



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:43 AM GMT

PDB ID : 3FKU
Title : Crystal structure of influenza hemagglutinin (H5) in complex with a broadly neutralizing antibody F10
Authors : Hwang, W.C.; Santelli, E.; Stec, B.; Wei, G.; Cadwell, G.; Bankston, L.A.; Sui, J.; Perez, S.; Aird, D.; Chen, L.M.; Ali, M.; Murakami, A.; Yammanuru, A.; Han, T.; Cox, N.; Donis, R.O.; Liddington, R.C.; Marasco, W.A.
Deposited on : 2008-12-17
Resolution : 3.20 Å(reported)

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

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

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

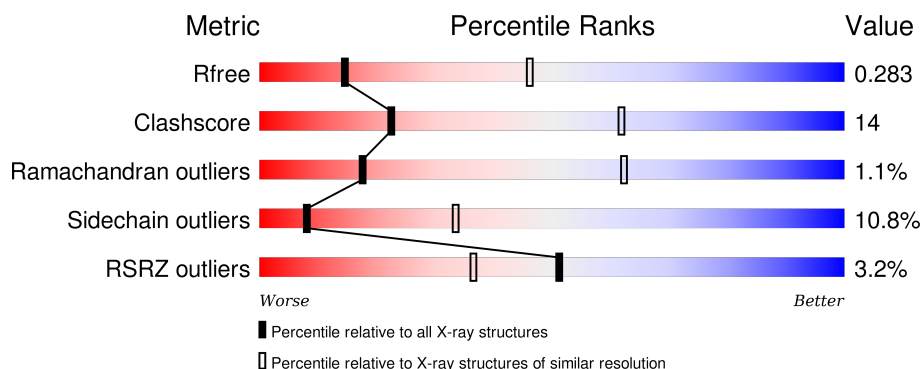
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	338	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>28%</div> <div>.</div> <div>.</div> </div> </div>
1	C	338	<div> <div>%</div> <div> <div></div> <div>63%</div> <div>30%</div> <div>.</div> <div>.</div> </div> </div>
1	E	338	<div> <div></div> <div> <div></div> <div>63%</div> <div>29%</div> <div>.</div> <div>.</div> </div> </div>
1	G	338	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>.</div> <div>.</div> </div> </div>
1	I	338	<div> <div>%</div> <div> <div></div> <div>64%</div> <div>27%</div> <div>.</div> <div>.</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	K	338	
2	B	182	
2	D	182	
2	F	182	
2	H	182	
2	J	182	
2	L	182	
3	S	280	
3	T	280	
3	U	280	
3	X	280	
3	Y	280	
3	Z	280	

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
5	NAG	G	601	X	-	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 34975 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2567	1621	443	488	15			
1	C	323	Total	C	N	O	S	0	0	0
			2567	1621	443	488	15			
1	E	323	Total	C	N	O	S	0	0	0
			2567	1621	443	488	15			
1	G	323	Total	C	N	O	S	0	0	0
			2567	1621	443	488	15			
1	I	323	Total	C	N	O	S	0	0	0
			2567	1621	443	488	15			
1	K	323	Total	C	N	O	S	0	0	0
			2567	1621	443	488	15			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	EXPRESSION TAG	UNP Q6DQ33
A	-2	ASP	-	EXPRESSION TAG	UNP Q6DQ33
A	-1	PRO	-	EXPRESSION TAG	UNP Q6DQ33
A	0	GLY	-	EXPRESSION TAG	UNP Q6DQ33
A	1	TYR	-	EXPRESSION TAG	UNP Q6DQ33
A	2	LEU	-	EXPRESSION TAG	UNP Q6DQ33
A	3	LEU	-	EXPRESSION TAG	UNP Q6DQ33
A	4	GLU	-	EXPRESSION TAG	UNP Q6DQ33
C	-3	ALA	-	EXPRESSION TAG	UNP Q6DQ33
C	-2	ASP	-	EXPRESSION TAG	UNP Q6DQ33
C	-1	PRO	-	EXPRESSION TAG	UNP Q6DQ33
C	0	GLY	-	EXPRESSION TAG	UNP Q6DQ33
C	1	TYR	-	EXPRESSION TAG	UNP Q6DQ33
C	2	LEU	-	EXPRESSION TAG	UNP Q6DQ33
C	3	LEU	-	EXPRESSION TAG	UNP Q6DQ33
C	4	GLU	-	EXPRESSION TAG	UNP Q6DQ33
E	-3	ALA	-	EXPRESSION TAG	UNP Q6DQ33

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	ASP	-	EXPRESSION TAG	UNP Q6DQ33
E	-1	PRO	-	EXPRESSION TAG	UNP Q6DQ33
E	0	GLY	-	EXPRESSION TAG	UNP Q6DQ33
E	1	TYR	-	EXPRESSION TAG	UNP Q6DQ33
E	2	LEU	-	EXPRESSION TAG	UNP Q6DQ33
E	3	LEU	-	EXPRESSION TAG	UNP Q6DQ33
E	4	GLU	-	EXPRESSION TAG	UNP Q6DQ33
G	-3	ALA	-	EXPRESSION TAG	UNP Q6DQ33
G	-2	ASP	-	EXPRESSION TAG	UNP Q6DQ33
G	-1	PRO	-	EXPRESSION TAG	UNP Q6DQ33
G	0	GLY	-	EXPRESSION TAG	UNP Q6DQ33
G	1	TYR	-	EXPRESSION TAG	UNP Q6DQ33
G	2	LEU	-	EXPRESSION TAG	UNP Q6DQ33
G	3	LEU	-	EXPRESSION TAG	UNP Q6DQ33
G	4	GLU	-	EXPRESSION TAG	UNP Q6DQ33
I	-3	ALA	-	EXPRESSION TAG	UNP Q6DQ33
I	-2	ASP	-	EXPRESSION TAG	UNP Q6DQ33
I	-1	PRO	-	EXPRESSION TAG	UNP Q6DQ33
I	0	GLY	-	EXPRESSION TAG	UNP Q6DQ33
I	1	TYR	-	EXPRESSION TAG	UNP Q6DQ33
I	2	LEU	-	EXPRESSION TAG	UNP Q6DQ33
I	3	LEU	-	EXPRESSION TAG	UNP Q6DQ33
I	4	GLU	-	EXPRESSION TAG	UNP Q6DQ33
K	-3	ALA	-	EXPRESSION TAG	UNP Q6DQ33
K	-2	ASP	-	EXPRESSION TAG	UNP Q6DQ33
K	-1	PRO	-	EXPRESSION TAG	UNP Q6DQ33
K	0	GLY	-	EXPRESSION TAG	UNP Q6DQ33
K	1	TYR	-	EXPRESSION TAG	UNP Q6DQ33
K	2	LEU	-	EXPRESSION TAG	UNP Q6DQ33
K	3	LEU	-	EXPRESSION TAG	UNP Q6DQ33
K	4	GLU	-	EXPRESSION TAG	UNP Q6DQ33

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1455	905	254	288	8			
2	D	180	Total	C	N	O	S	0	0	0
			1455	905	254	288	8			
2	F	180	Total	C	N	O	S	0	0	0
			1455	905	254	288	8			
2	H	174	Total	C	N	O	S	0	0	0
			1412	878	245	281	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	174	Total	C	N	O	S	0	0	0
			1412	878	245	281	8			
2	L	174	Total	C	N	O	S	0	0	0
			1412	878	245	281	8			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	177	ARG	-	EXPRESSION TAG	UNP Q2F4V2
B	178	SER	-	EXPRESSION TAG	UNP Q2F4V2
B	179	LEU	-	EXPRESSION TAG	UNP Q2F4V2
B	180	VAL	-	EXPRESSION TAG	UNP Q2F4V2
B	181	PRO	-	EXPRESSION TAG	UNP Q2F4V2
B	182	ARG	-	EXPRESSION TAG	UNP Q2F4V2
D	177	ARG	-	EXPRESSION TAG	UNP Q2F4V2
D	178	SER	-	EXPRESSION TAG	UNP Q2F4V2
D	179	LEU	-	EXPRESSION TAG	UNP Q2F4V2
D	180	VAL	-	EXPRESSION TAG	UNP Q2F4V2
D	181	PRO	-	EXPRESSION TAG	UNP Q2F4V2
D	182	ARG	-	EXPRESSION TAG	UNP Q2F4V2
F	177	ARG	-	EXPRESSION TAG	UNP Q2F4V2
F	178	SER	-	EXPRESSION TAG	UNP Q2F4V2
F	179	LEU	-	EXPRESSION TAG	UNP Q2F4V2
F	180	VAL	-	EXPRESSION TAG	UNP Q2F4V2
F	181	PRO	-	EXPRESSION TAG	UNP Q2F4V2
F	182	ARG	-	EXPRESSION TAG	UNP Q2F4V2
H	177	ARG	-	EXPRESSION TAG	UNP Q2F4V2
H	178	SER	-	EXPRESSION TAG	UNP Q2F4V2
H	179	LEU	-	EXPRESSION TAG	UNP Q2F4V2
H	180	VAL	-	EXPRESSION TAG	UNP Q2F4V2
H	181	PRO	-	EXPRESSION TAG	UNP Q2F4V2
H	182	ARG	-	EXPRESSION TAG	UNP Q2F4V2
J	177	ARG	-	EXPRESSION TAG	UNP Q2F4V2
J	178	SER	-	EXPRESSION TAG	UNP Q2F4V2
J	179	LEU	-	EXPRESSION TAG	UNP Q2F4V2
J	180	VAL	-	EXPRESSION TAG	UNP Q2F4V2
J	181	PRO	-	EXPRESSION TAG	UNP Q2F4V2
J	182	ARG	-	EXPRESSION TAG	UNP Q2F4V2
L	177	ARG	-	EXPRESSION TAG	UNP Q2F4V2
L	178	SER	-	EXPRESSION TAG	UNP Q2F4V2
L	179	LEU	-	EXPRESSION TAG	UNP Q2F4V2
L	180	VAL	-	EXPRESSION TAG	UNP Q2F4V2

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Chain	Residue	Modelled	Actual	Comment	Reference
L	181	PRO	-	EXPRESSION TAG	UNP Q2F4V2
L	182	ARG	-	EXPRESSION TAG	UNP Q2F4V2

- Molecule 3 is a protein called Neutralizing antibody F10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	235	Total	C	N	O	S	0	0	0
			1765	1094	311	352	8			
3	Y	235	Total	C	N	O	S	0	0	0
			1765	1094	311	352	8			
3	Z	236	Total	C	N	O	S	0	0	0
			1769	1096	312	353	8			
3	S	233	Total	C	N	O	S	0	0	0
			1753	1088	309	348	8			
3	T	234	Total	C	N	O	S	0	0	0
			1759	1091	310	350	8			
3	U	234	Total	C	N	O	S	0	0	0
			1759	1091	310	350	8			

- 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	C	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	2	Total	C	N	O	0	0
			28	16	2	10		

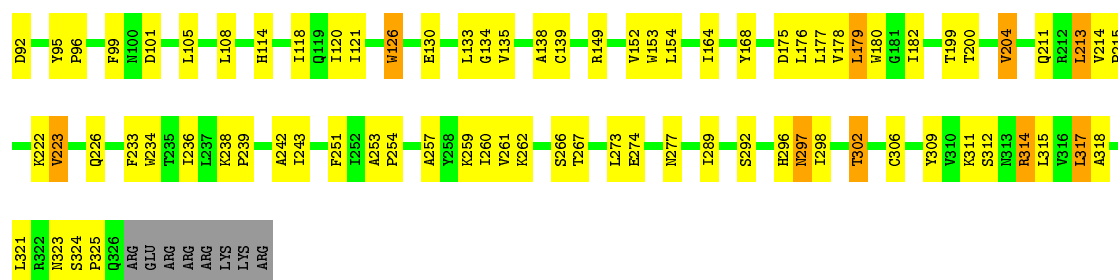
- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

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

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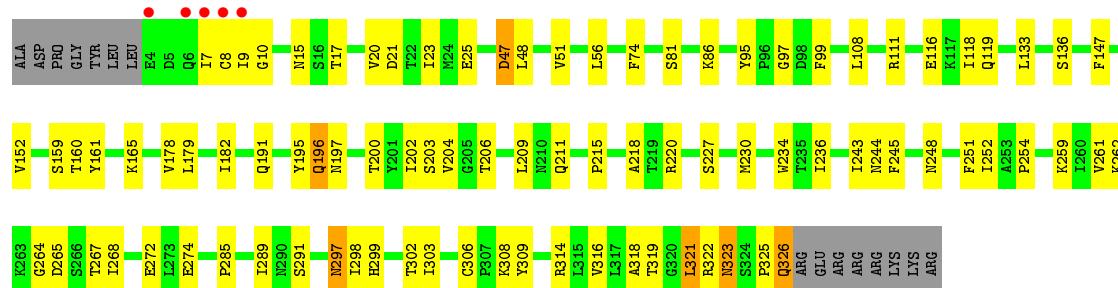
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	E	3	Total	C	N	O	0	0
			39	22	2	15		
5	G	3	Total	C	N	O	0	0
			39	22	2	15		
5	I	3	Total	C	N	O	0	0
			39	22	2	15		
5	K	3	Total	C	N	O	0	0
			39	22	2	15		



• Molecule 1: Hemagglutinin



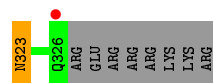
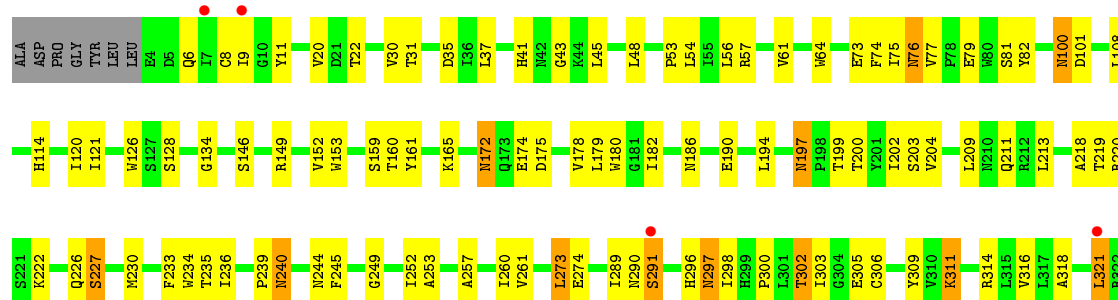
Chain G:



• Molecule 1: Hemagglutinin



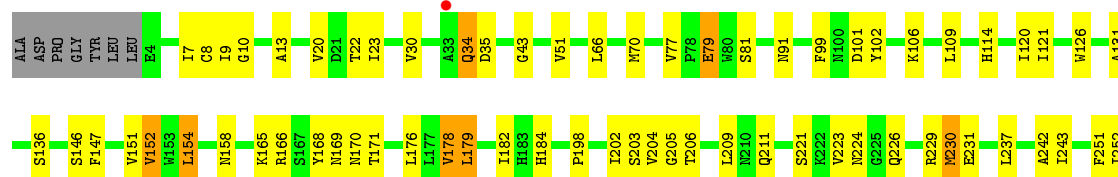
Chain I:

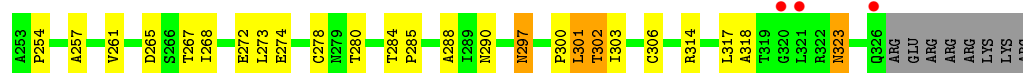


• Molecule 1: Hemagglutinin

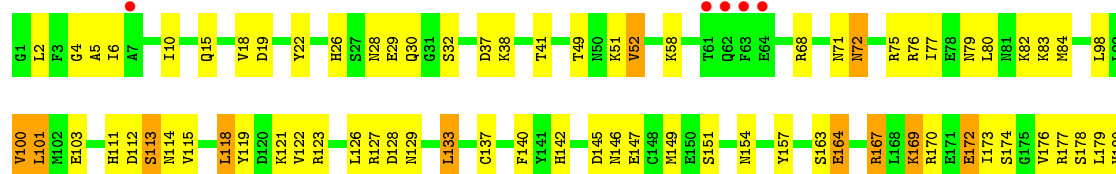


Chain K:



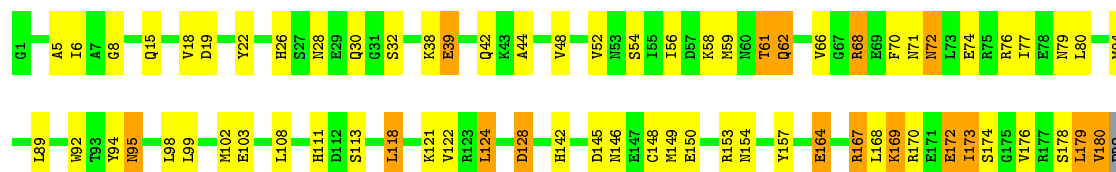


• Molecule 2: Hemagglutinin



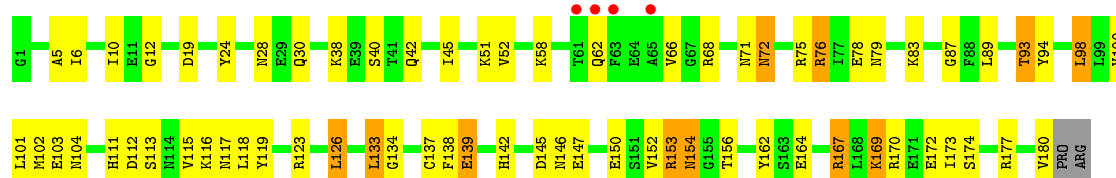
PRO
ARG

• Molecule 2: Hemagglutinin

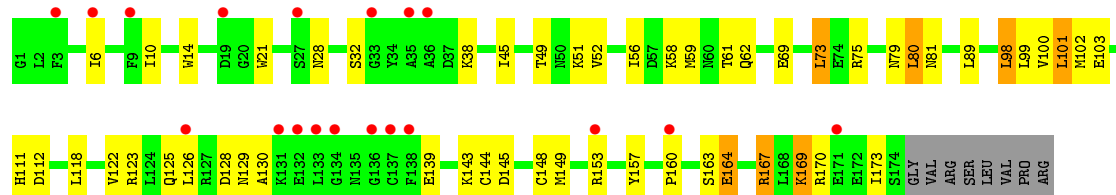


ARG

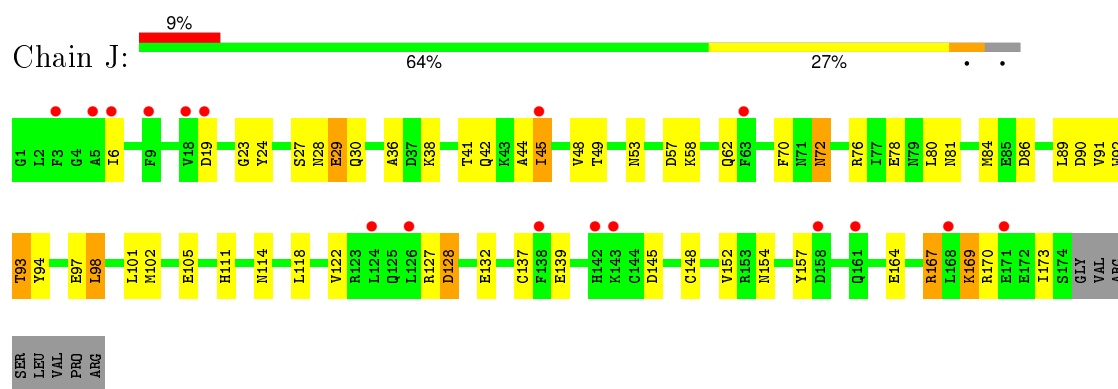
• Molecule 2: Hemagglutinin



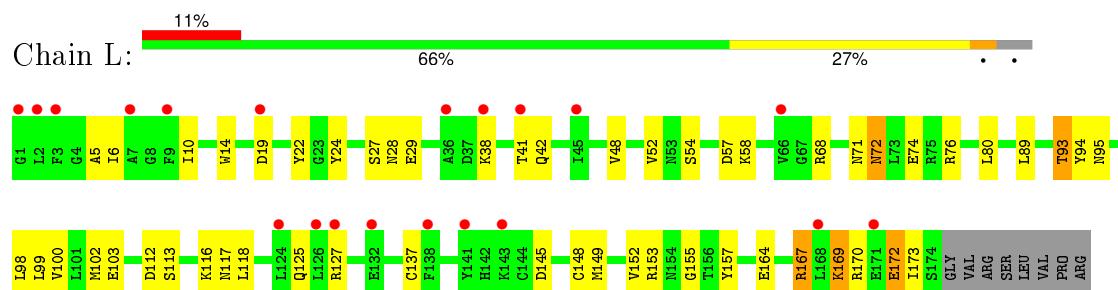
• Molecule 2: Hemagglutinin



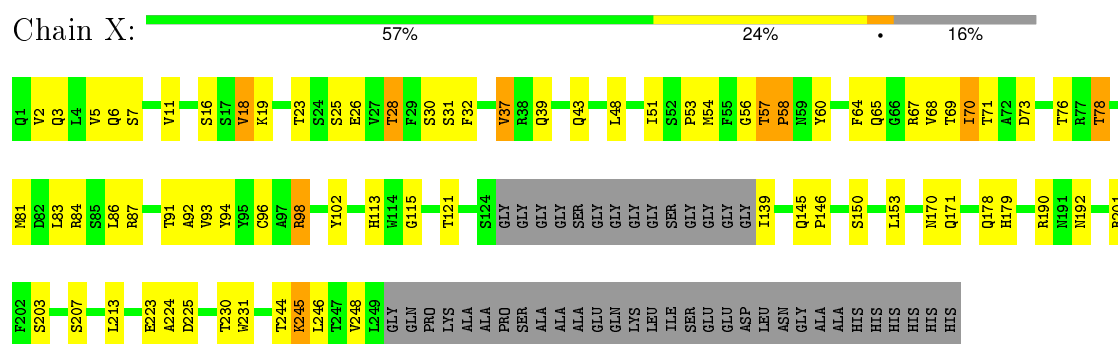
• Molecule 2: Hemagglutinin



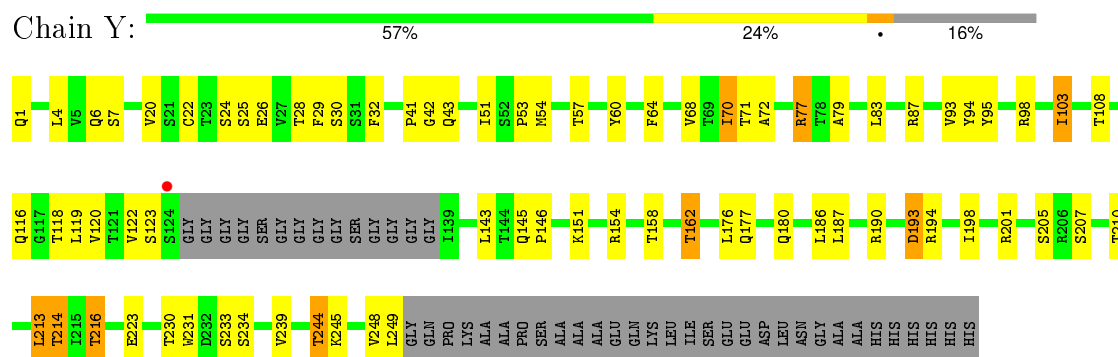
- Molecule 2: Hemagglutinin



- Molecule 3: Neutralizing antibody F10

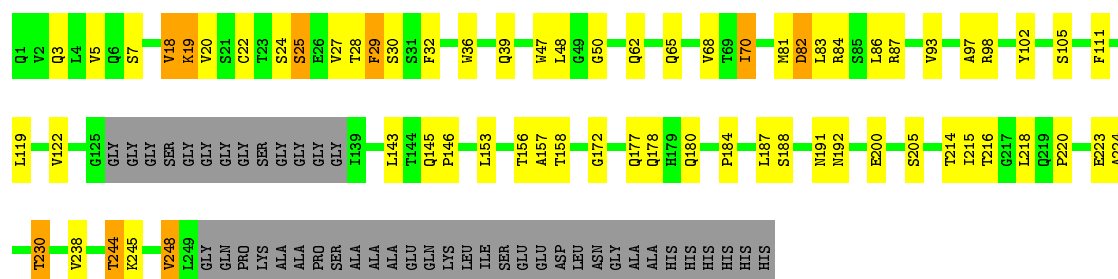


- Molecule 3: Neutralizing antibody F10



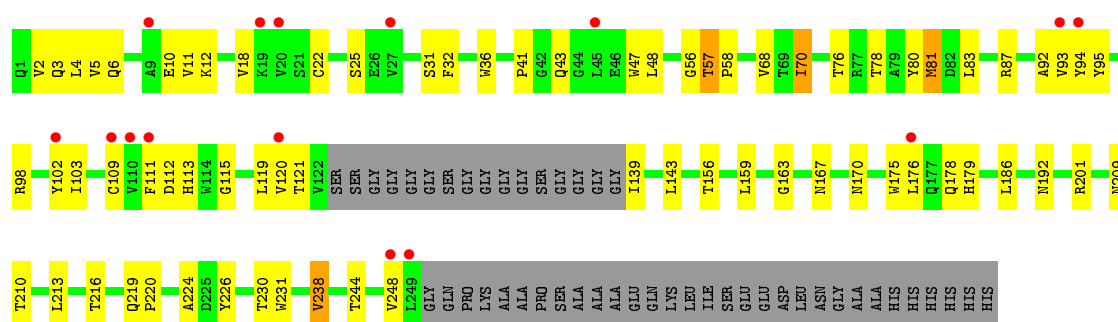
- Molecule 3: Neutralizing antibody F10

Chain Z: 



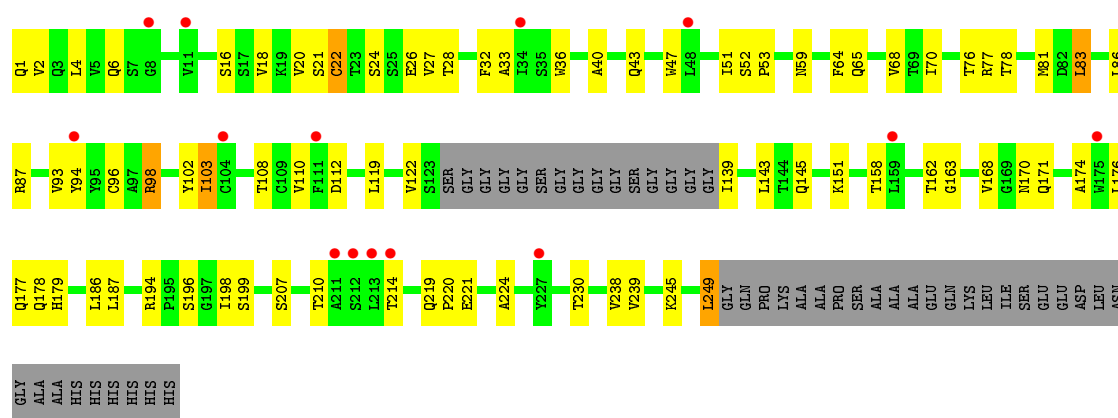
• Molecule 3: Neutralizing antibody F10

Chain S: 



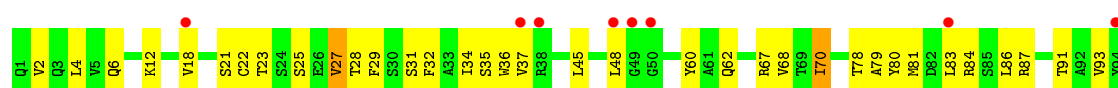
• Molecule 3: Neutralizing antibody F10

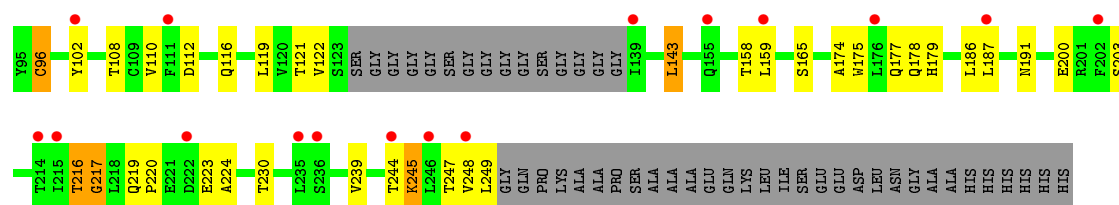
Chain T: 



• Molecule 3: Neutralizing antibody F10

Chain U: 





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	205.30Å 118.50Å 338.90Å 90.00° 99.60° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 93.77 – 3.20	Depositor EDS
% Data completeness (in resolution range)	85.0 (50.00-3.20) 85.0 (93.77-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.232 , 0.286 0.231 , 0.283	Depositor DCC
R_{free} test set	5676 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	70.8	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 84.0	EDS
Estimated twinning fraction	0.116 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.107 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	1 of 112570 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	34975	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.50	0/2629	0.66	0/3570
1	C	0.51	0/2629	0.68	0/3570
1	E	0.49	1/2629 (0.0%)	0.65	0/3570
1	G	0.48	0/2629	0.63	0/3570
1	I	0.46	0/2629	0.64	0/3570
1	K	0.48	0/2629	0.63	0/3570
2	B	0.64	0/1482	0.78	0/1992
2	D	0.62	0/1482	0.76	0/1992
2	F	0.63	0/1482	0.75	1/1992 (0.1%)
2	H	0.47	0/1439	0.61	0/1934
2	J	0.46	0/1439	0.60	0/1934
2	L	0.47	0/1439	0.60	0/1934
3	S	0.39	0/1791	0.57	0/2436
3	T	0.39	0/1797	0.57	0/2444
3	U	0.41	0/1797	0.59	0/2444
3	X	0.49	0/1803	0.65	0/2452
3	Y	0.52	0/1803	0.68	0/2452
3	Z	0.55	0/1807	0.72	0/2457
All	All	0.50	1/35335 (0.0%)	0.65	1/47883 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	E	0	3
1	G	0	1
1	I	0	1
1	K	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	Y	0	1
5	G	1	0
All	All	1	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	8	CYS	CB-SG	-5.67	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	76	ARG	NE-CZ-NH2	-5.45	117.57	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	601	NAG	C1

