1	1:C:78:GLU:OE1	2.49	0.46
1:L:124:ILE:O	1:L:255:GLU:HG3	2.15	0.46
2:D:41:THR:O	2:D:45:ILE:HG13	2.15	0.46
1:E:200:THR:O	1:E:214:VAL:HG13	2.15	0.46
1:J:55:GLY:N	1:J:278:ASN:OD1	2.45	0.46
2:I:6:ILE:HA	2:I:7:ALA:HA	1.67	0.46
1:L:283:THR:HG22	1:L:285:ILE:N	2.28	0.46
1:L:307:LYS:HA	1:L:307:LYS:HD3	1.64	0.46
1:L:97:CYS:HB2	1:L:139:CYS:CA	2.45	0.46
4:A:402:NAG:H61	4:A:403:NAG:HN2	1.79	0.46
1:J:33:LYS:HB2	3:J:401:NAG:C8	2.35	0.46
1:A:295:HIS:CD2	1:A:297:ILE:H	2.24	0.46
1:J:139:CYS:N	1:J:140:PRO:HD3	2.30	0.46
1:L:176:LEU:O	1:L:236:ILE:HA	2.15	0.46
2:B:146:ASN:O	2:B:150:GLU:HB2	2.16	0.46
2:M:9:PHE:CD1	2:M:10:ILE:HG13	2.50	0.46
1:E:22:THR:O	1:E:24:GLN:HG3	2.15	0.46
1:A:122:GLN:HB2	1:A:256:TYR:CE1	2.50	0.46
2:I:117:ASN:N	2:I:117:ASN:HD22	2.14	0.46
1:C:101:ASN:HB2	1:C:231:ASP:OD1	2.16	0.46
1:A:15:ILE:HD13	2:B:118:LEU:HD23	1.96	0.46
2:D:29:GLU:C	2:D:31:GLY:N	2.64	0.46
2:M:84:MET:HE3	2:M:85:GLU:HG3	1.98	0.46
1:H:97:CYS:HB2	1:H:138:ALA:O	2.16	0.45
1:H:52:CYS:HB3	1:H:277:CYS:O	2.16	0.45
1:C:295:HIS:CD2	1:C:297:ILE:H	2.32	0.45
1:L:275:GLY:O	1:L:276:ASN:HB2	2.16	0.45
1:H:50:LYS:HD3	1:H:275:GLY:HA3	1.97	0.45
1:J:202:ILE:HD11	1:J:251:PHE:HA	1.98	0.45
2:F:72:ASN:OD1	2:F:72:ASN:N	2.35	0.45
2:F:104:ASN:HD22	2:F:104:ASN:HA	1.57	0.45
2:K:24:TYR:CE2	2:K:153:ARG:HB3	2.52	0.45
1:H:96:ASP:CG	1:H:96(A):LEU:HD13	2.37	0.45
2:F:28:ASN:O	2:F:31:GLY:O	2.34	0.45
1:J:164:ILE:O	1:J:246:GLU:HA	2.16	0.45
1:L:15:ILE:HG23	2:M:118:LEU:HD23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:159:TYR:O	2:F:160:PRO:C	2.54	0.45
1:H:166:ARG:HH11	1:H:166:ARG:HG2	1.80	0.45
2:I:145:ASP:OD1	2:I:147:GLU:HB2	2.16	0.45
2:K:19:ASP:N	2:K:19:ASP:OD1	2.49	0.45
1:C:133:SER:O	1:C:133(A):SER:OG	2.30	0.45
1:J:91:ALA:HA	1:J:269:LYS:HE3	1.98	0.45
1:E:283:THR:HG22	1:E:285:ILE:H	1.82	0.45
1:H:182:ILE:HB	1:H:202:ILE:HD12	1.98	0.45
1:J:151:VAL:HG13	1:J:252:ILE:HG22	1.99	0.45
1:L:173:GLN:HE21	1:L:173:GLN:HB3	1.65	0.45
1:E:293:PRO:HG2	1:E:294:PHE:CD1	2.52	0.45
1:C:108:LEU:HB2	1:C:234:TRP:CE2	2.51	0.45
1:E:97:CYS:HB2	1:E:138:ALA:O	2.16	0.45
2:K:27:SER:HA	2:K:32:SER:OG	2.17	0.45
2:D:150:GLU:HA	2:D:153:ARG:HE	1.82	0.45
2:M:30:GLN:HE21	2:M:30:GLN:HB2	1.47	0.45
1:L:136:SER:OG	1:L:137:SER:N	2.50	0.45
2:M:15:GLN:HB2	2:M:15:GLN:HE21	1.62	0.45
1:L:265:SER:OG	1:L:266:ALA:N	2.50	0.45
1:H:301:THR:HB	1:H:305:CYS:SG	2.57	0.44
2:I:26:HIS:ND1	2:I:26:HIS:C	2.71	0.44
1:H:222:LYS:HB2	1:H:222:LYS:HE3	1.77	0.44
2:K:55:ILE:HG23	2:K:99:LEU:HD13	1.99	0.44
2:D:30:GLN:HG2	2:D:30:GLN:H	1.51	0.44
1:H:32:GLU:CD	1:H:321:ARG:HH22	2.19	0.44
1:C:301:THR:O	1:C:302:ILE:HD13	2.17	0.44
1:E:122:GLN:HG3	1:E:256:TYR:CE2	2.52	0.44
2:D:68:ARG:HH21	2:F:79:ASN:ND2	2.15	0.44
2:B:29:GLU:HB3	2:B:30:GLN:OE1	2.17	0.44
2:D:146:ASN:C	2:D:148:CYS:N	2.71	0.44
1:C:65:SER:OG	1:C:96:ASP:HA	2.17	0.44
1:A:247:SER:OG	1:A:251:PHE:HB2	2.16	0.44
1:C:304:GLU:H	1:C:304:GLU:HG2	1.61	0.44
1:L:42:ILE:O	1:L:293:PRO:HD2	2.17	0.44
2:I:37:ASP:O	2:I:41:THR:HB	2.17	0.44
2:B:131:LYS:HZ2	2:B:141:TYR:HE1	1.64	0.44
1:E:317:ALA:O	2:F:107:THR:HG21	2.18	0.44
2:D:106:ARG:HH22	2:F:106:ARG:HG3	1.82	0.44
1:L:295:HIS:HD2	1:L:297:ILE:N	2.14	0.44
1:E:38:HIS:HB2	1:E:318:THR:HG22	1.99	0.44
1:L:123:ILE:HG13	1:L:168:TYR:CG	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:129:ASN:ND2	2:M:142:HIS:NE2	2.49	0.44
2:D:80:LEU:CD1	2:D:80:LEU:C	2.83	0.44
1:A:293:PRO:HB2	1:A:294:PHE:CD2	2.53	0.44
1:H:47:HIS:CE1	1:H:285:ILE:HG22	2.53	0.44
1:J:42:ILE:O	1:J:293:PRO:HD2	2.17	0.44
2:D:145:ASP:O	2:D:148:CYS:N	2.45	0.43
1:E:240:ASN:HD21	4:E:403:NAG:H61	1.83	0.43
1:E:237:LEU:HD12	1:E:241:ASP:HB3	2.00	0.43
2:F:57:ASP:O	2:F:60:ASN:ND2	2.51	0.43
2:I:164:GLU:HG2	2:I:164:GLU:H	1.53	0.43
1:L:28:ILE:HA	1:L:28:ILE:HD13	1.86	0.43
2:F:149:MET:O	2:F:152:VAL:HG22	2.18	0.43
1:A:75:MET:CB	1:A:95:ASN:HD21	2.30	0.43
1:H:197:ASN:HA	1:H:198:PRO:HD3	1.72	0.43
1:C:38:HIS:HB3	1:C:318:THR:HG23	2.00	0.43
1:E:144:THR:HG23	1:E:145:PRO:HD2	2.00	0.43
1:A:15:ILE:HG23	2:B:118:LEU:HD23	1.99	0.43
1:L:23:GLU:OE2	1:L:39:ALA:HB3	2.19	0.43
2:B:11:GLU:CG	2:B:12:GLY:N	2.81	0.43
1:E:197:ASN:ND2	1:E:197:ASN:N	2.66	0.43
1:E:19(A):ASN:OD1	1:E:21:SER:HB2	2.19	0.43
1:L:295:HIS:CD2	1:L:297:ILE:HB	2.53	0.43
1:E:17:TYR:CZ	2:F:6:ILE:HG23	2.53	0.43
1:L:178:ILE:O	1:L:234:TRP:HA	2.19	0.43
1:L:197:ASN:ND2	1:L:197:ASN:N	2.64	0.43
1:C:147:PHE:O	1:C:148:PHE:C	2.55	0.43
1:L:164:ILE:O	1:L:246:GLU:HA	2.19	0.43
2:K:94:TYR:HD2	2:K:95:ASN:HD22	1.66	0.43
1:L:183:HIS:HB2	1:L:252:ILE:HD11	2.00	0.43
2:B:144:CYS:SG	2:B:149:MET:CG	3.07	0.43
1:H:239:PRO:O	1:H:240:ASN:HB2	2.18	0.43
2:D:42:GLN:HA	2:D:45:ILE:HD12	2.00	0.43
1:E:308:TYR:O	2:F:62:GLN:NE2	2.49	0.43
2:D:159:TYR:HB3	2:D:160:PRO:HD3	2.01	0.43
1:L:25:VAL:HG12	1:L:315:VAL:HG22	2.00	0.43
3:L:401:NAG:C2	3:L:403:NAG:O4	2.57	0.43
2:D:48:VAL:O	2:D:52:VAL:HG23	2.19	0.43
1:A:80:ILE:HA	1:A:80:ILE:HD13	1.90	0.43
1:C:293:PRO:CG	2:D:56:ILE:HD12	2.49	0.42
1:H:220:ARG:NH1	1:H:228:GLY:HA2	2.33	0.42
1:C:17:TYR:CZ	2:D:6:ILE:HG23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:27:THR:HG22	1:J:31:MET:H	1.82	0.42
2:B:128:ASP:OD1	2:B:159:TYR:OH	2.23	0.42
2:K:95:ASN:O	2:K:99:LEU:HB2	2.19	0.42
1:E:11:ASP:OD2	2:F:144:CYS:N	2.41	0.42
2:K:94:TYR:HD2	2:K:95:ASN:ND2	2.17	0.42
1:A:19(A):ASN:OD1	1:A:21:SER:HB2	2.19	0.42
1:L:209:LEU:HD22	1:L:235:THR:HG21	2.01	0.42
1:E:121:ILE:HG21	1:E:259:LYS:HD2	2.01	0.42
2:I:9:PHE:CE1	2:I:10:ILE:HG13	2.55	0.42
1:A:13:ILE:HB	2:B:149:MET:HE1	2.01	0.42
2:I:71:ASN:OD1	2:I:74:GLU:HG3	2.19	0.42
2:F:108:LEU:O	2:F:111:HIS:N	2.47	0.42
1:L:60:ILE:HG22	1:L:62:ARG:HG3	2.00	0.42
2:M:16:GLY:HA3	2:M:34:TYR:CE2	2.55	0.42
1:E:58:PRO:HB3	1:E:86:TYR:CZ	2.54	0.42
2:B:5:ALA:HB2	2:B:116:LYS:HB2	2.02	0.42
1:L:268:ILE:HD12	1:L:284:PRO:HA	2.01	0.42
1:A:10:GLY:N	2:B:139:GLU:OE2	2.52	0.42
2:D:146:ASN:O	2:D:149:MET:N	2.52	0.42
2:K:119:TYR:OH	2:K:132:GLU:OE1	2.29	0.42
1:H:296:ASN:HD22	1:H:296:ASN:C	2.23	0.42
1:A:31:MET:HE1	2:F:110:PHE:CZ	2.55	0.42
1:A:100:GLY:HA3	1:A:230:MET:O	2.19	0.42
1:E:283:THR:CG2	1:E:285:ILE:HG12	2.49	0.42
1:E:237:LEU:CD1	1:E:241:ASP:HB3	2.49	0.42
1:C:11:ASP:OD2	2:D:143:LYS:HD2	2.20	0.42
1:E:205:GLY:C	1:E:206:THR:CG2	2.88	0.42
2:M:129:ASN:HD21	2:M:142:HIS:CD2	2.35	0.42
2:M:129:ASN:OD1	2:M:157:TYR:OH	2.37	0.42
1:H:124:ILE:HG21	1:H:127:TRP:CZ2	2.55	0.42
2:D:3:PHE:HB2	2:D:112:ASP:OD2	2.19	0.42
2:B:79:ASN:HD22	2:F:68:ARG:HE	1.67	0.42
1:C:298:HIS:O	1:C:308:TYR:CD1	2.73	0.42
1:A:78:GLU:O	1:A:78:GLU:HG2	2.20	0.42
1:C:197:ASN:HA	1:C:198:PRO:HD3	1.74	0.42
1:C:307:LYS:HB3	2:D:62:GLN:OE1	2.19	0.42
2:M:4:GLY:O	2:M:8:GLY:HA3	2.20	0.42
1:L:50:LYS:HB3	1:L:50:LYS:HE2	1.73	0.42
1:L:131:GLU:OE2	1:L:131:GLU:CA	2.64	0.41
1:E:77:ASP:CG	1:E:149:ARG:HD2	2.39	0.41
1:A:25:VAL:HG12	1:A:315:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:164:ILE:O	1:H:246:GLU:HA	2.20	0.41
2:B:53:ASN:N	2:B:53:ASN:HD22	2.17	0.41
2:K:29:GLU:HB2	2:K:143:LYS:NZ	2.34	0.41
2:I:102:MET:O	2:I:106:ARG:HG3	2.20	0.41
1:L:97:CYS:HB2	1:L:139:CYS:HA	2.01	0.41
2:K:85:GLU:O	2:K:89:LEU:HG	2.20	0.41
1:H:38:HIS:C	1:H:318:THR:HG22	2.40	0.41
1:A:77:ASP:OD1	1:A:149:ARG:HD2	2.20	0.41
1:L:128:SER:OG	1:L:129:ASP:N	2.53	0.41
1:H:125(A):LYS:HG2	1:H:132:ALA:HB1	2.01	0.41