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	TRP	Peptide
1	A	290	ASN	Peptide
1	E	126	TRP	Peptide
1	E	323	ASN	Peptide
1	E	324	SER	Peptide
1	G	321	LEU	Peptide
1	I	290	ASN	Peptide
1	K	290	ASN	Peptide
3	Y	42	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2567	0	2507	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2567	0	2507	73	0
1	E	2567	0	2507	70	0
1	G	2567	0	2505	61	0
1	I	2567	0	2507	77	0
1	K	2567	0	2507	69	0
2	B	1455	0	1369	60	0
2	D	1455	0	1369	69	0
2	F	1455	0	1369	74	0
2	H	1412	0	1320	59	0
2	J	1412	0	1319	42	0
2	L	1412	0	1319	33	0
3	S	1753	0	1693	61	0
3	T	1759	0	1698	53	0
3	U	1759	0	1698	46	0
3	X	1765	0	1703	57	0
3	Y	1765	0	1703	39	0
3	Z	1769	0	1706	39	0
4	A	28	0	25	0	0
4	C	28	0	25	2	0
4	E	28	0	25	1	0
4	G	28	0	23	0	0
4	I	28	0	25	0	0
4	K	28	0	25	1	0
5	A	39	0	34	0	0
5	C	39	0	34	0	0
5	E	39	0	34	0	0
5	G	39	0	34	2	0
5	I	39	0	34	0	0
5	K	39	0	34	0	0
All	All	34975	0	33658	938	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 (938) 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:C:302:THR:HG21	1:C:306:CYS:SG	1.63	1.36
3:Y:158:THR:HG22	3:Y:214:THR:HG23	1.21	1.15
2:B:169:LYS:NZ	2:B:173:ILE:HG21	1.62	1.14
2:H:98:LEU:HD21	2:H:102:MET:HE1	1.27	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:THR:CG2	1:C:306:CYS:SG	2.37	1.13
1:A:108:LEU:HD21	1:A:236:ILE:HD11	1.37	1.04
1:I:204:VAL:HG23	1:I:209:LEU:HD23	1.42	1.00
2:H:98:LEU:HD21	2:H:102:MET:CE	1.93	0.98
1:A:7:ILE:HD12	2:B:149:MET:HE3	1.43	0.98
1:A:187:ASP:OD1	1:A:189:ALA:HB3	1.64	0.97
2:D:71:ASN:OD1	2:D:72:ASN:N	2.03	0.92
1:G:9:ILE:HD11	2:H:122:VAL:HG21	1.51	0.91
3:Y:162:THR:HG23	3:Y:210:THR:HB	1.53	0.91
2:B:169:LYS:HZ2	2:B:173:ILE:HG21	1.30	0.90
3:S:178:GLN:O	3:S:224:ALA:HB1	1.71	0.90
2:D:169:LYS:NZ	2:D:173:ILE:HG21	1.86	0.90
1:G:302:THR:CG2	1:G:306:CYS:SG	2.62	0.87
1:G:302:THR:HG22	1:G:306:CYS:SG	2.15	0.87
3:Z:158:THR:OG1	3:Z:214:THR:HG22	1.73	0.86
1:I:172:ASN:N	1:I:172:ASN:HD22	1.72	0.86
2:B:169:LYS:HZ3	2:B:173:ILE:HG21	1.36	0.85
3:X:68:VAL:HG22	3:X:83:LEU:HD13	1.57	0.84
3:Z:18:VAL:O	3:Z:82:ASP:HB2	1.77	0.84
1:A:230:MET:SD	1:A:252:ILE:HD11	2.19	0.83
1:I:108:LEU:HD13	1:I:236:ILE:HD11	1.61	0.82
2:B:123:ARG:O	2:B:126:LEU:O	1.98	0.81
1:I:100:ASN:HD22	1:I:101:ASP:N	1.77	0.81
1:K:20:VAL:HG21	1:K:318:ALA:HB2	1.61	0.81
1:A:156:LYS:NZ	1:A:192:THR:O	2.12	0.80
3:Z:87:ARG:O	3:Z:122:VAL:HG21	1.81	0.80
4:C:501:NAG:H4	4:C:502:NAG:N2	1.97	0.80
2:H:52:VAL:CG2	3:U:28:THR:HG22	2.12	0.79
1:I:204:VAL:HG23	1:I:209:LEU:CD2	2.13	0.78
2:D:169:LYS:HZ2	2:D:173:ILE:HG21	1.48	0.78
3:Y:158:THR:CG2	3:Y:214:THR:HG23	2.10	0.78
1:A:9:ILE:HD11	2:B:122:VAL:HG21	1.66	0.78
1:C:191:GLN:HE21	1:C:250:ASN:HD21	1.30	0.78
2:F:42:GLN:HE22	3:X:102:TYR:H	1.32	0.77
1:E:213:LEU:HD12	1:E:233:PHE:CZ	2.19	0.77
1:K:230:MET:SD	1:K:252:ILE:HD11	2.24	0.77
2:H:98:LEU:CD2	2:H:102:MET:CE	2.63	0.77
1:C:121:ILE:O	1:C:121:ILE:HG22	1.84	0.77
1:A:213:LEU:HD11	1:A:233:PHE:CE1	2.20	0.77
3:Y:87:ARG:O	3:Y:122:VAL:HG21	1.84	0.77
1:C:9:ILE:HD11	2:D:122:VAL:HG21	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HD12	2:B:149:MET:CE	2.16	0.76
1:C:48:LEU:HD22	1:C:303:ILE:CD1	2.15	0.76
3:Y:158:THR:HG22	3:Y:214:THR:CG2	2.11	0.76
3:U:248:VAL:HG23	3:U:249:LEU:HD12	1.67	0.76
1:I:20:VAL:HG11	1:I:318:ALA:HB2	1.66	0.76
3:U:4:LEU:HD22	3:U:22:CYS:SG	2.26	0.76
2:B:169:LYS:HZ2	2:B:173:ILE:CG2	1.98	0.75
1:I:180:TRP:HZ3	1:I:235:THR:HG22	1.49	0.75
1:I:45:LEU:HD12	1:I:273:LEU:O	1.86	0.75
2:B:169:LYS:NZ	2:B:173:ILE:CG2	2.46	0.75
1:A:302:THR:CG2	1:A:306:CYS:SG	2.75	0.75
3:S:76:THR:OG1	3:S:78:THR:HG22	1.87	0.74
1:E:251:PHE:CE2	1:E:253:ALA:HB2	2.22	0.74
2:J:30:GLN:HE21	2:J:145:ASP:HB2	1.52	0.74
1:A:302:THR:HG21	1:A:306:CYS:SG	2.27	0.74
3:T:52:SER:HB2	3:T:103:ILE:HD12	1.69	0.74
2:F:173:ILE:HD12	2:F:173:ILE:C	2.09	0.73
3:Z:68:VAL:HG22	3:Z:83:LEU:HB3	1.70	0.73
1:A:297:ASN:C	1:A:297:ASN:HD22	1.91	0.73
1:I:43:GLY:O	1:I:273:LEU:HD13	1.87	0.73
2:L:169:LYS:HZ2	2:L:173:ILE:HG12	1.53	0.73
3:S:43:GLN:HG2	3:S:139:ILE:HG21	1.69	0.73
1:E:302:THR:HG23	1:E:306:CYS:SG	2.29	0.73
3:X:37:VAL:HG12	3:X:37:VAL:O	1.88	0.73
1:I:9:ILE:HD11	2:J:122:VAL:HG21	1.69	0.73
3:X:91:THR:HG23	3:X:121:THR:HA	1.69	0.73
3:X:76:THR:OG1	3:X:78:THR:HG23	1.89	0.73
1:E:108:LEU:HD13	1:E:236:ILE:HD11	1.70	0.72
3:T:177:GLN:HB2	3:T:187:LEU:HD11	1.71	0.72
1:A:108:LEU:HD21	1:A:236:ILE:CD1	2.17	0.72
3:T:52:SER:CB	3:T:103:ILE:HD12	2.20	0.72
3:T:176:LEU:HD23	3:T:186:LEU:HA	1.71	0.72
3:X:230:THR:HG22	3:X:231:TRP:N	2.06	0.71
1:K:284:THR:HG22	1:K:302:THR:OG1	1.89	0.71
1:I:204:VAL:CG2	1:I:209:LEU:CD2	2.69	0.71
2:B:129:ASN:ND2	2:B:157:TYR:OH	2.23	0.71
1:K:126:TRP:CD2	1:K:154:LEU:HD11	2.26	0.71
1:A:289:ILE:HG12	1:A:298:ILE:HD12	1.71	0.71
2:D:30:GLN:NE2	2:D:146:ASN:H	1.88	0.71
3:T:158:THR:HG22	3:T:214:THR:HG23	1.73	0.70
1:G:230:MET:SD	1:G:252:ILE:HD11	2.30	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:169:LYS:HZ2	2:D:173:ILE:HD13	1.54	0.70
2:F:169:LYS:HZ1	2:F:173:ILE:HG21	1.56	0.70
1:I:204:VAL:CG2	1:I:209:LEU:HD23	2.20	0.70
1:A:11:TYR:CE1	2:B:6:ILE:HG23	2.26	0.70
3:X:51:ILE:HB	3:X:70:ILE:HD11	1.74	0.70
1:G:51:VAL:HG12	1:G:81:SER:HB2	1.73	0.70
1:A:66:LEU:HD23	1:A:179:LEU:HD12	1.72	0.69
1:K:204:VAL:HG22	1:K:211:GLN:HB3	1.74	0.69
3:S:6:GLN:HE21	3:S:115:GLY:HA3	1.57	0.69
1:K:317:LEU:HD13	2:L:52:VAL:HG12	1.74	0.69
3:Z:146:PRO:O	3:Z:244:THR:HB	1.91	0.69
2:F:28:ASN:HD21	2:F:146:ASN:ND2	1.90	0.69
2:B:126:LEU:HD22	2:B:140:PHE:HE2	1.56	0.69
3:T:87:ARG:O	3:T:122:VAL:HG21	1.93	0.68
1:A:325:PRO:HB3	2:B:15:GLN:NE2	2.08	0.68
2:D:179:LEU:N	2:D:179:LEU:HD12	2.09	0.68
2:H:80:LEU:CD2	2:J:80:LEU:HD21	2.24	0.68
3:S:159:LEU:HD23	3:S:244:THR:CG2	2.24	0.67
1:G:21:ASP:O	2:H:101:LEU:HD12	1.95	0.67
3:Y:177:GLN:HB2	3:Y:187:LEU:HD11	1.76	0.67
1:E:176:LEU:HD11	1:E:257:ALA:HB3	1.77	0.67
4:K:501:NAG:H4	4:K:502:NAG:N2	2.09	0.67
1:C:213:LEU:HD13	1:C:233:PHE:CE1	2.29	0.67
3:T:6:GLN:NE2	3:T:94:TYR:O	2.24	0.67
2:D:98:LEU:HD23	2:D:98:LEU:C	2.15	0.66
1:K:297:ASN:HD22	1:K:297:ASN:C	1.97	0.66
1:C:289:ILE:CD1	1:C:298:ILE:HD12	2.25	0.66
2:F:133:LEU:HB2	2:F:137:CYS:O	1.96	0.66
3:Z:18:VAL:HG22	3:Z:86:LEU:HD22	1.77	0.66
1:E:182:ILE:HD11	1:E:215:PRO:HG3	1.77	0.66
3:Y:201:ARG:HD2	3:Y:216:THR:O	1.95	0.66
1:C:75:ILE:HD12	1:C:75:ILE:O	1.96	0.66
3:U:78:THR:HG21	3:U:80:TYR:CZ	2.31	0.66
1:C:9:ILE:CD1	2:D:122:VAL:HG21	2.26	0.66
1:E:138:ALA:HB2	1:E:226:GLN:NE2	2.11	0.66
1:K:204:VAL:HG23	1:K:209:LEU:HD23	1.77	0.65
1:E:200:THR:O	1:E:214:VAL:HG13	1.96	0.65
1:I:172:ASN:N	1:I:172:ASN:ND2	2.44	0.65
2:H:98:LEU:CD2	2:H:102:MET:HE2	2.26	0.65
3:X:6:GLN:HE21	3:X:115:GLY:HA3	1.60	0.65
1:E:179:LEU:HD23	1:E:179:LEU:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:169:LYS:NZ	2:F:173:ILE:CG2	2.60	0.65
3:Z:172:GLY:O	3:Z:230:THR:HG21	1.97	0.65
1:G:302:THR:HG21	1:G:306:CYS:SG	2.36	0.64
3:X:64:PHE:HB3	3:X:68:VAL:HG23	1.80	0.64
3:X:60:TYR:HE2	3:X:70:ILE:HG23	1.62	0.64
1:E:134:GLY:HA3	1:E:153:TRP:HB3	1.79	0.64
1:A:204:VAL:HG12	1:A:245:PHE:CD2	2.32	0.64
2:D:169:LYS:HZ3	2:D:173:ILE:HG21	1.61	0.64
2:F:173:ILE:HD12	2:F:174:SER:N	2.13	0.64
1:I:180:TRP:CZ3	1:I:235:THR:HG22	2.31	0.64
1:K:7:ILE:HD12	2:L:149:MET:HE3	1.80	0.64
1:E:213:LEU:HD12	1:E:233:PHE:HZ	1.62	0.64
2:F:98:LEU:HD21	2:F:102:MET:HE1	1.80	0.64
2:F:180:VAL:HG12	2:F:180:VAL:O	1.95	0.64
1:G:204:VAL:HG12	1:G:245:PHE:CD2	2.32	0.64
1:A:230:MET:SD	1:A:252:ILE:CD1	2.86	0.64
3:S:3:GLN:HB2	3:S:25:SER:HB2	1.80	0.63
1:A:58:ASP:HB3	1:A:90:VAL:HG22	1.79	0.63
1:C:119:GLN:NE2	1:C:122:PRO:HA	2.13	0.63
1:E:302:THR:CG2	1:E:306:CYS:SG	2.86	0.63
1:A:120:ILE:HG22	1:A:168:TYR:CE1	2.34	0.63
1:A:120:ILE:HG22	1:A:168:TYR:CZ	2.33	0.63
2:H:130:ALA:HB1	2:H:139:GLU:O	1.98	0.63
2:B:84:MET:HE3	2:D:84:MET:HA	1.81	0.63
3:U:87:ARG:O	3:U:122:VAL:HG21	1.98	0.63
2:D:42:GLN:HE22	3:Z:102:TYR:H	1.47	0.63
1:C:289:ILE:HD11	1:C:298:ILE:HD12	1.81	0.63
2:B:83:LYS:HE3	2:F:66:VAL:HG22	1.81	0.62
1:A:7:ILE:O	1:A:7:ILE:HG23	1.99	0.62
1:G:297:ASN:C	1:G:297:ASN:HD22	2.02	0.62
1:A:45:LEU:HD11	1:A:84:VAL:HG11	1.81	0.62
1:I:100:ASN:C	1:I:100:ASN:HD22	2.01	0.62
3:S:2:VAL:HG21	3:S:113:HIS:CG	2.35	0.62
3:Y:30:SER:HA	3:Y:53:PRO:HB2	1.82	0.62
3:T:20:VAL:HG12	3:T:81:MET:HE2	1.81	0.62
2:B:49:THR:O	2:B:52:VAL:HG23	2.00	0.62
1:I:41:HIS:HB3	1:I:298:ILE:HD13	1.80	0.62
1:E:11:TYR:CE1	2:F:6:ILE:HG23	2.34	0.62
1:G:191:GLN:NE2	1:G:197:ASN:O	2.32	0.62
2:B:37:ASP:OD1	2:B:118:LEU:HD11	1.99	0.62
3:Y:60:TYR:HE2	3:Y:70:ILE:HG23	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:30:GLN:NE2	2:J:145:ASP:HB2	2.14	0.62
3:S:93:VAL:HG13	3:S:119:LEU:HD13	1.80	0.62
3:Y:70:ILE:HD12	3:Y:71:THR:N	2.15	0.61
3:U:110:VAL:HG11	3:U:174:ALA:HB2	1.81	0.61
1:E:175:ASP:O	1:E:260:ILE:HD12	1.99	0.61
1:C:17:THR:O	1:C:17:THR:HG22	2.00	0.61
2:B:5:ALA:HB1	2:B:115:VAL:HG12	1.82	0.61
3:U:18:VAL:HG13	3:U:86:LEU:HD22	1.81	0.61
1:G:204:VAL:HG22	1:G:211:GLN:HB3	1.82	0.61
1:C:302:THR:HG22	1:C:303:ILE:N	2.16	0.61
3:Y:30:SER:O	3:Y:54:MET:HB2	1.99	0.61
2:F:52:VAL:HG21	3:X:28:THR:HG23	1.81	0.61
3:Y:143:LEU:HG	3:Y:239:VAL:HG13	1.83	0.61
2:D:176:VAL:O	2:D:179:LEU:HD13	2.00	0.61
3:T:110:VAL:CG1	3:T:174:ALA:HB2	2.31	0.61
1:A:261:VAL:HG12	1:A:262:LYS:N	2.15	0.61
1:C:120:ILE:HG22	1:C:168:TYR:CE1	2.36	0.60
1:A:244:ASN:HB2	1:C:219:THR:HG23	1.84	0.60
1:G:20:VAL:HG21	1:G:318:ALA:HB2	1.82	0.60
1:C:204:VAL:HG22	1:C:245:PHE:CD2	2.36	0.60
3:S:78:THR:HG23	3:S:80:TYR:CE2	2.37	0.60
3:U:143:LEU:HD22	3:U:239:VAL:HG23	1.83	0.60
2:D:66:VAL:HG22	2:F:83:LYS:HE3	1.83	0.60
1:K:300:PRO:HB3	2:L:89:LEU:HD11	1.83	0.60
3:Y:6:GLN:NE2	3:Y:94:TYR:O	2.34	0.60
3:U:18:VAL:HG13	3:U:86:LEU:CD2	2.32	0.60
1:K:126:TRP:CE3	1:K:154:LEU:HD11	2.37	0.60
3:S:11:VAL:HG13	3:S:121:THR:O	2.02	0.60
1:C:108:LEU:HD13	1:C:236:ILE:HD11	1.84	0.60
3:S:68:VAL:HG22	3:S:83:LEU:HD13	1.83	0.59
3:X:153:LEU:HD13	3:X:248:VAL:HG11	1.83	0.59
2:F:169:LYS:NZ	2:F:173:ILE:HG21	2.16	0.59
2:H:125:GLN:HE21	2:H:157:TYR:HB3	1.66	0.59
3:Y:20:VAL:HG21	3:Y:118:THR:HG21	1.85	0.59
2:F:98:LEU:HD21	2:F:102:MET:CE	2.33	0.59
2:B:52:VAL:HG21	3:Y:28:THR:HG22	1.85	0.59
3:T:178:GLN:O	3:T:224:ALA:HB1	2.01	0.59
1:K:152:VAL:HG22	1:K:154:LEU:CD2	2.33	0.59
3:S:226:TYR:O	3:S:244:THR:HG22	2.03	0.59
1:I:182:ILE:HG13	1:I:202:ILE:HD12	1.84	0.59
1:G:206:THR:HG22	1:G:243:ILE:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:3:GLN:H	3:Z:25:SER:HB3	1.66	0.59
3:U:245:LYS:HE3	3:U:247:THR:HG23	1.84	0.59
3:U:220:PRO:HA	3:U:248:VAL:HG21	1.85	0.58
2:H:129:ASN:ND2	2:H:157:TYR:OH	2.37	0.58
3:U:223:GLU:OE2	3:U:247:THR:HG22	2.03	0.58
1:K:7:ILE:HG13	2:L:149:MET:HE1	1.86	0.58
3:S:156:THR:HG22	3:S:216:THR:HA	1.85	0.58
1:E:53:PRO:HB3	1:E:82:TYR:CE2	2.38	0.58
3:T:207:SER:O	3:T:210:THR:HG22	2.04	0.58
1:E:325:PRO:HG2	2:F:12:GLY:HA2	1.84	0.58