2:D:150:GLU:CA	2:D:153:ARG:HH21	2.33	0.41
1:C:290:SER:OG	1:C:291:SER:N	2.54	0.41
2:K:107:THR:O	2:K:110:PHE:HB3	2.21	0.41
1:H:268:ILE:HD12	1:H:284:PRO:HG3	2.01	0.41
1:L:83:GLU:OE2	1:L:262:LYS:NZ	2.41	0.41
1:H:134:GLY:C	1:H:135:VAL:HG13	2.41	0.41
1:C:184:HIS:HB3	1:C:220:ARG:NH2	2.36	0.41
1:J:37:THR:HG23	1:J:320:LEU:O	2.20	0.41
2:D:135:ASN:HA	2:D:135:ASN:HD22	1.62	0.41
2:B:51:LYS:HA	1:C:28:ILE:O	2.21	0.41
2:M:9:PHE:CE1	2:M:10:ILE:HG13	2.56	0.41
1:E:282:GLN:HG3	1:E:283:THR:N	2.35	0.41
2:M:102:MET:O	2:M:106:ARG:HG3	2.20	0.41
2:F:85:GLU:O	2:F:89:LEU:HD22	2.20	0.41
1:L:38:HIS:C	1:L:318:THR:HG22	2.41	0.41
1:A:180:TRP:CE2	1:A:204:VAL:HG21	2.55	0.41
1:A:38:HIS:HB2	1:A:318:THR:HG22	2.02	0.41
1:C:73:ASN:HA	1:C:74:PRO:HD3	1.98	0.41
1:E:240:ASN:HD21	4:E:403:NAG:C6	2.34	0.41
1:H:268:ILE:HA	1:H:268:ILE:HD13	1.92	0.41
1:A:121:ILE:HG13	1:A:121:ILE:O	2.20	0.41
1:C:307:LYS:HD3	1:C:307:LYS:HA	1.64	0.41
1:A:176:LEU:HD12	1:A:259:LYS:HA	2.03	0.41
1:J:131:GLU:HG2	1:J:133(A):SER:HB2	2.02	0.41
1:C:47:HIS:CE1	1:C:285:ILE:HG13	2.56	0.41
1:E:98:TYR:HA	1:E:99:PRO:HD3	1.89	0.41
1:E:283:THR:CG2	1:E:285:ILE:H	2.33	0.41
2:M:87:GLY:O	2:M:91:VAL:HG23	2.21	0.41
1:E:142:GLN:NE2	1:E:142:GLN:HA	2.36	0.41
1:E:34:ASN:OD1	3:E:401:NAG:C1	2.69	0.41
1:J:14:CYS:O	2:K:24:TYR:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:GLN:HE21	1:A:125:PRO:HA	1.86	0.41
1:E:42:ILE:O	1:E:293:PRO:HD2	2.19	0.41
1:E:293:PRO:HG2	1:E:294:PHE:HD1	1.85	0.41
1:C:73:ASN:HB3	1:C:76:CYS:SG	2.60	0.41
1:E:200:THR:HG23	1:E:215:PRO:HD2	2.02	0.41
1:L:101:ASN:HB2	1:L:231:ASP:OD1	2.21	0.41
1:H:234:TRP:HZ3	1:H:236:ILE:HD13	1.86	0.41
1:J:73:ASN:HB3	1:J:76:CYS:SG	2.61	0.41
2:D:38:LYS:HG2	2:D:39:GLU:H	1.86	0.41
2:K:37:ASP:O	2:K:41:THR:HB	2.20	0.41
1:L:33:LYS:CB	3:L:402:NAG:H81	2.50	0.41
1:E:53:ASP:OD1	1:E:274:TYR:OH	2.23	0.41
1:C:42:ILE:HG12	1:C:314:LEU:O	2.21	0.40
2:I:101:LEU:HD12	2:I:101:LEU:HA	1.90	0.40
2:D:168:LEU:HA	2:D:168:LEU:HD13	1.71	0.40
1:C:43:LEU:HB2	1:C:314:LEU:HB2	2.03	0.40
1:C:44:GLU:HG3	1:C:290:SER:OG	2.21	0.40
1:C:156:LYS:HB3	1:C:195:TYR:HA	2.03	0.40
2:D:17:MET:HE2	2:D:17:MET:HB2	1.86	0.40
1:E:77:ASP:OD1	1:E:149:ARG:HD2	2.21	0.40
2:K:62:GLN:HG2	2:K:63:PHE:N	2.36	0.40
2:M:14:TRP:CE3	2:M:17:MET:HE2	2.57	0.40
2:D:107:THR:O	2:D:110:PHE:HB3	2.21	0.40
1:A:53:ASP:OD1	1:A:274:TYR:OH	2.27	0.40
1:J:17:TYR:CZ	2:K:6:ILE:HG23	2.57	0.40
2:B:133:LEU:HA	2:B:133:LEU:HD23	1.73	0.40
1:A:269:LYS:HE3	1:A:269:LYS:HB3	1.92	0.40
1:C:209:LEU:HD22	1:C:235:THR:HG21	2.04	0.40
1:E:205:GLY:O	1:E:206:THR:CG2	2.69	0.40
1:J:105:TYR:HB3	1:J:106:GLU:OE1	2.21	0.40
1:E:184:HIS:HB3	1:E:220:ARG:NH2	2.36	0.40
2:M:54:SER:O	2:M:58:LYS:HB2	2.21	0.40
2:D:95:ASN:HD22	2:D:95:ASN:HA	1.57	0.40
1:C:186:ASN:HD21	1:C:227:SER:C	2.23	0.40
1:A:122:GLN:NE2	1:A:125:PRO:HA	2.36	0.40
4:A:402:NAG:H81	1:C:221:SER:HB3	2.03	0.40
1:C:247:SER:OG	1:C:251:PHE:HB2	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	319/329 (97%)	305 (96%)	13 (4%)	1 (0%)	46	79
1	C	319/329 (97%)	305 (96%)	14 (4%)	0	100	100
1	E	320/329 (97%)	296 (92%)	22 (7%)	2 (1%)	30	65
1	H	319/329 (97%)	299 (94%)	20 (6%)	0	100	100
1	J	319/329 (97%)	298 (93%)	21 (7%)	0	100	100
1	L	317/329 (96%)	288 (91%)	29 (9%)	0	100	100
2	B	168/182 (92%)	159 (95%)	9 (5%)	0	100	100
2	D	170/182 (93%)	161 (95%)	9 (5%)	0	100	100
2	F	170/182 (93%)	154 (91%)	15 (9%)	1 (1%)	30	65
2	I	168/182 (92%)	154 (92%)	14 (8%)	0	100	100
2	K	170/182 (93%)	157 (92%)	11 (6%)	2 (1%)	16	47
2	M	167/182 (92%)	155 (93%)	12 (7%)	0	100	100
All	All	2926/3066 (95%)	2731 (93%)	189 (6%)	6 (0%)	52	84

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	161	GLN
1	E	140	PRO
1	A	77	ASP
1	E	78	GLU
2	K	39	GLU
2	F	18	VAL

### 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	286/292 (98%)	265 (93%)	21 (7%)	17	44
1	C	286/292 (98%)	258 (90%)	28 (10%)	10	28
1	E	287/292 (98%)	256 (89%)	31 (11%)	8	23
1	H	286/292 (98%)	262 (92%)	24 (8%)	14	37
1	J	286/292 (98%)	259 (91%)	27 (9%)	11	31
1	L	285/292 (98%)	259 (91%)	26 (9%)	12	33
2	B	145/156 (93%)	121 (83%)	24 (17%)	3	8
2	D	147/156 (94%)	126 (86%)	21 (14%)	4	12
2	F	147/156 (94%)	124 (84%)	23 (16%)	3	9
2	I	145/156 (93%)	117 (81%)	28 (19%)	2	5
2	K	147/156 (94%)	122 (83%)	25 (17%)	2	7
2	M	144/156 (92%)	119 (83%)	25 (17%)	2	7
All	All	2591/2688 (96%)	2288 (88%)	303 (12%)	7	20

All (303) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	35(A)	THR
1	A	36	VAL
1	A	37	THR
1	A	46	THR
1	A	63	ASP
1	A	144	THR
1	A	194	LEU
1	A	211	GLN
1	A	221	SER
1	A	238	LYS
1	A	268	ILE
1	A	279	THR
1	A	283	THR
1	A	302	ILE
1	A	312	ASN
1	A	315	VAL
1	A	316	LEU