1:E:20:VAL:HG21	1:E:318:ALA:HB2	1.85	0.58
3:Z:36:TRP:CE2	3:Z:81:MET:HB2	2.38	0.58
2:H:52:VAL:CG2	3:U:28:THR:CG2	2.81	0.58
3:X:70:ILE:HD12	3:X:70:ILE:C	2.24	0.58
3:S:111:PHE:O	3:S:186:LEU:HD13	2.04	0.58
1:C:204:VAL:HG22	1:C:245:PHE:HD2	1.68	0.58
1:E:114:HIS:HB3	1:E:262:LYS:HB2	1.85	0.58
3:X:171:GLN:O	3:X:190:ARG:HD2	2.04	0.58
2:F:123:ARG:O	2:F:126:LEU:O	2.20	0.57
1:G:8:CYS:HG	2:H:14:TRP:HZ2	1.51	0.57
1:A:195:TYR:O	1:A:196:GLN:HB3	2.04	0.57
2:H:81:ASN:OD1	2:J:80:LEU:HD12	2.05	0.57
1:K:7:ILE:HD12	2:L:149:MET:CE	2.34	0.57
1:A:222:LYS:HG3	1:A:227:SER:HB2	1.86	0.57
1:K:317:LEU:HD13	2:L:52:VAL:CG1	2.33	0.57
1:A:170:ASN:HB2	1:A:237:LEU:HD23	1.85	0.57
1:A:302:THR:HG22	1:A:303:ILE:N	2.18	0.57
3:X:230:THR:CG2	3:X:231:TRP:N	2.68	0.57
3:Z:145:GLN:NE2	3:Z:244:THR:HG22	2.20	0.57
2:B:169:LYS:HZ2	2:B:173:ILE:HD13	1.70	0.57
2:B:5:ALA:HB1	2:B:115:VAL:CG1	2.34	0.57
1:C:230:MET:SD	1:C:252:ILE:HD11	2.45	0.57
1:E:309:TYR:CE2	2:F:89:LEU:HD13	2.40	0.57
2:J:169:LYS:NZ	2:J:173:ILE:HG21	2.18	0.57
3:T:2:VAL:HG13	3:T:26:GLU:HB3	1.87	0.57
3:S:179:HIS:CD2	3:S:224:ALA:HB2	2.40	0.57
3:S:47:TRP:CD2	3:S:238:VAL:HG23	2.39	0.57
2:H:79:ASN:HD22	2:L:68:ARG:HE	1.53	0.57
2:F:30:GLN:HE21	2:F:146:ASN:H	1.51	0.57
2:D:167:ARG:HB3	2:D:170:ARG:CZ	2.34	0.57
1:K:169:ASN:O	1:K:171:THR:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:169:LYS:HZ2	2:D:173:ILE:CD1	2.18	0.56
2:D:66:VAL:HG22	2:F:83:LYS:CE	2.35	0.56
2:H:56:ILE:HD11	3:U:27:VAL:HG12	1.87	0.56
2:B:80:LEU:C	2:B:80:LEU:HD23	2.26	0.56
1:A:243:ILE:HG23	1:A:243:ILE:O	2.05	0.56
1:K:9:ILE:HD11	2:L:24:TYR:CE2	2.39	0.56
1:A:289:ILE:HG12	1:A:298:ILE:CD1	2.35	0.56
1:G:108:LEU:HD13	1:G:236:ILE:HD11	1.88	0.56
2:L:42:GLN:HE21	3:T:102:TYR:HD1	1.51	0.56
2:D:169:LYS:HZ2	2:D:173:ILE:CG2	2.17	0.56
1:A:302:THR:CG2	1:A:303:ILE:N	2.68	0.56
3:Z:32:PHE:CB	3:Z:98:ARG:HD2	2.35	0.56
2:H:61:THR:HG21	1:I:311:LYS:HD3	1.88	0.56
2:J:49:THR:HG21	3:S:32:PHE:CZ	2.40	0.56
1:K:66:LEU:HD23	1:K:179:LEU:HD12	1.88	0.56
1:A:47:ASP:O	1:A:280:THR:HG22	2.05	0.56
3:U:178:GLN:O	3:U:224:ALA:HB1	2.06	0.56
3:Y:24:SER:O	3:Y:77:ARG:HD3	2.06	0.56
1:I:230:MET:SD	1:I:252:ILE:HD11	2.46	0.56
1:E:96:PRO:HB3	1:E:223:VAL:HG23	1.88	0.56
3:Z:28:THR:O	3:Z:28:THR:HG23	2.06	0.56
1:I:204:VAL:HG22	1:I:211:GLN:HB3	1.88	0.56
3:U:158:THR:C	3:U:159:LEU:HD12	2.26	0.56
1:A:38:GLU:OE1	1:A:291:SER:HB2	2.06	0.56
2:D:169:LYS:NZ	2:D:173:ILE:HD13	2.21	0.55
3:X:70:ILE:HD12	3:X:71:THR:N	2.21	0.55
2:B:68:ARG:NE	2:D:79:ASN:HD22	2.04	0.55
1:E:176:LEU:HD11	1:E:257:ALA:CB	2.35	0.55
3:S:93:VAL:CG1	3:S:119:LEU:HD13	2.36	0.55
1:G:309:TYR:CE2	2:H:89:LEU:HD13	2.42	0.55
2:B:71:ASN:OD1	2:B:72:ASN:N	2.40	0.55
2:J:72:ASN:O	2:J:72:ASN:ND2	2.39	0.55
1:I:204:VAL:HA	1:I:244:ASN:O	2.07	0.55
2:H:52:VAL:HG23	3:U:28:THR:CG2	2.35	0.55
1:E:45:LEU:HD12	1:E:273:LEU:HB2	1.89	0.55
1:I:175:ASP:OD1	1:I:239:PRO:HD3	2.07	0.55
1:E:72:ASP:O	1:E:74:PHE:N	2.38	0.55
2:D:169:LYS:NZ	2:D:173:ILE:CG2	2.67	0.55
1:A:314:ARG:HD3	1:A:316:VAL:HG23	1.89	0.55
1:C:180:TRP:HZ3	1:C:235:THR:HG22	1.71	0.55
3:S:143:LEU:HD22	3:S:163:GLY:HA3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:167:ARG:HB3	2:B:170:ARG:NH2	2.22	0.55
3:S:57:THR:HG21	3:S:103:ILE:HD12	1.87	0.55
3:Y:70:ILE:HD12	3:Y:70:ILE:C	2.27	0.55
1:A:297:ASN:C	1:A:297:ASN:ND2	2.59	0.55
2:H:56:ILE:HD11	3:U:27:VAL:CG1	2.36	0.55
1:C:74:PHE:O	1:C:77:VAL:HG13	2.06	0.55
1:A:325:PRO:HB3	2:B:15:GLN:HE21	1.72	0.55
1:G:321:LEU:CD2	2:H:111:HIS:HB3	2.37	0.55
1:I:204:VAL:HG21	1:I:209:LEU:HD21	1.89	0.54
1:I:79:GLU:HB3	1:I:114:HIS:CG	2.42	0.54
3:Z:153:LEU:HD21	3:Z:220:PRO:HD3	1.90	0.54
1:A:72:ASP:O	1:A:75:ILE:HG23	2.07	0.54
3:U:179:HIS:CD2	3:U:224:ALA:HB2	2.42	0.54
1:I:204:VAL:CG2	1:I:209:LEU:HD21	2.36	0.54
3:Y:32:PHE:CB	3:Y:98:ARG:HD2	2.38	0.54
2:H:169:LYS:HZ2	2:H:173:ILE:HG12	1.71	0.54
3:S:43:GLN:CG	3:S:139:ILE:HG21	2.37	0.54
2:L:52:VAL:HG23	3:T:28:THR:HG22	1.89	0.54
3:S:143:LEU:HD21	3:S:167:ASN:ND2	2.23	0.54
2:L:99:LEU:O	2:L:99:LEU:HD12	2.07	0.54
3:S:159:LEU:HD23	3:S:244:THR:HG23	1.88	0.54
1:E:138:ALA:HB2	1:E:226:GLN:HE21	1.69	0.54
1:I:152:VAL:CG1	1:I:253:ALA:HB3	2.38	0.54
1:K:182:ILE:HD13	1:K:184:HIS:CE1	2.43	0.54
1:C:61:VAL:HG11	1:C:109:LEU:HD22	1.90	0.54
2:B:113:SER:O	2:B:114:ASN:C	2.45	0.53
1:K:302:THR:CG2	1:K:306:CYS:SG	2.96	0.53
3:U:70:ILE:HG22	3:U:81:MET:HG2	1.89	0.53
1:K:7:ILE:CG1	2:L:149:MET:HE1	2.39	0.53
3:X:153:LEU:HA	3:X:248:VAL:HG13	1.90	0.53
2:D:167:ARG:HB3	2:D:170:ARG:NH2	2.23	0.53
3:T:187:LEU:HD23	3:T:198:ILE:HD12	1.90	0.53
1:A:195:TYR:O	1:A:196:GLN:CB	2.56	0.53
2:F:167:ARG:HB3	2:F:170:ARG:CZ	2.38	0.53
3:S:56:GLY:O	3:S:58:PRO:HD3	2.09	0.53
1:G:9:ILE:O	2:H:10:ILE:HD13	2.08	0.53
2:B:28:ASN:HD22	2:B:145:ASP:HA	1.73	0.53
1:I:213:LEU:HD11	1:I:233:PHE:CZ	2.44	0.53
3:X:76:THR:O	3:X:78:THR:HG22	2.08	0.53
3:T:6:GLN:HG2	3:T:22:CYS:HB3	1.91	0.53
3:S:176:LEU:HD23	3:S:186:LEU:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:152:VAL:HG12	1:I:253:ALA:HB3	1.90	0.53
1:E:317:LEU:HD23	2:F:104:ASN:OD1	2.09	0.53
3:U:177:GLN:HB2	3:U:187:LEU:HD21	1.90	0.53
2:B:126:LEU:HD22	2:B:140:PHE:CE2	2.43	0.53
2:F:51:LYS:HE2	2:F:103:GLU:OE1	2.09	0.53
1:K:151:VAL:HB	1:K:252:ILE:HG22	1.91	0.53
2:D:80:LEU:O	2:D:80:LEU:HD23	2.08	0.53
1:K:20:VAL:HG21	1:K:318:ALA:CB	2.35	0.52
5:G:601:NAG:C6	5:G:602:NAG:H82	2.40	0.52
3:T:143:LEU:HD11	3:T:230:THR:HG22	1.91	0.52
1:E:126:TRP:CZ3	1:E:164:ILE:HD13	2.45	0.52
3:U:2:VAL:HG23	3:U:2:VAL:O	2.08	0.52
3:S:3:GLN:HA	3:S:3:GLN:HE21	1.75	0.52
1:E:55:ILE:HG22	1:E:57:ARG:HG3	1.89	0.52
2:H:98:LEU:HD23	2:H:102:MET:HE2	1.89	0.52
1:K:20:VAL:HG22	1:K:30:VAL:HG11	1.90	0.52
1:A:289:ILE:CD1	1:A:298:ILE:HD12	2.39	0.52
1:K:317:LEU:CD1	2:L:52:VAL:HG12	2.38	0.52
3:T:143:LEU:HD21	3:T:168:VAL:HG23	1.92	0.52
1:K:267:THR:HB	1:K:303:ILE:HD13	1.91	0.52
1:G:285:PRO:HG2	1:G:299:HIS:CD2	2.43	0.52
1:E:311:LYS:HG2	2:F:93:THR:HG21	1.92	0.52
3:S:92:ALA:HB3	3:S:94:TYR:CE1	2.44	0.52
3:T:20:VAL:CG1	3:T:81:MET:HE2	2.40	0.52
1:E:297:ASN:C	1:E:297:ASN:HD22	2.11	0.52
2:F:24:TYR:CD1	2:F:153:ARG:HG3	2.45	0.52
1:G:20:VAL:HG12	1:G:316:VAL:HG12	1.92	0.52
3:S:32:PHE:HB3	3:S:98:ARG:HD3	1.92	0.52
1:E:126:TRP:CZ2	1:E:154:LEU:HD11	2.44	0.52
2:L:167:ARG:HA	2:L:170:ARG:HB2	1.90	0.52
3:T:151:LYS:O	3:T:249:LEU:HD23	2.10	0.52
1:C:53:PRO:HB3	1:C:82:TYR:CE2	2.44	0.52
2:J:91:VAL:HG12	2:J:92:TRP:N	2.23	0.52
2:D:176:VAL:O	2:D:179:LEU:CD1	2.57	0.52
3:T:36:TRP:CE2	3:T:81:MET:HB2	2.45	0.52
3:U:68:VAL:HG22	3:U:83:LEU:HB3	1.91	0.52
1:E:289:ILE:CD1	1:E:298:ILE:HD12	2.40	0.52
1:K:182:ILE:HG22	1:K:231:GLU:HB3	1.91	0.52
3:X:68:VAL:HG22	3:X:83:LEU:CD1	2.36	0.52
3:T:16:SER:O	3:T:86:LEU:HB2	2.10	0.52
1:A:25:GLU:HB3	1:A:28:VAL:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:52:VAL:HG23	3:U:28:THR:HG22	1.92	0.51
3:Y:193:ASP:N	3:Y:193:ASP:OD2	2.43	0.51
2:F:173:ILE:CD1	2:F:173:ILE:C	2.79	0.51
3:U:12:LYS:HG3	3:U:18:VAL:HG12	1.91	0.51
1:A:182:ILE:HD11	1:A:215:PRO:HG3	1.92	0.51
3:X:146:PRO:O	3:X:244:THR:HB	2.10	0.51
1:G:95:TYR:CD2	1:G:230:MET:HG2	2.46	0.51
3:X:30:SER:HA	3:X:53:PRO:HB2	1.93	0.51
3:Z:177:GLN:O	3:Z:184:PRO:HA	2.10	0.51
1:E:321:LEU:CD2	2:F:111:HIS:CG	2.93	0.51
2:D:98:LEU:HD21	2:D:102:MET:CE	2.41	0.51
1:I:311:LYS:H	2:J:93:THR:HG1	1.55	0.51
2:L:6:ILE:HD12	2:L:112:ASP:HA	1.90	0.51
1:K:121:ILE:HD12	1:K:254:PRO:HD2	1.92	0.51
3:S:48:LEU:N	3:S:48:LEU:HD12	2.26	0.51
1:A:289:ILE:CG1	1:A:298:ILE:HD12	2.37	0.51
3:T:110:VAL:HG11	3:T:174:ALA:HB2	1.91	0.51
3:T:47:TRP:CE3	3:T:238:VAL:HG23	2.45	0.51
1:I:20:VAL:HG12	1:I:316:VAL:HG12	1.91	0.51
1:K:302:THR:HG23	1:K:306:CYS:SG	2.50	0.51
3:T:158:THR:HG22	3:T:214:THR:CG2	2.40	0.51
1:K:297:ASN:ND2	1:K:297:ASN:C	2.64	0.51
1:K:20:VAL:HG22	1:K:30:VAL:CG1	2.40	0.51
3:X:230:THR:HG22	3:X:231:TRP:O	2.11	0.51
1:G:147:PHE:HE1	1:G:230:MET:HE2	1.75	0.51
1:G:204:VAL:CG2	1:G:209:LEU:HD21	2.40	0.51
1:I:230:MET:SD	1:I:252:ILE:CD1	2.99	0.51
1:E:289:ILE:HD13	1:E:298:ILE:HD12	1.92	0.51
2:B:174:SER:HB2	2:B:176:VAL:HG13	1.91	0.51
1:G:7:ILE:HD12	2:H:149:MET:HE3	1.93	0.51
2:H:49:THR:HG21	3:U:32:PHE:CZ	2.46	0.51
1:I:260:ILE:O	1:I:260:ILE:HG22	2.10	0.51
3:Y:6:GLN:HE22	3:Y:95:TYR:HA	1.76	0.51
2:J:93:THR:HG22	2:J:94:TYR:N	2.25	0.51
1:C:178:VAL:C	1:C:179:LEU:HD23	2.32	0.51
1:C:187:ASP:OD1	1:C:189:ALA:HB3	2.11	0.51
3:Y:143:LEU:HG	3:Y:239:VAL:CG1	2.41	0.51
1:I:54:LEU:HD11	1:I:77:VAL:HG12	1.91	0.51
2:D:26:HIS:HB3	2:D:149:MET:CE	2.41	0.51
3:X:43:GLN:HG2	3:X:139:ILE:HG21	1.92	0.51
2:L:72:ASN:C	2:L:72:ASN:HD22	2.15	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:202:ILE:HD11	1:K:251:PHE:HA	1.92	0.50
2:L:48:VAL:O	2:L:52:VAL:HG22	2.11	0.50
1:K:102:TYR:CE2	1:K:106:LYS:HD2	2.46	0.50
2:B:38:LYS:HD3	3:Y:103:ILE:HG21	1.92	0.50
3:Y:72:ALA:HA	3:Y:79:ALA:HA	1.93	0.50
2:D:38:LYS:NZ	3:Z:105:SER:OG	2.40	0.50
3:Y:230:THR:HG23	3:Y:231:TRP:N	2.25	0.50
3:U:4:LEU:HD22	3:U:96:CYS:SG	2.52	0.50
3:S:159:LEU:HD23	3:S:244:THR:HG21	1.92	0.50
1:I:302:THR:HG23	1:I:306:CYS:SG	2.52	0.50
3:S:12:LYS:HD2	3:S:18:VAL:HG12	1.94	0.50
1:I:31:THR:HG22	1:I:323:ASN:OD1	2.11	0.50
1:E:120:ILE:HG22	1:E:168:TYR:CE1	2.47	0.50
1:A:11:TYR:HB2	1:A:321:LEU:HD13	1.93	0.50
2:H:169:LYS:NZ	2:H:173:ILE:HG21	2.27	0.50
2:D:44:ALA:O	2:D:48:VAL:HG23	2.12	0.50
1:K:43:GLY:O	1:K:273:LEU:HD22	2.12	0.50
1:G:108:LEU:CD1	1:G:236:ILE:HD11	2.41	0.50
3:U:36:TRP:NE1	3:U:81:MET:HB2	2.27	0.50
1:K:34:GLN:HE21	1:K:34:GLN:HA	1.76	0.50
1:A:302:THR:O	1:A:303:ILE:HG23	2.11	0.50
1:K:7:ILE:HG23	1:K:7:ILE:O	2.11	0.50
3:S:3:GLN:HA	3:S:3:GLN:NE2	2.27	0.50
1:A:84:VAL:HG12	1:A:84:VAL:O	2.11	0.50
2:H:128:ASP:N	2:H:128:ASP:OD1	2.43	0.50
3:X:19:LYS:HA	3:X:81:MET:O	2.12	0.50
2:B:164:GLU:OE2	2:B:164:GLU:N	2.44	0.50
3:Y:213:LEU:HD22	3:Y:214:THR:N	2.27	0.50
1:A:164:ILE:O	1:A:246:GLU:HA	2.12	0.50
1:I:159:SER:O	1:I:160:THR:HG23	2.12	0.50
1:A:179:LEU:N	1:A:179:LEU:HD23	2.27	0.49
1:E:178:VAL:C	1:E:179:LEU:HD23	2.32	0.49
3:T:18:VAL:CG1	3:T:86:LEU:HD11	2.42	0.49
1:C:313:ASN:HD22	1:C:313:ASN:C	2.14	0.49
3:Y:60:TYR:CE2	3:Y:70:ILE:HG23	2.45	0.49
2:B:30:GLN:NE2	2:B:146:ASN:H	2.10	0.49
1:C:243:ILE:O	1:C:243:ILE:HG23	2.12	0.49
2:B:79:ASN:HD22	2:F:68:ARG:NE	2.10	0.49
1:A:302:THR:HG23	1:A:306:CYS:SG	2.52	0.49
3:T:179:HIS:CD2	3:T:224:ALA:HB2	2.47	0.49
1:K:267:THR:CG2	1:K:268:ILE:N	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:219:GLN:HB3	3:S:220:PRO:HD2	1.94	0.49
3:Z:18:VAL:HG22	3:Z:86:LEU:CD2	2.42	0.49
3:Z:145:GLN:NE2	3:Z:244:THR:CG2	2.76	0.49
1:I:11:TYR:CZ	2:J:6:ILE:HG23	2.46	0.49
1:C:156:LYS:HE2	1:C:193:LYS:O	2.12	0.49
1:I:321:LEU:HD23	2:J:111:HIS:CG	2.48	0.49
3:Z:7:SER:HB3	3:Z:20:VAL:HG13	1.94	0.49
1:I:37:LEU:HD12	1:I:296:HIS:HA	1.93	0.49
1:K:131:ALA:HB1	1:K:152:VAL:HG21	1.95	0.49
2:D:30:GLN:HE21	2:D:146:ASN:H	1.58	0.49