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Mol	Chain	Res	Type
1	A	318	THR
1	A	320	LEU
1	A	323	SER
2	B	9	PHE
2	B	19	ASP
2	B	22	TYR
2	B	24	TYR
2	B	26	HIS
2	B	34	TYR
2	B	42	GLN
2	B	57	ASP
2	B	60	ASN
2	B	78	GLU
2	B	84	MET
2	B	86	ASP
2	B	89	LEU
2	B	101	LEU
2	B	107	THR
2	B	108	LEU
2	B	113	SER
2	B	121	LYS
2	B	124	LEU
2	B	128	ASP
2	B	129	ASN
2	B	139	GLU
2	B	163	SER
2	B	164	GLU
1	C	23	GLU
1	C	26	ASP
1	C	28	ILE
1	C	35(A)	THR
1	C	46	THR
1	C	62	ARG
1	C	71	LEU
1	C	80	ILE
1	C	111	LEU
1	C	114	ARG
1	C	136	SER
1	C	151	VAL
1	C	167	SER
1	C	173	GLN
1	C	179	LEU

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Mol	Chain	Res	Type
1	C	185	SER
1	C	195	TYR
1	C	200	THR
1	C	211	GLN
1	C	235	THR
1	C	244	ASN
1	C	269	LYS
1	C	276	ASN
1	C	285	ILE
1	C	291	SER
1	C	300	LEU
1	C	315	VAL
1	C	322	ASN
2	D	22	TYR
2	D	30	GLN
2	D	32	SER
2	D	38	LYS
2	D	45	ILE
2	D	46	ASP
2	D	54	SER
2	D	80	LEU
2	D	83	LYS
2	D	84	MET
2	D	86	ASP
2	D	99	LEU
2	D	106	ARG
2	D	108	LEU
2	D	113	SER
2	D	135	ASN
2	D	144	CYS
2	D	147	GLU
2	D	149	MET
2	D	168	LEU
2	D	171	GLU
1	E	11	ASP
1	E	22	THR
1	E	23	GLU
1	E	46	THR
1	E	53(A)	LEU
1	E	54	ASP
1	E	63	ASP
1	E	81	ASN

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Mol	Chain	Res	Type
1	E	82	VAL
1	E	112	LEU
1	E	114	ARG
1	E	129	ASP
1	E	133	SER
1	E	149	ARG
1	E	161	TYR
1	E	179	LEU
1	E	195	TYR
1	E	200	THR
1	E	206	THR
1	E	219	THR
1	E	221	SER
1	E	244	ASN
1	E	246	GLU
1	E	283	THR
1	E	291	SER
1	E	300	LEU
1	E	314	LEU
1	E	316	LEU
1	E	318	THR
1	E	320	LEU
1	E	322	ASN
2	F	18	VAL
2	F	21	TRP
2	F	22	TYR
2	F	24	TYR
2	F	26	HIS
2	F	39	GLU
2	F	43	LYS
2	F	51	LYS
2	F	58	LYS
2	F	60	ASN
2	F	69	GLU
2	F	72	ASN
2	F	75	ARG
2	F	77	ILE
2	F	89	LEU
2	F	101	LEU
2	F	107	THR
2	F	108	LEU
2	F	113	SER

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Mol	Chain	Res	Type
2	F	126	LEU
2	F	149	MET
2	F	165	GLU
2	F	167	ARG
1	H	22	THR
1	H	23	GLU
1	H	28	ILE
1	H	36	VAL
1	H	62	ARG
1	H	81	ASN
1	H	92	ASN
1	H	97	CYS
1	H	112	LEU
1	H	114	ARG
1	H	129	ASP
1	H	161	TYR
1	H	166	ARG
1	H	185	SER
1	H	190	GLU
1	H	195	TYR
1	H	197	ASN
1	H	208	THR
1	H	227	SER
1	H	292	MET
1	H	296	ASN
1	H	302	ILE
1	H	310	LYS
1	H	315	VAL
2	I	11	GLU
2	I	32	SER
2	I	41	THR
2	I	42	GLN
2	I	54	SER
2	I	60	ASN
2	I	61	THR
2	I	72	ASN
2	I	81	ASN
2	I	84	MET
2	I	89	LEU
2	I	101	LEU
2	I	105	GLU
2	I	106	ARG

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Mol	Chain	Res	Type
2	I	108	LEU
2	I	117	ASN
2	I	124	LEU
2	I	129	ASN
2	I	133	LEU
2	I	143	LYS
2	I	145	ASP
2	I	151	SER
2	I	152	VAL
2	I	156	THR
2	I	157	TYR
2	I	164	GLU
2	I	165	GLU
2	I	170	ARG
1	J	22	THR
1	J	63	ASP
1	J	66	VAL
1	J	71	LEU
1	J	75	MET
1	J	89	GLU
1	J	114	ARG
1	J	151	VAL
1	J	186	ASN
1	J	191	GLN
1	J	195	TYR
1	J	196	GLN
1	J	197	ASN
1	J	208	THR
1	J	211	GLN
1	J	220	ARG
1	J	221	SER
1	J	222	LYS
1	J	227	SER
1	J	268	ILE
1	J	273	GLU
1	J	277	CYS
1	J	279	THR
1	J	283	THR
1	J	311	SER
1	J	314	LEU
1	J	320	LEU
2	K	19	ASP

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Mol	Chain	Res	Type
2	K	22	TYR
2	K	24	TYR
2	K	32	SER
2	K	38	LYS
2	K	39	GLU
2	K	41	THR
2	K	43	LYS
2	K	57	ASP
2	K	72	ASN
2	K	80	LEU
2	K	83	LYS
2	K	86	ASP
2	K	99	LEU
2	K	101	LEU
2	K	113	SER
2	K	116	LYS
2	K	132	GLU
2	K	148	CYS
2	K	153	ARG
2	K	154	ASN
2	K	156	THR
2	K	161	GLN
2	K	164	GLU
2	K	169	LYS
1	L	22	THR
1	L	26	ASP
1	L	45	LYS
1	L	46	THR
1	L	54	ASP
1	L	63	ASP
1	L	90	LYS
1	L	119	GLU
1	L	123	ILE
1	L	136	SER
1	L	145	PRO
1	L	146	SER
1	L	173	GLN
1	L	185	SER
1	L	186	ASN
1	L	191	GLN
1	L	219	THR
1	L	220	ARG

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Mol	Chain	Res	Type
1	L	221	SER
1	L	268	ILE
1	L	280	LYS
1	L	283	THR
1	L	291	SER
1	L	311	SER
1	L	315	VAL
1	L	320	LEU
2	M	15	GLN
2	M	19	ASP
2	M	21	TRP
2	M	24	TYR
2	M	25	HIS
2	M	30	GLN
2	M	42	GLN
2	M	43	LYS
2	M	45	ILE
2	M	51	LYS
2	M	60	ASN
2	M	69	GLU
2	M	72	ASN
2	M	75	ARG
2	M	84	MET
2	M	89	LEU
2	M	104	ASN
2	M	108	LEU
2	M	128	ASP
2	M	129	ASN
2	M	139	GLU
2	M	140	PHE
2	M	145	ASP
2	M	157	TYR
2	M	163	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	18	HIS
1	A	95	ASN
1	A	122	GLN
1	A	142	GLN

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Mol	Chain	Res	Type
1	A	173	GLN
1	A	186	ASN
1	A	224	ASN
1	A	240	ASN
1	A	295	HIS
2	B	26	HIS
2	B	50	ASN
2	B	53	ASN
2	B	60	ASN
2	B	79	ASN
2	B	95	ASN
2	B	111	HIS
2	B	117	ASN
2	B	125	GLN
2	B	129	ASN
2	B	161	GLN
1	C	18	HIS
1	C	92	ASN
1	C	95	ASN
1	C	103	ASN
1	C	116	ASN
1	C	197	ASN
1	C	295	HIS
1	C	322	ASN
2	D	50	ASN
2	D	79	ASN
2	D	95	ASN
2	D	117	ASN
2	D	125	GLN
2	D	129	ASN
2	D	135	ASN
1	E	24	GLN
1	E	34	ASN
1	E	38	HIS
1	E	95	ASN
1	E	130	HIS
1	E	142	GLN
1	E	186	ASN
1	E	196	GLN
1	E	197	ASN
1	E	226	GLN
1	E	295	HIS

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Mol	Chain	Res	Type
2	F	15	GLN
2	F	25	HIS
2	F	26	HIS
2	F	42	GLN
2	F	60	ASN
2	F	79	ASN
2	F	104	ASN
2	F	111	HIS
2	F	125	GLN
2	F	154	ASN
1	H	18	HIS
1	H	34	ASN
1	H	142	GLN
1	H	173	GLN
1	H	196	GLN
1	H	240	ASN
1	H	295	HIS
1	H	296	ASN
2	I	26	HIS
2	I	42	GLN
2	I	53	ASN
2	I	60	ASN
2	I	79	ASN
2	I	95	ASN
2	I	111	HIS
2	I	117	ASN
2	I	129	ASN
2	I	154	ASN
1	J	34	ASN
1	J	95	ASN
1	J	197	ASN
1	J	295	HIS
2	K	26	HIS
2	K	50	ASN
2	K	62	GLN
2	K	95	ASN
2	K	117	ASN
2	K	125	GLN
2	K	129	ASN
1	L	24	GLN
1	L	38	HIS
1	L	130	HIS

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Mol	Chain	Res	Type
1	L	142	GLN
1	L	173	GLN
1	L	186	ASN
1	L	197	ASN
1	L	295	HIS
1	L	322	ASN
2	M	25	HIS
2	M	42	GLN
2	M	79	ASN
2	M	104	ASN
2	M	111	HIS
2	M	154	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

6 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	$\# Z  > 2$
4	NAG	A	402	1,4	14,14,15	0.85	0	15,19,21	1.61	1 (6%)
4	NAG	A	403	4	14,14,15	0.71	0	15,19,21	1.90	4 (26%)
4	NAG	E	402	1,4	14,14,15	0.76	0	15,19,21	2.98	5 (33%)
4	NAG	E	403	4	14,14,15	0.57	0	15,19,21	0.97	1 (6%)
4	NAG	H	402	1,4	14,14,15	1.03	1 (7%)	15,19,21	2.75	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	H	403	4	14,14,15	0.42	0	15,19,21	1.93	4 (26%)