1:G:116:GLU:HB3	1:G:259:LYS:HB2	1.95	0.49
3:T:112:ASP:HA	3:T:186:LEU:HD22	1.93	0.49
1:E:19:GLN:NE2	1:E:27:ASN:OD1	2.46	0.49
1:G:289:ILE:HG22	1:G:291:SER:OG	2.13	0.49
3:Y:51:ILE:HB	3:Y:70:ILE:HD11	1.94	0.49
1:I:121:ILE:HG21	1:I:126:TRP:CZ2	2.48	0.49
1:C:202:ILE:O	1:C:212:ARG:HA	2.13	0.49
3:Z:158:THR:OG1	3:Z:214:THR:CG2	2.53	0.49
1:A:321:LEU:HD23	2:B:111:HIS:CG	2.48	0.49
2:D:179:LEU:O	2:D:180:VAL:HG13	2.13	0.49
3:U:68:VAL:HG22	3:U:83:LEU:CB	2.42	0.49
1:K:121:ILE:HG23	1:K:166:ARG:NH1	2.28	0.49
1:I:48:LEU:HD22	1:I:303:ILE:CD1	2.43	0.49
1:A:171:THR:CB	1:G:118:ILE:HG22	2.42	0.49
1:E:7:ILE:HG23	1:E:7:ILE:O	2.12	0.49
2:F:30:GLN:NE2	2:F:146:ASN:H	2.11	0.49
3:Y:187:LEU:HA	3:Y:198:ILE:HG13	1.94	0.49
3:Y:146:PRO:O	3:Y:244:THR:HG23	2.13	0.49
2:B:4:GLY:N	2:B:112:ASP:OD2	2.46	0.49
1:A:41:HIS:HB3	1:A:298:ILE:HD13	1.95	0.48
3:X:51:ILE:HD11	3:X:56:GLY:O	2.13	0.48
1:C:180:TRP:CE2	1:C:204:VAL:HG21	2.48	0.48
3:Y:26:GLU:OE2	3:Y:98:ARG:NE	2.46	0.48
1:C:317:LEU:HD13	2:D:52:VAL:HG22	1.95	0.48
2:D:71:ASN:HB3	2:D:74:GLU:HG3	1.95	0.48
1:A:11:TYR:CZ	2:B:6:ILE:HG23	2.49	0.48
2:H:80:LEU:HD21	2:J:80:LEU:HD21	1.92	0.48
1:K:79:GLU:HB2	1:K:114:HIS:HB2	1.95	0.48
2:F:145:ASP:OD1	2:F:145:ASP:C	2.51	0.48
3:S:57:THR:CG2	3:S:103:ILE:HD12	2.43	0.48
3:S:210:THR:HG23	3:S:210:THR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:601:NAG:H61	5:G:602:NAG:H82	1.94	0.48
3:S:230:THR:HG22	3:S:231:TRP:N	2.29	0.48
3:U:78:THR:HG22	3:U:79:ALA:N	2.28	0.48
1:E:95:TYR:N	1:E:139:CYS:SG	2.87	0.48
3:X:32:PHE:HB3	3:X:98:ARG:HD3	1.94	0.48
1:C:30:VAL:HG11	2:D:108:LEU:HD21	1.95	0.48
1:C:303:ILE:HD12	1:C:303:ILE:C	2.34	0.48
1:C:114:HIS:HB2	1:C:262:LYS:HZ1	1.77	0.48
3:U:6:GLN:H	3:U:116:GLN:HE22	1.61	0.48
2:D:30:GLN:NE2	2:D:145:ASP:HB2	2.28	0.48
2:H:164:GLU:HA	2:H:167:ARG:HD2	1.96	0.48
2:D:145:ASP:OD1	2:D:145:ASP:C	2.52	0.48
1:G:321:LEU:HD23	2:H:111:HIS:HB3	1.96	0.48
1:G:179:LEU:O	1:G:254:PRO:HB3	2.14	0.48
1:G:308:LYS:HZ2	2:H:62:GLN:HB3	1.79	0.48
3:U:112:ASP:HA	3:U:186:LEU:HD22	1.96	0.48
3:T:139:ILE:O	3:T:139:ILE:HG23	2.13	0.48
3:X:170:ASN:HB2	3:X:171:GLN:OE1	2.14	0.48
3:Z:32:PHE:HB2	3:Z:98:ARG:HD2	1.95	0.48
1:C:53:PRO:HB3	1:C:82:TYR:CZ	2.49	0.48
1:E:9:ILE:HG13	2:F:119:TYR:HA	1.96	0.48
2:H:144:CYS:SG	2:H:145:ASP:N	2.87	0.48
1:G:161:TYR:HB2	1:G:195:TYR:O	2.13	0.48
1:C:237:LEU:CD1	1:C:241:ASP:HB3	2.44	0.48
1:E:315:LEU:HG	2:F:100:VAL:HG21	1.95	0.48
2:J:152:VAL:HG22	2:J:157:TYR:CD1	2.49	0.48
3:Y:64:PHE:HB3	3:Y:68:VAL:HG13	1.96	0.48
1:I:297:ASN:C	1:I:297:ASN:HD22	2.16	0.48
2:F:180:VAL:CG1	2:F:180:VAL:O	2.62	0.47
2:B:72:ASN:HD22	2:B:75:ARG:NH2	2.12	0.47
1:A:135:VAL:HG23	1:A:145:SER:HB3	1.96	0.47
2:B:169:LYS:NZ	2:B:173:ILE:HD13	2.29	0.47
2:F:24:TYR:CE1	2:F:153:ARG:HG3	2.49	0.47
3:Y:176:LEU:HD23	3:Y:186:LEU:HA	1.95	0.47
3:T:219:GLN:HB2	3:T:220:PRO:CD	2.44	0.47
1:C:13:ALA:HB1	2:D:15:GLN:HE21	1.77	0.47
3:U:37:VAL:CG1	3:U:45:LEU:HD12	2.44	0.47
3:S:143:LEU:HD22	3:S:163:GLY:CA	2.45	0.47
1:I:48:LEU:HD22	1:I:303:ILE:HD13	1.97	0.47
2:B:51:LYS:HE3	1:C:24:MET:HE2	1.96	0.47
1:A:9:ILE:HG13	2:B:119:TYR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:178:VAL:C	1:K:179:LEU:HD23	2.35	0.47
1:E:222:LYS:O	1:E:223:VAL:HG13	2.14	0.47
2:B:30:GLN:HE21	2:B:146:ASN:H	1.63	0.47
1:K:280:THR:HG21	1:K:288:ALA:HB1	1.95	0.47
1:G:47:ASP:N	1:G:47:ASP:OD1	2.46	0.47
1:E:177:LEU:HD12	1:E:178:VAL:N	2.30	0.47
3:S:68:VAL:HG12	3:S:70:ILE:CG2	2.45	0.47
2:J:48:VAL:O	2:J:49:THR:C	2.53	0.47
3:U:48:LEU:HD22	3:U:81:MET:SD	2.54	0.47
1:C:261:VAL:HG22	1:C:262:LYS:N	2.28	0.47
3:T:219:GLN:HB2	3:T:220:PRO:HD2	1.96	0.47
3:T:4:LEU:HD23	3:T:96:CYS:SG	2.55	0.47
3:U:219:GLN:O	3:U:248:VAL:HG11	2.13	0.47
1:K:152:VAL:HG22	1:K:154:LEU:HD23	1.95	0.47
2:J:169:LYS:HZ2	2:J:173:ILE:HG12	1.80	0.47
1:K:109:LEU:HB3	1:K:268:ILE:HD11	1.97	0.47
2:B:51:LYS:HE3	1:C:24:MET:CE	2.44	0.47
3:X:223:GLU:HB2	3:X:246:LEU:O	2.14	0.47
2:F:154:ASN:HD22	2:F:154:ASN:C	2.18	0.47
1:G:202:ILE:HD11	1:G:251:PHE:HA	1.97	0.47
2:L:28:ASN:ND2	2:L:145:ASP:HA	2.29	0.47
1:A:87:ALA:HB2	1:A:272:GLU:OE2	2.14	0.47
2:H:99:LEU:HD13	2:J:98:LEU:HD11	1.95	0.47
1:G:309:TYR:HE2	2:H:89:LEU:HD13	1.79	0.47
1:G:179:LEU:CD2	1:G:234:TRP:HB3	2.44	0.47
1:I:211:GLN:OE1	1:I:213:LEU:HD12	2.15	0.47
1:E:9:ILE:O	2:F:10:ILE:HD13	2.15	0.47
3:X:92:ALA:HB3	3:X:94:TYR:CE1	2.50	0.47
1:K:230:MET:SD	1:K:252:ILE:CD1	3.01	0.47
1:K:205:GLY:HA2	1:K:209:LEU:O	2.14	0.47
3:Z:178:GLN:O	3:Z:224:ALA:HB1	2.15	0.47
1:I:22:THR:HB	2:J:105:GLU:HB2	1.97	0.47
2:D:71:ASN:HB3	2:D:74:GLU:CG	2.45	0.46
3:Y:6:GLN:H	3:Y:116:GLN:HE22	1.63	0.46
1:C:237:LEU:HD11	1:C:241:ASP:HB3	1.97	0.46
2:J:44:ALA:HB2	2:J:114:ASN:HD22	1.80	0.46
3:Y:119:LEU:HD23	3:Y:120:VAL:N	2.30	0.46
3:Z:50:GLY:C	3:Z:70:ILE:HD11	2.35	0.46
3:T:52:SER:HB3	3:T:103:ILE:HD12	1.97	0.46
2:F:169:LYS:HZ2	2:F:173:ILE:CG2	2.27	0.46
1:K:9:ILE:HD12	2:L:118:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:99:PHE:O	1:K:102:TYR:HB2	2.15	0.46
1:I:48:LEU:HB3	1:I:81:SER:OG	2.16	0.46
1:E:58:ASP:HB3	1:E:90:VAL:HG22	1.95	0.46
1:C:95:TYR:N	1:C:139:CYS:SG	2.89	0.46
3:S:70:ILE:HG22	3:S:81:MET:HG2	1.96	0.46
2:F:126:LEU:HD21	2:F:152:VAL:CG2	2.46	0.46
2:L:93:THR:HG22	2:L:94:TYR:N	2.30	0.46
1:A:97:GLY:HA3	1:A:230:MET:O	2.16	0.46
1:G:297:ASN:HD22	1:G:298:ILE:N	2.13	0.46
1:E:321:LEU:HD23	2:F:111:HIS:CG	2.50	0.46
1:I:303:ILE:HD12	1:I:303:ILE:C	2.35	0.46
1:G:25:GLU:OE2	1:G:322:ARG:NH2	2.47	0.46
1:K:120:ILE:HD13	1:K:257:ALA:HB2	1.97	0.46
3:S:226:TYR:HB2	3:S:244:THR:HG23	1.97	0.46
2:D:6:ILE:HD11	2:D:111:HIS:HB3	1.97	0.46
1:G:182:ILE:HD11	1:G:215:PRO:CA	2.46	0.46
1:K:13:ALA:HB1	1:K:323:ASN:ND2	2.30	0.46
1:E:261:VAL:O	1:E:261:VAL:CG1	2.63	0.46
2:J:128:ASP:OD1	2:J:128:ASP:N	2.48	0.46
2:D:169:LYS:HZ2	2:D:173:ILE:CG1	2.29	0.46
1:E:32:HIS:CD2	3:X:54:MET:HG3	2.50	0.46
3:S:70:ILE:HG22	3:S:81:MET:CG	2.45	0.46
3:U:60:TYR:HE2	3:U:70:ILE:HG23	1.81	0.46
3:T:47:TRP:CD2	3:T:238:VAL:HG23	2.51	0.46
1:C:239:PRO:O	1:C:240:ASN:HB2	2.16	0.46
3:Z:191:ASN:O	3:Z:192:ASN:HB2	2.14	0.46
1:K:206:THR:HG22	1:K:243:ILE:HA	1.98	0.46
1:C:120:ILE:HG22	1:C:168:TYR:CZ	2.51	0.46
3:T:143:LEU:HD12	3:T:239:VAL:HG12	1.97	0.46
1:I:300:PRO:HB3	2:J:89:LEU:HD11	1.96	0.46
3:X:178:GLN:O	3:X:224:ALA:HB1	2.16	0.46
1:E:243:ILE:O	1:E:243:ILE:HG23	2.16	0.46
2:J:169:LYS:HZ2	2:J:173:ILE:HG21	1.80	0.46
1:G:195:TYR:O	1:G:196:GLN:HB3	2.15	0.46
2:L:113:SER:O	2:L:117:ASN:ND2	2.49	0.46
1:C:164:ILE:O	1:C:246:GLU:HA	2.16	0.46
1:A:53:PRO:HB3	1:A:82:TYR:CE2	2.51	0.46
2:F:72:ASN:HD22	2:F:75:ARG:NH2	2.14	0.46
2:J:23:GLY:HA3	2:J:36:ALA:HA	1.97	0.46
3:T:76:THR:O	3:T:78:THR:N	2.49	0.46
2:B:169:LYS:HZ2	2:B:173:ILE:CG1	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:THR:HG21	1:A:306:CYS:CB	2.46	0.45
2:J:28:ASN:HD22	2:J:145:ASP:HA	1.80	0.45
3:X:179:HIS:HA	3:X:224:ALA:HB1	1.98	0.45
1:I:190:GLU:O	1:I:194:LEU:HD13	2.17	0.45
1:C:218:ALA:HB3	1:C:220:ARG:NH1	2.31	0.45
3:X:3:GLN:H	3:X:25:SER:HB3	1.80	0.45
1:I:200:THR:HG21	1:I:249:GLY:HA3	1.97	0.45
3:T:93:VAL:CG1	3:T:119:LEU:HD12	2.46	0.45
3:S:179:HIS:NE2	3:S:224:ALA:HB2	2.31	0.45
2:F:98:LEU:CD2	2:F:102:MET:CE	2.93	0.45
3:S:93:VAL:HG13	3:S:119:LEU:CD1	2.46	0.45
1:A:291:SER:OG	1:A:292:SER:N	2.48	0.45
3:U:175:TRP:HB3	3:U:187:LEU:HD12	1.98	0.45
3:X:225:ASP:OD1	3:X:245:LYS:HE3	2.16	0.45
3:S:43:GLN:CB	3:S:139:ILE:HG21	2.47	0.45
1:A:23:ILE:CG2	2:F:51:LYS:HG3	2.46	0.45
1:C:11:TYR:HB2	1:C:321:LEU:CD1	2.47	0.45
3:X:18:VAL:HG22	3:X:86:LEU:CD2	2.47	0.45
2:J:167:ARG:HA	2:J:170:ARG:HB2	1.98	0.45
2:H:102:MET:SD	2:L:102:MET:HE3	2.56	0.45
3:S:112:ASP:HA	3:S:186:LEU:HB2	1.98	0.45
3:U:216:THR:HG22	3:U:217:GLY:H	1.81	0.45
1:E:238:LYS:HG3	1:E:239:PRO:HD2	1.99	0.45
1:I:100:ASN:ND2	1:I:101:ASP:N	2.55	0.45
2:D:98:LEU:HD21	2:D:102:MET:HE2	1.98	0.45
1:G:297:ASN:ND2	1:G:297:ASN:C	2.68	0.45
1:C:191:GLN:NE2	1:C:250:ASN:HD21	2.05	0.45
2:L:169:LYS:NZ	2:L:173:ILE:HG21	2.32	0.45
3:Z:32:PHE:CD2	3:Z:98:ARG:NH1	2.85	0.45
3:T:51:ILE:HB	3:T:70:ILE:CD1	2.47	0.45
1:I:174:GLU:OE1	1:I:174:GLU:N	2.49	0.45
2:F:45:ILE:HD13	3:X:102:TYR:HB2	1.99	0.45
1:G:8:CYS:SG	2:H:14:TRP:HZ2	2.39	0.45
2:D:70:PHE:CE2	2:D:77:ILE:HG13	2.52	0.45
3:S:43:GLN:HG2	3:S:139:ILE:CG2	2.42	0.45
1:C:213:LEU:CD1	1:C:233:PHE:CE1	2.98	0.45
1:I:6:GLN:HG2	2:J:27:SER:HB3	1.99	0.45
1:K:300:PRO:HG2	1:K:301:LEU:HD13	1.98	0.45
1:K:102:TYR:CZ	1:K:106:LYS:HD2	2.52	0.45
3:S:10:GLU:O	3:S:120:VAL:HA	2.17	0.45
3:Z:47:TRP:CG	3:Z:238:VAL:HB	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:77:ARG:NH2	3:T:77:ARG:HB3	2.32	0.45
1:G:289:ILE:HD11	1:G:298:ILE:HD12	1.97	0.45
1:C:239:PRO:O	1:C:240:ASN:CB	2.65	0.45
2:D:172:GLU:C	2:D:174:SER:H	2.20	0.45
1:I:186:ASN:HD21	1:I:227:SER:HB3	1.81	0.45
1:E:6:GLN:HE21	2:F:139:GLU:HB2	1.82	0.45
1:C:302:THR:CG2	1:C:303:ILE:N	2.79	0.44
1:A:180:TRP:HZ3	1:A:235:THR:HG22	1.82	0.44
2:D:61:THR:HG21	1:E:311:LYS:HE2	1.98	0.44
1:A:171:THR:HB	1:G:118:ILE:HG22	1.99	0.44
1:K:10:GLY:HA2	2:L:10:ILE:HD13	1.99	0.44
1:E:204:VAL:HG22	1:E:211:GLN:HB3	1.99	0.44
1:C:102:TYR:CE2	1:C:106:LYS:HD2	2.53	0.44
2:J:41:THR:CG2	3:S:102:TYR:CZ	3.00	0.44
1:G:321:LEU:HD21	2:H:111:HIS:HB3	1.98	0.44
2:H:164:GLU:HA	2:H:167:ARG:CD	2.47	0.44
3:Z:29:PHE:CD2	3:Z:29:PHE:C	2.88	0.44
1:A:291:SER:OG	1:A:293:MET:N	2.49	0.44
2:F:154:ASN:ND2	2:F:156:THR:HG23	2.32	0.44
1:E:60:SER:HB3	1:E:92:ASP:HA	1.98	0.44
3:T:33:ALA:HA	3:T:53:PRO:HD3	1.98	0.44
2:D:164:GLU:OE2	2:D:164:GLU:N	2.51	0.44
1:E:6:GLN:HB2	2:F:138:PHE:O	2.18	0.44
1:A:201:TYR:HA	1:A:213:LEU:O	2.17	0.44
1:K:13:ALA:HB1	1:K:323:ASN:HD21	1.83	0.44
2:F:71:ASN:C	2:F:71:ASN:OD1	2.56	0.44
2:D:118:LEU:O	2:D:121:LYS:HB3	2.18	0.44
2:H:21:TRP:CZ3	2:H:45:ILE:HG13	2.52	0.44
1:G:111:ARG:O	1:G:264:GLY:N	2.49	0.44
2:B:140:PHE:HB3	2:B:142:HIS:O	2.18	0.44
3:X:6:GLN:NE2	3:X:115:GLY:HA3	2.30	0.44
1:G:8:CYS:SG	2:H:14:TRP:CZ2	3.10	0.44
1:C:237:LEU:HD22	1:C:243:ILE:HB	2.00	0.44
2:D:56:ILE:HD11	3:Z:27:VAL:HG11	2.00	0.44
1:A:7:ILE:CG2	1:A:7:ILE:O	2.66	0.44
1:C:126:TRP:CE3	1:C:166:ARG:NH1	2.82	0.44
3:S:6:GLN:HE22	3:S:95:TYR:HA	1.82	0.44
1:A:180:TRP:CZ2	1:A:204:VAL:HG21	2.53	0.44
1:K:182:ILE:CG2	1:K:231:GLU:HB3	2.46	0.44
1:E:120:ILE:HG22	1:E:168:TYR:CZ	2.52	0.44
1:E:105:LEU:HD13	1:E:234:TRP:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:86:ASP:O	2:J:90:ASP:OD2	2.34	0.44
1:K:176:LEU:HB3	1:K:237:LEU:HB3	2.00	0.44
2:B:133:LEU:HB2	2:B:137:CYS:O	2.18	0.44
1:I:179:LEU:CD2	1:I:234:TRP:HB3	2.48	0.44
2:B:100:VAL:HG12	2:B:101:LEU:N	2.32	0.44
3:X:23:THR:HG23	3:X:78:THR:HB	1.99	0.43
3:X:51:ILE:CB	3:X:70:ILE:HD11	2.44	0.43
2:F:177:ARG:O	2:F:180:VAL:HG23	2.18	0.43
1:G:204:VAL:HG21	1:G:209:LEU:HD21	1.98	0.43
1:C:238:LYS:HG3	1:C:239:PRO:HD2	2.00	0.43
1:I:218:ALA:HB3	1:I:220:ARG:NH1	2.32	0.43
3:S:4:LEU:HD22	3:S:22:CYS:SG	2.58	0.43