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	402	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	403	4	-	0/6/23/26	0/1/1/1
4	NAG	E	402	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	403	4	-	0/6/23/26	0/1/1/1
4	NAG	H	402	1,4	-	0/6/23/26	0/1/1/1
4	NAG	H	403	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	402	NAG	O4-C4	3.07	1.50	1.43

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	402	NAG	O4-C4-C5	-8.68	86.23	109.24
4	E	402	NAG	C2-N2-C7	-8.47	112.16	123.04
4	A	402	NAG	C2-N2-C7	-4.61	117.12	123.04
4	H	402	NAG	C4-C3-C2	-3.25	106.18	111.23
4	E	402	NAG	O4-C4-C5	-3.13	100.93	109.24
4	E	403	NAG	C4-C3-C2	-2.78	106.91	111.23
4	H	403	NAG	O7-C7-C8	-2.75	117.02	122.06
4	A	403	NAG	C3-C4-C5	2.01	113.70	110.20
4	E	402	NAG	O3-C3-C4	2.15	115.17	110.34
4	E	402	NAG	C1-O5-C5	2.20	115.04	112.25
4	H	403	NAG	C8-C7-N2	2.54	120.96	116.11
4	A	403	NAG	C3-C2-N2	2.55	116.66	110.56
4	A	403	NAG	C1-O5-C5	2.74	115.73	112.25
4	H	402	NAG	C1-O5-C5	2.92	115.95	112.25
4	H	402	NAG	O5-C5-C6	3.36	114.62	107.35
4	H	403	NAG	C3-C4-C5	3.73	116.70	110.20
4	A	403	NAG	C2-N2-C7	4.43	128.74	123.04
4	H	403	NAG	C1-O5-C5	4.55	118.02	112.25
4	E	402	NAG	O4-C4-C3	5.61	122.98	110.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	402	NAG	2	0
4	A	403	NAG	1	0
4	E	402	NAG	3	0
4	E	403	NAG	2	0
4	H	402	NAG	2	0

## 5.6 Ligand geometry [i](#)

10 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	$\# Z  > 2$
3	NAG	A	401	1	14,14,15	0.48	0	15,19,21	1.58	2 (13%)
3	NAG	C	401	1	14,14,15	0.54	0	15,19,21	1.73	4 (26%)
3	NAG	C	402	1	14,14,15	0.75	1 (7%)	15,19,21	1.78	5 (33%)
3	NAG	E	401	1	14,14,15	0.58	0	15,19,21	1.71	4 (26%)
3	NAG	H	401	1	14,14,15	0.49	0	15,19,21	1.57	2 (13%)
3	NAG	J	401	1	14,14,15	0.57	0	15,19,21	1.28	1 (6%)
3	NAG	J	402	1	14,14,15	0.54	0	15,19,21	0.69	0
3	NAG	L	401	3	14,14,15	0.56	0	15,19,21	0.97	1 (6%)
3	NAG	L	402	1	14,14,15	0.63	0	15,19,21	1.54	3 (20%)
3	NAG	L	403	1,3	14,14,15	0.56	0	15,19,21	1.77	3 (20%)

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	401	1	-	0/6/23/26	0/1/1/1
3	NAG	C	401	1	-	0/6/23/26	0/1/1/1
3	NAG	C	402	1	-	0/6/23/26	0/1/1/1
3	NAG	E	401	1	-	0/6/23/26	0/1/1/1
3	NAG	H	401	1	-	0/6/23/26	0/1/1/1
3	NAG	J	401	1	-	0/6/23/26	0/1/1/1
3	NAG	J	402	1	-	0/6/23/26	0/1/1/1
3	NAG	L	401	3	-	0/6/23/26	0/1/1/1
3	NAG	L	402	1	-	0/6/23/26	0/1/1/1
3	NAG	L	403	1,3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	NAG	O5-C1	-2.27	1.39	1.43

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	NAG	C2-N2-C7	-4.43	117.35	123.04
3	L	401	NAG	C4-C3-C2	-2.78	106.91	111.23
3	C	402	NAG	O3-C3-C4	-2.71	104.23	110.34
3	L	403	NAG	C4-C3-C2	-2.65	107.11	111.23
3	L	403	NAG	O3-C3-C2	-2.55	104.06	109.11
3	C	401	NAG	O7-C7-C8	-2.25	117.93	122.06
3	E	401	NAG	C3-C4-C5	2.02	113.72	110.20
3	L	402	NAG	O5-C5-C6	2.16	112.02	107.35
3	C	402	NAG	C2-N2-C7	2.17	125.83	123.04
3	C	401	NAG	O4-C4-C3	2.19	115.27	110.34
3	C	402	NAG	C1-O5-C5	2.31	115.18	112.25
3	C	401	NAG	C1-O5-C5	2.35	115.24	112.25
3	E	401	NAG	O3-C3-C2	2.49	114.05	109.11
3	C	402	NAG	C4-C3-C2	2.50	115.11	111.23
3	H	401	NAG	C3-C4-C5	2.60	114.74	110.20
3	L	402	NAG	C2-N2-C7	2.62	126.40	123.04
3	A	401	NAG	C3-C4-C5	2.63	114.79	110.20
3	E	401	NAG	O5-C5-C6	3.07	114.00	107.35
3	J	401	NAG	C1-O5-C5	3.28	116.41	112.25
3	L	402	NAG	C1-O5-C5	3.66	116.89	112.25
3	E	401	NAG	C1-O5-C5	3.78	117.04	112.25
3	C	402	NAG	C3-C4-C5	3.83	116.88	110.20
3	L	403	NAG	C1-O5-C5	4.08	117.42	112.25
3	H	401	NAG	C1-O5-C5	4.38	117.81	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NAG	C1-O5-C5	4.44	117.89	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAG	2	0
3	E	401	NAG	5	0
3	H	401	NAG	1	0
3	J	401	NAG	7	0
3	J	402	NAG	1	0
3	L	401	NAG	2	0
3	L	402	NAG	2	0
3	L	403	NAG	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	321/329 (97%)	-0.34	0 100 100	19, 36, 54, 81	0
1	C	321/329 (97%)	-0.23	0 100 100	20, 39, 55, 71	0
1	E	322/329 (97%)	-0.27	1 (0%) 94 92	19, 36, 57, 93	0
1	H	321/329 (97%)	-0.18	1 (0%) 94 92	20, 40, 59, 80	0
1	J	321/329 (97%)	-0.21	1 (0%) 94 92	20, 38, 55, 65	0
1	L	319/329 (96%)	-0.19	3 (0%) 85 79	20, 40, 65, 95	0
2	B	170/182 (93%)	0.49	15 (8%) 12 6	17, 58, 92, 104	0
2	D	172/182 (94%)	0.12	1 (0%) 90 86	23, 55, 72, 84	0
2	F	172/182 (94%)	0.51	18 (10%) 8 4	18, 55, 95, 102	0
2	I	170/182 (93%)	0.27	5 (2%) 55 43	18, 56, 84, 91	0
2	K	172/182 (94%)	0.06	3 (1%) 73 63	19, 50, 75, 99	0
2	M	169/182 (92%)	0.61	24 (14%) 4 2	17, 63, 106, 122	0
All	All	2950/3066 (96%)	-0.04	72 (2%) 62 50	17, 41, 81, 122	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	168	LEU	6.2
2	M	141	TYR	4.7
2	F	35	ALA	4.5
1	L	20	ASN	4.5
2	B	31	GLY	4.4
2	B	32	SER	4.3
2	F	33	GLY	4.2
2	M	143	LYS	4.2
2	F	160	PRO	4.1
2	M	168	LEU	4.1
2	F	158	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
2	M	33	GLY	3.8
1	L	12	GLN	3.8
2	B	158	ASP	3.7
2	M	131	LYS	3.7
2	B	29	GLU	3.6
2	F	161	GLN	3.5
2	M	160	PRO	3.5
2	M	138	PHE	3.1
2	F	164	GLU	3.1
2	M	167	ARG	3.1
1	E	22	THR	3.0
2	M	32	SER	3.0
2	F	169	LYS	3.0
2	B	141	TYR	3.0
2	M	35	ALA	2.9
2	B	157	TYR	2.9
2	M	144	CYS	2.9
2	M	140	PHE	2.9
2	F	144	CYS	2.8
2	B	11	GLU	2.8
1	J	218	ALA	2.8
2	K	164	GLU	2.8
2	M	148	CYS	2.7
1	H	19	ALA	2.7
2	I	19	ASP	2.7
2	I	16	GLY	2.7
2	I	29	GLU	2.7
2	F	140	PHE	2.7
2	F	38	LYS	2.6
2	M	27	SER	2.6
2	M	31	GLY	2.6
2	B	19	ASP	2.6
2	F	34	TYR	2.6
2	D	164	GLU	2.6
2	M	18	VAL	2.6
2	B	169	LYS	2.5
2	M	145	ASP	2.5
2	B	33	GLY	2.4
2	M	149	MET	2.4
2	K	172	GLU	2.4
2	F	31	GLY	2.4
2	B	140	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	I	141	TYR	2.3
2	B	28	ASN	2.3
2	I	162	TYR	2.3
2	M	34	TYR	2.3
2	F	32	SER	2.3
2	M	20	GLY	2.2
2	M	28	ASN	2.2
2	M	11	GLU	2.2
2	B	1	GLY	2.2
2	M	139	GLU	2.1
2	F	29	GLU	2.1
1	L	22	THR	2.1
2	M	132	GLU	2.1
2	K	168	LEU	2.1
2	F	17	MET	2.1
2	F	141	TYR	2.0
2	F	146	ASN	2.0
2	B	168	LEU	2.0
2	B	3	PHE	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	E	402	14/15	0.92	0.19	1.14	49,55,61,71	0
4	NAG	H	402	14/15	0.93	0.17	0.61	54,64,79,80	0
4	NAG	A	402	14/15	0.91	0.13	-0.75	33,47,56,61	0
4	NAG	H	403	14/15	0.84	0.35	-	81,92,100,104	0
4	NAG	A	403	14/15	0.92	0.25	-	62,75,81,93	0
4	NAG	E	403	14/15	0.78	0.38	-	91,97,107,108	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	J	402	14/15	0.85	0.20	2.20	39,55,68,68	0
3	NAG	C	402	14/15	0.92	0.18	1.02	52,59,64,73	0
3	NAG	L	403	14/15	0.89	0.17	0.92	57,65,83,84	0
3	NAG	A	401	14/15	0.84	0.26	-	89,95,105,119	0
3	NAG	E	401	14/15	0.82	0.23	-	71,84,90,92	0
3	NAG	L	402	14/15	0.80	0.35	-	78,88,95,97	0
3	NAG	H	401	14/15	0.75	0.30	-	91,99,112,113	0
3	NAG	L	401	14/15	0.69	0.35	-	85,93,108,114	0
3	NAG	J	401	14/15	0.73	0.42	-	94,106,111,113	0
3	NAG	C	401	14/15	0.82	0.36	-	82,88,98,98	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.