3:T:64:PHE:O	3:T:65:GLN:C	2.56	0.43
1:I:240:ASN:OD1	1:I:240:ASN:N	2.50	0.43
3:T:68:VAL:HG12	3:T:83:LEU:HG	1.99	0.43
2:F:133:LEU:HD12	2:F:133:LEU:HA	1.81	0.43
3:T:18:VAL:HG12	3:T:86:LEU:HD11	1.99	0.43
2:L:94:TYR:HD2	2:L:95:ASN:HD22	1.66	0.43
3:Z:97:ALA:HB1	3:Z:111:PHE:HB3	2.00	0.43
2:J:70:PHE:CD1	2:J:78:GLU:HA	2.53	0.43
1:I:56:LEU:HA	1:I:74:PHE:CZ	2.53	0.43
3:Z:19:LYS:HG2	3:Z:82:ASP:HB3	2.01	0.43
3:S:43:GLN:HB3	3:S:139:ILE:HG21	2.00	0.43
3:U:18:VAL:CG2	3:U:83:LEU:HD23	2.48	0.43
2:B:163:SER:O	2:B:167:ARG:HG3	2.18	0.43
2:B:30:GLN:NE2	2:B:145:ASP:HB2	2.34	0.43
1:E:297:ASN:C	1:E:297:ASN:ND2	2.72	0.43
3:Z:39:GLN:OE1	3:Z:178:GLN:OE1	2.35	0.43
1:K:20:VAL:CG2	1:K:30:VAL:HG11	2.48	0.43
2:F:126:LEU:HD21	2:F:152:VAL:HG22	2.00	0.43
2:D:26:HIS:HB3	2:D:149:MET:HE2	2.00	0.43
1:E:168:TYR:O	1:E:242:ALA:HA	2.17	0.43
3:X:32:PHE:N	3:X:32:PHE:CD1	2.86	0.43
2:D:99:LEU:HD12	2:D:103:GLU:HG2	2.01	0.43
1:A:323:ASN:ND2	1:A:323:ASN:O	2.52	0.43
3:T:170:ASN:N	3:T:170:ASN:HD22	2.15	0.43
2:L:172:GLU:OE2	2:L:173:ILE:N	2.51	0.43
1:I:9:ILE:HG23	2:J:118:LEU:HD23	2.00	0.43
2:F:30:GLN:HE21	2:F:145:ASP:HB2	1.83	0.43
1:C:313:ASN:C	1:C:313:ASN:ND2	2.72	0.43
3:U:93:VAL:HG22	3:U:119:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:75:ILE:HG13	1:I:76:ASN:N	2.34	0.43
2:D:142:HIS:CE1	2:D:157:TYR:OH	2.71	0.43
1:G:56:LEU:HA	1:G:74:PHE:CZ	2.53	0.43
2:D:124:LEU:HD13	2:F:134:GLY:HA2	2.00	0.43
2:D:28:ASN:HD22	2:D:145:ASP:HA	1.83	0.43
2:D:179:LEU:N	2:D:179:LEU:CD1	2.78	0.43
2:D:66:VAL:HG22	2:F:83:LYS:NZ	2.34	0.43
3:X:43:GLN:OE1	3:X:139:ILE:HG21	2.18	0.43
1:A:106:LYS:HB3	1:A:268:ILE:HD12	2.00	0.43
1:K:70:MET:CE	1:K:91:ASN:HD21	2.32	0.43
2:D:68:ARG:NE	2:F:79:ASN:HD22	2.17	0.43
1:A:117:LYS:NZ	1:A:150:ASN:HD21	2.17	0.43
2:D:59:MET:HE2	2:F:94:TYR:CE1	2.53	0.43
1:I:20:VAL:HG22	1:I:30:VAL:CG1	2.49	0.43
2:D:26:HIS:CB	2:D:149:MET:CE	2.97	0.43
1:E:38:GLU:O	1:E:296:HIS:HA	2.18	0.43
1:I:197:ASN:N	1:I:197:ASN:OD1	2.51	0.43
3:T:249:LEU:HD23	3:T:249:LEU:N	2.33	0.43
1:I:64:TRP:HZ2	1:I:77:VAL:HG21	1.83	0.43
1:I:134:GLY:HA3	1:I:153:TRP:HB3	2.00	0.43
2:D:72:ASN:ND2	2:D:72:ASN:O	2.52	0.43
1:A:289:ILE:HG22	1:A:290:ASN:N	2.34	0.43
3:S:36:TRP:CE2	3:S:81:MET:HB2	2.54	0.43
3:Y:7:SER:HB2	3:Y:20:VAL:HG23	2.00	0.43
2:D:62:GLN:HG2	2:D:92:TRP:CD2	2.54	0.43
2:F:142:HIS:CD2	2:F:162:TYR:CD1	3.07	0.43
2:F:5:ALA:HB1	2:F:115:VAL:CG1	2.48	0.43
3:X:11:VAL:HG22	3:X:121:THR:HB	1.99	0.43
1:G:97:GLY:HA3	1:G:230:MET:O	2.19	0.43
2:H:80:LEU:HD21	2:L:80:LEU:CD2	2.49	0.43
3:Z:36:TRP:CD2	3:Z:81:MET:HB2	2.54	0.43
1:E:180:TRP:CZ2	1:E:204:VAL:HG21	2.54	0.43
2:D:124:LEU:N	2:D:124:LEU:HD23	2.34	0.43
1:C:299:HIS:HA	1:C:300:PRO:HD3	1.83	0.43
3:U:91:THR:CG2	3:U:121:THR:HG23	2.49	0.43
2:F:98:LEU:CD2	2:F:102:MET:HE2	2.49	0.42
1:E:11:TYR:CZ	2:F:6:ILE:HG23	2.54	0.42
1:K:285:PRO:HD3	1:K:301:LEU:O	2.19	0.42
1:G:10:GLY:HA3	2:H:14:TRP:CZ2	2.54	0.42
1:G:7:ILE:HD12	2:H:149:MET:CE	2.49	0.42
1:C:20:VAL:HG21	1:C:318:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:118:LEU:O	2:H:122:VAL:HG23	2.19	0.42
2:H:28:ASN:ND2	2:H:145:ASP:HA	2.33	0.42
2:D:94:TYR:HD2	2:D:95:ASN:HD22	1.67	0.42
2:L:125:GLN:HE22	2:L:155:GLY:C	2.22	0.42
2:H:80:LEU:HD23	2:J:80:LEU:HD21	1.98	0.42
1:C:17:THR:O	1:C:17:THR:CG2	2.67	0.42
3:T:143:LEU:HD23	3:T:163:GLY:HA3	2.00	0.42
2:H:167:ARG:HA	2:H:170:ARG:HB2	2.02	0.42
2:F:71:ASN:OD1	2:F:72:ASN:N	2.52	0.42
3:Z:47:TRP:CD2	3:Z:238:VAL:HB	2.54	0.42
2:D:68:ARG:CZ	2:F:79:ASN:HD22	2.32	0.42
1:C:310:VAL:C	1:C:312:SER:H	2.23	0.42
3:X:57:THR:HA	3:X:58:PRO:HD3	1.85	0.42
3:U:244:THR:O	3:U:244:THR:HG23	2.18	0.42
2:F:45:ILE:HD13	3:X:102:TYR:CB	2.49	0.42
3:Z:177:GLN:HB2	3:Z:187:LEU:HD11	2.01	0.42
1:I:204:VAL:HG12	1:I:245:PHE:CD2	2.55	0.42
1:K:146:SER:OG	1:K:147:PHE:N	2.51	0.42
2:H:163:SER:O	2:H:167:ARG:HG3	2.19	0.42
3:U:37:VAL:HG11	3:U:45:LEU:HD12	2.01	0.42
2:J:42:GLN:HE22	3:S:102:TYR:N	2.18	0.42
1:G:200:THR:HA	1:G:248:ASN:OD1	2.19	0.42
2:B:177:ARG:C	2:B:179:LEU:H	2.22	0.42
1:I:108:LEU:CD1	1:I:236:ILE:HD11	2.41	0.42
1:E:309:TYR:HE2	2:F:89:LEU:HD13	1.84	0.42
1:G:323:ASN:HD22	1:G:325:PRO:HD3	1.83	0.42
1:A:147:PHE:CZ	1:A:148:PHE:HD1	2.38	0.42
1:I:120:ILE:HD13	1:I:257:ALA:HB2	2.02	0.42
2:H:73:LEU:HD22	1:K:101:ASP:OD2	2.19	0.42
3:X:203:SER:O	3:X:213:LEU:HD12	2.18	0.42
2:J:169:LYS:HZ3	2:J:173:ILE:HG21	1.84	0.42
2:H:45:ILE:HD12	3:U:102:TYR:CG	2.54	0.42
1:K:70:MET:HE2	1:K:91:ASN:HD21	1.85	0.42
3:Z:93:VAL:HG22	3:Z:119:LEU:HD13	2.01	0.42
1:C:54:LEU:HD23	1:C:83:ILE:HG12	2.02	0.42
1:A:62:ALA:HB2	1:A:102:TYR:CE1	2.54	0.42
1:A:174:GLU:OE1	1:A:259:LYS:NZ	2.52	0.42
3:S:170:ASN:N	3:S:170:ASN:HD22	2.18	0.42
3:Z:156:THR:OG1	3:Z:216:THR:HG22	2.20	0.42
3:X:64:PHE:O	3:X:65:GLN:C	2.58	0.42
1:I:56:LEU:HD11	1:I:61:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:59:MET:CE	2:F:94:TYR:CE1	3.02	0.42
1:C:105:LEU:HD22	1:C:234:TRP:CD2	2.55	0.42
2:L:5:ALA:HB2	2:L:116:LYS:HB2	2.02	0.42
1:K:51:VAL:HG12	1:K:81:SER:HB2	2.02	0.42
3:X:73:ASP:OD2	3:X:76:THR:N	2.38	0.42
2:D:179:LEU:C	2:D:180:VAL:HG22	2.39	0.42
2:J:93:THR:HG23	2:J:97:GLU:OE1	2.20	0.42
1:E:30:VAL:HG23	1:E:32:HIS:H	1.85	0.42
1:A:96:PRO:HB3	1:A:223:VAL:HG11	2.01	0.42
2:H:51:LYS:HZ3	2:H:103:GLU:HG3	1.84	0.42
2:L:71:ASN:HB2	2:L:74:GLU:OE1	2.19	0.42
2:B:169:LYS:HZ2	2:B:173:ILE:CD1	2.31	0.41
2:F:6:ILE:N	2:F:112:ASP:OD1	2.51	0.41
3:Y:20:VAL:CG2	3:Y:118:THR:HG21	2.48	0.41
3:T:27:VAL:HG13	3:T:77:ARG:NH1	2.35	0.41
2:B:101:LEU:HD23	2:F:58:LYS:HE3	2.02	0.41
1:G:325:PRO:O	1:G:326:GLN:C	2.58	0.41
2:H:101:LEU:HA	2:H:101:LEU:HD12	1.94	0.41
3:S:18:VAL:HG11	3:S:120:VAL:CG1	2.50	0.41
2:J:98:LEU:HD21	2:J:102:MET:HE1	2.02	0.41
1:C:300:PRO:HG3	1:C:309:TYR:CE2	2.55	0.41
1:A:118:ILE:HG21	1:A:259:LYS:HD2	2.02	0.41
3:Z:223:GLU:HB2	3:Z:248:VAL:HG23	2.02	0.41
1:G:267:THR:HG22	1:G:268:ILE:N	2.36	0.41
3:U:110:VAL:CG1	3:U:174:ALA:HB2	2.50	0.41
2:J:97:GLU:O	2:J:101:LEU:HD13	2.20	0.41
1:C:82:TYR:CE1	1:C:269:MET:HE2	2.54	0.41
1:C:187:ASP:HA	1:C:217:ILE:HG21	2.01	0.41
1:I:6:GLN:CG	2:J:27:SER:HB3	2.50	0.41
1:A:323:ASN:HD22	1:A:323:ASN:C	2.22	0.41
3:S:175:TRP:CG	3:S:213:LEU:HD22	2.56	0.41
2:D:89:LEU:HA	2:D:89:LEU:HD23	1.91	0.41
1:A:7:ILE:HB	2:B:149:MET:HE1	2.02	0.41
1:I:9:ILE:HD13	2:J:24:TYR:CD2	2.56	0.41
3:T:187:LEU:CD2	3:T:198:ILE:HD12	2.51	0.41
1:C:180:TRP:CZ3	1:C:235:THR:HG22	2.52	0.41
1:K:267:THR:HG22	1:K:268:ILE:N	2.35	0.41
1:I:321:LEU:HD23	2:J:111:HIS:ND1	2.34	0.41
2:H:167:ARG:HB3	2:H:170:ARG:CZ	2.50	0.41
1:I:289:ILE:HG22	1:I:291:SER:H	1.85	0.41
1:G:48:LEU:HB3	1:G:81:SER:OG	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:112:ASP:OD1	3:S:113:HIS:N	2.53	0.41
1:G:308:LYS:HZ1	2:H:62:GLN:H	1.69	0.41
1:C:283:GLN:OE1	1:C:288:ALA:HB2	2.19	0.41
1:A:10:GLY:HA2	2:B:10:ILE:HG21	2.02	0.41
3:Z:5:VAL:O	3:Z:22:CYS:HA	2.21	0.41
2:B:169:LYS:O	2:B:172:GLU:HG3	2.20	0.41
1:E:31:THR:HG23	1:E:321:LEU:O	2.21	0.41
2:H:49:THR:HG21	3:U:32:PHE:HZ	1.84	0.41
1:A:259:LYS:NZ	1:G:119:GLN:HE22	2.18	0.41
2:H:123:ARG:O	2:H:126:LEU:O	2.37	0.41
4:C:501:NAG:H61	4:C:502:NAG:O7	2.21	0.41
3:Y:32:PHE:CD2	3:Y:98:ARG:HD2	2.55	0.41
3:X:26:GLU:OE2	3:X:98:ARG:NH1	2.54	0.41
2:H:6:ILE:HD12	2:H:112:ASP:HA	2.02	0.41
3:X:68:VAL:HG12	3:X:69:THR:N	2.36	0.41
1:I:100:ASN:C	1:I:100:ASN:ND2	2.72	0.41
2:F:169:LYS:HZ2	2:F:173:ILE:HG22	1.86	0.41
1:I:121:ILE:HG22	1:I:121:ILE:O	2.21	0.41
3:Y:151:LYS:O	3:Y:248:VAL:HA	2.21	0.41
3:Y:162:THR:HG23	3:Y:210:THR:CB	2.37	0.41
3:X:60:TYR:CE2	3:X:70:ILE:HG23	2.49	0.41
3:X:153:LEU:HD13	3:X:248:VAL:CG1	2.50	0.41
1:G:178:VAL:O	1:G:179:LEU:HD23	2.20	0.41
1:I:309:TYR:CD2	2:J:89:LEU:HD13	2.56	0.41
2:F:75:ARG:O	2:F:78:GLU:HB3	2.21	0.41
3:X:225:ASP:OD1	3:X:245:LYS:CE	2.69	0.41
2:J:45:ILE:HD12	3:S:102:TYR:HB2	2.03	0.41
2:D:59:MET:HE3	2:F:94:TYR:HE1	1.86	0.41
1:E:121:ILE:HD12	1:E:254:PRO:HG2	2.02	0.41
3:T:40:ALA:HB3	3:T:43:GLN:OE1	2.21	0.41
3:S:209:ASN:HD22	3:S:209:ASN:N	2.18	0.41
2:D:5:ALA:O	2:D:8:GLY:N	2.53	0.41
1:E:118:ILE:HG21	1:E:259:LYS:HD2	2.02	0.41
1:C:121:ILE:HG21	1:C:126:TRP:CZ2	2.56	0.41
3:T:20:VAL:HG22	3:T:21:SER:N	2.36	0.41
3:X:145:GLN:HA	3:X:146:PRO:HD2	1.95	0.41
1:G:195:TYR:O	1:G:196:GLN:CB	2.69	0.41
3:X:16:SER:O	3:X:86:LEU:HG	2.21	0.41
2:B:133:LEU:HD12	2:B:133:LEU:HA	1.95	0.41
1:K:221:SER:O	1:K:229:ARG:NH2	2.53	0.41
1:E:130:GLU:HG2	1:E:133:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:172:ASN:H	1:I:172:ASN:HD22	1.64	0.40
2:B:72:ASN:ND2	2:B:72:ASN:O	2.55	0.40
2:B:98:LEU:CB	2:F:58:LYS:HZ3	2.34	0.40
3:T:32:PHE:CB	3:T:98:ARG:HD2	2.51	0.40
3:X:67:ARG:NH1	3:X:84:ARG:O	2.54	0.40
2:F:113:SER:OG	2:F:117:ASN:ND2	2.54	0.40
1:E:314:ARG:CG	1:E:314:ARG:HH11	2.34	0.40
2:F:145:ASP:OD1	2:F:147:GLU:N	2.52	0.40
3:T:162:THR:CG2	3:T:163:GLY:N	2.85	0.40
3:T:47:TRP:CD2	3:T:238:VAL:CG2	3.04	0.40
3:S:219:GLN:O	3:S:248:VAL:HG21	2.21	0.40
1:C:105:LEU:HD22	1:C:234:TRP:CG	2.56	0.40
2:B:2:LEU:O	2:F:113:SER:OG	2.39	0.40
1:K:168:TYR:O	1:K:242:ALA:HA	2.21	0.40
1:I:53:PRO:HB3	1:I:82:TYR:CE2	2.57	0.40
1:C:296:HIS:HD2	1:C:307:PRO:HB2	1.86	0.40
2:D:38:LYS:O	2:D:39:GLU:C	2.59	0.40
3:X:2:VAL:HG21	3:X:113:HIS:CG	2.56	0.40
2:D:30:GLN:HE21	2:D:145:ASP:HB2	1.87	0.40
1:C:203:SER:HB3	1:C:212:ARG:HG3	2.04	0.40
1:C:13:ALA:HB1	2:D:15:GLN:NE2	2.35	0.40
1:K:10:GLY:HA3	2:L:14:TRP:CZ2	2.56	0.40
2:B:98:LEU:HB2	2:F:58:LYS:HZ3	1.87	0.40
1:A:117:LYS:HG3	1:A:256:TYR:HB3	2.03	0.40
1:E:68:ASN:OD1	1:E:70:MET:HG2	2.21	0.40
3:Z:157:ALA:HB2	3:Z:218:LEU:HD11	2.02	0.40
1:E:152:VAL:CG1	1:E:253:ALA:HB3	2.51	0.40
1:K:202:ILE:HG22	1:K:203:SER:N	2.36	0.40
3:S:12:LYS:CD	3:S:18:VAL:HG12	2.51	0.40
3:X:39:GLN:C	3:X:92:ALA:HB1	2.42	0.40
4:E:502:NAG:H83	4:E:502:NAG:O3	2.22	0.40
2:L:152:VAL:HG22	2:L:157:TYR:CD1	2.56	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	321/338 (95%)	278 (87%)	37 (12%)	6 (2%)	10	50
1	C	321/338 (95%)	282 (88%)	36 (11%)	3 (1%)	21	67
1	E	321/338 (95%)	271 (84%)	47 (15%)	3 (1%)	21	67
1	G	321/338 (95%)	280 (87%)	37 (12%)	4 (1%)	16	60
1	I	321/338 (95%)	282 (88%)	37 (12%)	2 (1%)	30	75
1	K	321/338 (95%)	287 (89%)	30 (9%)	4 (1%)	16	60
2	B	178/182 (98%)	159 (89%)	16 (9%)	3 (2%)	11	52
2	D	178/182 (98%)	155 (87%)	20 (11%)	3 (2%)	11	52
2	F	178/182 (98%)	153 (86%)	24 (14%)	1 (1%)	30	75
2	H	172/182 (94%)	150 (87%)	19 (11%)	3 (2%)	11	52
2	J	172/182 (94%)	146 (85%)	23 (13%)	3 (2%)	11	52
2	L	172/182 (94%)	158 (92%)	13 (8%)	1 (1%)	30	75
3	S	229/280 (82%)	206 (90%)	21 (9%)	2 (1%)	21	67
3	T	230/280 (82%)	204 (89%)	25 (11%)	1 (0%)	39	80
3	U	230/280 (82%)	204 (89%)	25 (11%)	1 (0%)	39	80
3	X	231/280 (82%)	204 (88%)	25 (11%)	2 (1%)	21	67
3	Y	231/280 (82%)	203 (88%)	25 (11%)	3 (1%)	15	59
3	Z	232/280 (83%)	201 (87%)	29 (12%)	2 (1%)	21	67
All	All	4359/4800 (91%)	3823 (88%)	489 (11%)	47 (1%)	17	62

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	196	GLN
1	E	73	GLU
3	Y	43	GLN
2	B	128	ASP
2	B	178	SER
2	D	128	ASP
1	G	196	GLN
1	G	218	ALA
2	H	143	LYS

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Mol	Chain	Res	Type
2	J	127	ARG
2	J	132	GLU
2	B	32	SER
2	J	29	GLU
3	Z	65	GLN
3	S	109	CYS
3	T	196	SER
1	A	158	ASN
1	C	240	ASN
1	E	15	ASN
1	E	277	ASN
2	F	87	GLY
1	I	57	ARG
1	I	261	VAL
1	K	170	ASN
3	Y	123	SER
1	A	73	GLU
1	A	148	PHE
1	C	198	PRO
2	D	178	SER
1	G	15	ASN
2	H	32	SER
1	K	158	ASN
1	K	198	PRO
2	L	127	ARG
3	Z	180	GLN
1	A	34	GLN
1	K	261	VAL
3	U	217	GLY
1	G	261	VAL
1	A	261	VAL
2	D	173	ILE
2	H	160	PRO
3	X	58	PRO
3	Y	41	PRO
3	S	41	PRO
1	C	75	ILE
3	X	37	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	291/304 (96%)	264 (91%)	27 (9%)	11	41
1	C	291/304 (96%)	263 (90%)	28 (10%)	10	39
1	E	291/304 (96%)	264 (91%)	27 (9%)	11	41
1	G	291/304 (96%)	266 (91%)	25 (9%)	13	46
1	I	291/304 (96%)	261 (90%)	30 (10%)	9	36
1	K	291/304 (96%)	265 (91%)	26 (9%)	12	44
2	B	154/156 (99%)	126 (82%)	28 (18%)	2	10
2	D	154/156 (99%)	126 (82%)	28 (18%)	2	10
2	F	154/156 (99%)	133 (86%)	21 (14%)	5	22
2	H	149/156 (96%)	134 (90%)	15 (10%)	9	36
2	J	149/156 (96%)	127 (85%)	22 (15%)	4	18
2	L	149/156 (96%)	127 (85%)	22 (15%)	4	18
3	S	194/220 (88%)	185 (95%)	9 (5%)	33	74
3	T	195/220 (89%)	180 (92%)	15 (8%)	16	54
3	U	195/220 (89%)	173 (89%)	22 (11%)	7	31
3	X	196/220 (89%)	178 (91%)	18 (9%)	11	41
3	Y	196/220 (89%)	166 (85%)	30 (15%)	3	17
3	Z	196/220 (89%)	176 (90%)	20 (10%)	9	36
All	All	3827/4080 (94%)	3414 (89%)	413 (11%)	8	33

All (413) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	17	THR
1	A	25	GLU
1	A	73	GLU
1	A	86	LYS
1	A	88	ASN

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Mol	Chain	Res	Type
1	A	99	PHE
1	A	135	VAL
1	A	149	ARG
1	A	178	VAL
1	A	179	LEU
1	A	199	THR
1	A	203	SER
1	A	213	LEU
1	A	226	GLN
1	A	244	ASN
1	A	263	LYS
1	A	267	THR
1	A	274	GLU
1	A	278	CYS
1	A	292	SER
1	A	297	ASN
1	A	312	SER
1	A	314	ARG
1	A	322	ARG
1	A	323	ASN
1	A	324	SER
2	B	18	VAL
2	B	19	ASP
2	B	22	TYR
2	B	26	HIS
2	B	29	GLU
2	B	41	THR
2	B	52	VAL
2	B	58	LYS
2	B	72	ASN
2	B	76	ARG
2	B	77	ILE
2	B	82	LYS
2	B	100	VAL
2	B	101	LEU
2	B	103	GLU
2	B	113	SER
2	B	118	LEU
2	B	121	LYS
2	B	127	ARG
2	B	133	LEU
2	B	147	GLU

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Mol	Chain	Res	Type
2	B	151	SER
2	B	154	ASN
2	B	164	GLU
2	B	167	ARG
2	B	169	LYS
2	B	172	GLU
2	B	180	VAL
1	C	8	CYS
1	C	16	SER
1	C	23	ILE
1	C	35	ASP
1	C	40	LYS
1	C	58	ASP
1	C	73	GLU
1	C	79	GLU
1	C	99	PHE
1	C	113	ASN
1	C	117	LYS
1	C	146	SER
1	C	152	VAL
1	C	160	THR
1	C	178	VAL
1	C	199	THR
1	C	226	GLN
1	C	244	ASN
1	C	250	ASN
1	C	260	ILE
1	C	261	VAL
1	C	266	SER
1	C	267	THR
1	C	278	CYS
1	C	290	ASN
1	C	313	ASN
1	C	321	LEU
1	C	326	GLN
2	D	18	VAL
2	D	19	ASP
2	D	22	TYR
2	D	32	SER
2	D	39	GLU
2	D	54	SER
2	D	58	LYS

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Mol	Chain	Res	Type
2	D	61	THR
2	D	62	GLN
2	D	68	ARG
2	D	72	ASN
2	D	76	ARG
2	D	95	ASN
2	D	113	SER
2	D	118	LEU
2	D	124	LEU
2	D	128	ASP
2	D	148	CYS
2	D	150	GLU
2	D	153	ARG
2	D	154	ASN
2	D	164	GLU
2	D	167	ARG
2	D	168	LEU
2	D	169	LYS
2	D	172	GLU
2	D	179	LEU
2	D	180	VAL
1	E	4	GLU
1	E	6	GLN
1	E	8	CYS
1	E	17	THR
1	E	22	THR
1	E	23	ILE
1	E	70	MET
1	E	75	ILE
1	E	86	LYS
1	E	99	PHE
1	E	101	ASP
1	E	135	VAL
1	E	149	ARG
1	E	179	LEU
1	E	199	THR
1	E	204	VAL
1	E	213	LEU
1	E	223	VAL
1	E	266	SER
1	E	267	THR
1	E	274	GLU

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Mol	Chain	Res	Type
1	E	292	SER
1	E	297	ASN
1	E	302	THR
1	E	312	SER
1	E	314	ARG
1	E	317	LEU
2	F	19	ASP
2	F	38	LYS
2	F	40	SER
2	F	62	GLN
2	F	72	ASN
2	F	76	ARG
2	F	93	THR
2	F	98	LEU
2	F	101	LEU
2	F	116	LYS
2	F	118	LEU
2	F	126	LEU
2	F	133	LEU
2	F	139	GLU
2	F	150	GLU
2	F	153	ARG
2	F	154	ASN
2	F	164	GLU
2	F	167	ARG
2	F	169	LYS
2	F	172	GLU
1	G	17	THR
1	G	23	ILE
1	G	47	ASP
1	G	86	LYS
1	G	99	PHE
1	G	133	LEU
1	G	136	SER
1	G	152	VAL
1	G	159	SER
1	G	160	THR
1	G	165	LYS
1	G	203	SER
1	G	220	ARG
1	G	227	SER
1	G	244	ASN

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Mol	Chain	Res	Type
1	G	262	LYS
1	G	265	ASP
1	G	272	GLU
1	G	274	GLU
1	G	297	ASN
1	G	303	ILE
1	G	314	ARG
1	G	319	THR
1	G	323	ASN
1	G	326	GLN
2	H	38	LYS
2	H	58	LYS
2	H	59	MET
2	H	69	GLU
2	H	73	LEU
2	H	75	ARG
2	H	80	LEU
2	H	98	LEU
2	H	100	VAL
2	H	101	LEU
2	H	148	CYS
2	H	153	ARG
2	H	164	GLU
2	H	167	ARG
2	H	169	LYS
1	I	8	CYS
1	I	35	ASP
1	I	73	GLU
1	I	76	ASN
1	I	100	ASN
1	I	128	SER
1	I	146	SER
1	I	149	ARG
1	I	161	TYR
1	I	165	LYS
1	I	172	ASN
1	I	178	VAL
1	I	197	ASN
1	I	199	THR
1	I	203	SER
1	I	219	THR
1	I	222	LYS

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Mol	Chain	Res	Type
1	I	226	GLN
1	I	227	SER
1	I	240	ASN
1	I	273	LEU
1	I	274	GLU
1	I	291	SER
1	I	297	ASN
1	I	302	THR
1	I	305	GLU
1	I	311	LYS
1	I	314	ARG
1	I	321	LEU
1	I	323	ASN
2	J	19	ASP
2	J	29	GLU
2	J	38	LYS
2	J	45	ILE
2	J	53	ASN
2	J	57	ASP
2	J	58	LYS
2	J	62	GLN
2	J	72	ASN
2	J	76	ARG
2	J	81	ASN
2	J	84	MET
2	J	93	THR
2	J	98	LEU
2	J	128	ASP
2	J	137	CYS
2	J	139	GLU
2	J	148	CYS
2	J	154	ASN
2	J	164	GLU
2	J	167	ARG
2	J	169	LYS
1	K	8	CYS
1	K	22	THR
1	K	23	ILE
1	K	34	GLN
1	K	35	ASP
1	K	77	VAL
1	K	79	GLU

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Mol	Chain	Res	Type
1	K	136	SER
1	K	152	VAL
1	K	154	LEU
1	K	165	LYS
1	K	178	VAL
1	K	179	LEU
1	K	223	VAL
1	K	224	ASN
1	K	226	GLN
1	K	230	MET
1	K	265	ASP
1	K	272	GLU
1	K	274	GLU
1	K	278	CYS
1	K	297	ASN
1	K	301	LEU
1	K	302	THR
1	K	314	ARG
1	K	323	ASN
2	L	19	ASP
2	L	22	TYR
2	L	27	SER
2	L	29	GLU
2	L	38	LYS
2	L	41	THR
2	L	54	SER
2	L	57	ASP
2	L	58	LYS
2	L	72	ASN
2	L	76	ARG
2	L	93	THR
2	L	98	LEU
2	L	100	VAL
2	L	103	GLU
2	L	137	CYS
2	L	148	CYS
2	L	153	ARG
2	L	164	GLU
2	L	167	ARG
2	L	169	LYS
2	L	172	GLU
3	X	5	VAL

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Mol	Chain	Res	Type
3	X	7	SER
3	X	18	VAL
3	X	28	THR
3	X	31	SER
3	X	48	LEU
3	X	57	THR
3	X	70	ILE
3	X	78	THR
3	X	87	ARG
3	X	93	VAL
3	X	96	CYS
3	X	98	ARG
3	X	150	SER
3	X	192	ASN
3	X	201	ARG
3	X	207	SER
3	X	245	LYS
3	Y	1	GLN
3	Y	4	LEU
3	Y	22	CYS
3	Y	25	SER
3	Y	29	PHE
3	Y	57	THR
3	Y	70	ILE
3	Y	77	ARG
3	Y	83	LEU
3	Y	93	VAL
3	Y	103	ILE
3	Y	108	THR
3	Y	145	GLN
3	Y	154	ARG
3	Y	162	THR
3	Y	180	GLN
3	Y	190	ARG
3	Y	193	ASP
3	Y	194	ARG
3	Y	205	SER
3	Y	207	SER
3	Y	213	LEU
3	Y	214	THR
3	Y	216	THR
3	Y	223	GLU

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Mol	Chain	Res	Type
3	Y	233	SER
3	Y	234	SER
3	Y	244	THR
3	Y	245	LYS
3	Y	249	LEU
3	Z	18	VAL
3	Z	19	LYS
3	Z	24	SER
3	Z	25	SER
3	Z	29	PHE
3	Z	30	SER
3	Z	48	LEU
3	Z	62	GLN
3	Z	70	ILE
3	Z	82	ASP
3	Z	84	ARG
3	Z	143	LEU
3	Z	188	SER
3	Z	200	GLU
3	Z	205	SER
3	Z	215	ILE
3	Z	230	THR
3	Z	244	THR
3	Z	245	LYS
3	Z	248	VAL
3	S	5	VAL
3	S	31	SER
3	S	57	THR
3	S	70	ILE
3	S	81	MET
3	S	87	ARG
3	S	192	ASN
3	S	201	ARG
3	S	238	VAL
3	T	1	GLN
3	T	22	CYS
3	T	24	SER
3	T	59	ASN
3	T	83	LEU
3	T	98	ARG
3	T	103	ILE
3	T	108	THR

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Mol	Chain	Res	Type
3	T	145	GLN
3	T	171	GLN
3	T	194	ARG
3	T	199	SER
3	T	221	GLU
3	T	245	LYS
3	T	249	LEU
3	U	21	SER
3	U	23	THR
3	U	25	SER
3	U	27	VAL
3	U	29	PHE
3	U	31	SER
3	U	34	ILE
3	U	35	SER
3	U	62	GLN
3	U	67	ARG
3	U	70	ILE
3	U	84	ARG
3	U	96	CYS
3	U	108	THR
3	U	143	LEU
3	U	165	SER
3	U	191	ASN
3	U	200	GLU
3	U	203	SER
3	U	216	THR
3	U	230	THR
3	U	245	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	88	ASN
1	A	150	ASN
1	A	226	GLN
1	A	297	ASN
1	A	323	ASN
2	B	15	GLN
2	B	30	GLN
2	B	42	GLN

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Mol	Chain	Res	Type
2	B	72	ASN
2	B	79	ASN
2	B	95	ASN
2	B	114	ASN
2	B	129	ASN
2	B	142	HIS
2	B	146	ASN
2	B	154	ASN
1	C	19	GLN
1	C	91	ASN
1	C	113	ASN
1	C	142	GLN
1	C	186	ASN
1	C	191	GLN
1	C	226	GLN
1	C	240	ASN
1	C	299	HIS
1	C	313	ASN
2	D	15	GLN
2	D	30	GLN
2	D	42	GLN
2	D	53	ASN
2	D	62	GLN
2	D	72	ASN
2	D	79	ASN
2	D	95	ASN
2	D	125	GLN
2	D	142	HIS
2	D	146	ASN
1	E	6	GLN
1	E	19	GLN
1	E	119	GLN
1	E	150	ASN
1	E	226	GLN
1	E	297	ASN
2	F	30	GLN
2	F	42	GLN
2	F	72	ASN
2	F	79	ASN
2	F	117	ASN
2	F	125	GLN
2	F	142	HIS

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Mol	Chain	Res	Type
2	F	146	ASN
2	F	154	ASN
1	G	91	ASN
1	G	113	ASN
1	G	114	HIS
1	G	119	GLN
1	G	224	ASN
1	G	226	GLN
1	G	244	ASN
1	G	297	ASN
1	G	323	ASN
2	H	53	ASN
2	H	60	ASN
2	H	72	ASN
2	H	79	ASN
2	H	95	ASN
2	H	125	GLN
2	H	129	ASN
2	H	142	HIS
2	H	146	ASN
1	I	6	GLN
1	I	91	ASN
1	I	100	ASN
1	I	113	ASN
1	I	172	ASN
1	I	226	GLN
1	I	277	ASN
1	I	297	ASN
2	J	26	HIS
2	J	30	GLN
2	J	42	GLN
2	J	72	ASN
2	J	79	ASN
2	J	95	ASN
2	J	125	GLN
2	J	142	HIS
2	J	146	ASN
1	K	6	GLN
1	K	34	GLN
1	K	91	ASN
1	K	100	ASN
1	K	224	ASN

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Mol	Chain	Res	Type
1	K	226	GLN
1	K	297	ASN
1	K	299	HIS
1	K	323	ASN
2	L	28	ASN
2	L	42	GLN
2	L	71	ASN
2	L	95	ASN
2	L	125	GLN
2	L	142	HIS
2	L	146	ASN
3	X	6	GLN
3	X	170	ASN
3	Y	1	GLN
3	Y	171	GLN
3	Y	209	ASN
3	Z	43	GLN
3	Z	62	GLN
3	Z	170	ASN
3	Z	178	GLN
3	Z	191	ASN
3	S	6	GLN
3	S	170	ASN
3	T	1	GLN
3	T	39	GLN
3	T	62	GLN
3	T	170	ASN
3	T	171	GLN
3	U	140	GLN
3	U	171	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

30 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	501	1,4	14,14,15	0.57	0	15,19,21	0.75	0
4	NAG	A	502	4	14,14,15	0.53	0	15,19,21	1.50	1 (6%)
5	NAG	A	601	1,5	14,14,15	0.67	0	15,19,21	1.23	1 (6%)
5	NAG	A	602	5	14,14,15	0.39	0	15,19,21	0.75	0
5	BMA	A	603	5	11,11,12	0.52	0	14,15,17	1.39	1 (7%)
4	NAG	C	501	1,4	14,14,15	0.50	0	15,19,21	1.51	1 (6%)
4	NAG	C	502	4	14,14,15	0.67	1 (7%)	15,19,21	1.15	1 (6%)
5	NAG	C	601	1,5	14,14,15	0.52	0	15,19,21	0.62	0
5	NAG	C	602	5	14,14,15	0.48	0	15,19,21	0.88	0
5	BMA	C	603	5	11,11,12	0.35	0	14,15,17	0.98	1 (7%)
4	NAG	E	501	1,4	14,14,15	0.55	0	15,19,21	1.65	4 (26%)
4	NAG	E	502	4	14,14,15	0.78	0	15,19,21	1.26	2 (13%)
5	NAG	E	601	1,5	14,14,15	0.56	0	15,19,21	0.69	0
5	NAG	E	602	5	14,14,15	0.43	0	15,19,21	0.78	0
5	BMA	E	603	5	11,11,12	0.48	0	14,15,17	0.93	1 (7%)
4	NAG	G	501	1,4	14,14,15	0.59	0	15,19,21	1.10	2 (13%)
4	NAG	G	502	4	14,14,15	0.66	0	15,19,21	1.24	1 (6%)
5	NAG	G	601	1,5	14,14,15	0.67	0	15,19,21	1.04	1 (6%)
5	NAG	G	602	5	14,14,15	0.64	0	15,19,21	0.99	0
5	BMA	G	603	5	11,11,12	0.70	0	14,15,17	1.69	3 (21%)
4	NAG	I	501	1,4	14,14,15	0.47	0	15,19,21	1.80	3 (20%)
4	NAG	I	502	4	14,14,15	0.77	0	15,19,21	1.07	0
5	NAG	I	601	1,5	14,14,15	0.58	0	15,19,21	0.96	1 (6%)
5	NAG	I	602	5	14,14,15	0.59	0	15,19,21	1.02	1 (6%)
5	BMA	I	603	5	11,11,12	0.63	0	14,15,17	1.33	1 (7%)
4	NAG	K	501	1,4	14,14,15	0.38	0	15,19,21	1.83	2 (13%)
4	NAG	K	502	4	14,14,15	0.76	1 (7%)	15,19,21	1.47	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	K	601	1,5	14,14,15	0.57	0	15,19,21	0.99	1 (6%)
5	NAG	K	602	5	14,14,15	0.62	0	15,19,21	1.14	1 (6%)
5	BMA	K	603	5	11,11,12	0.54	0	14,15,17	0.86	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	501	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	502	4	-	0/6/23/26	0/1/1/1
5	NAG	A	601	1,5	-	1/6/23/26	0/1/1/1
5	NAG	A	602	5	-	0/6/23/26	0/1/1/1
5	BMA	A	603	5	-	0/2/19/22	0/1/1/1
4	NAG	C	501	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	502	4	-	0/6/23/26	0/1/1/1
5	NAG	C	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	602	5	-	0/6/23/26	0/1/1/1
5	BMA	C	603	5	-	0/2/19/22	0/1/1/1
4	NAG	E	501	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	502	4	-	1/6/23/26	0/1/1/1
5	NAG	E	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	602	5	-	0/6/23/26	0/1/1/1
5	BMA	E	603	5	-	0/2/19/22	0/1/1/1
4	NAG	G	501	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	502	4	-	0/6/23/26	0/1/1/1
5	NAG	G	601	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	G	602	5	-	0/6/23/26	0/1/1/1
5	BMA	G	603	5	-	0/2/19/22	0/1/1/1
4	NAG	I	501	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	502	4	-	0/6/23/26	0/1/1/1
5	NAG	I	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	602	5	-	0/6/23/26	0/1/1/1
5	BMA	I	603	5	-	0/2/19/22	0/1/1/1
4	NAG	K	501	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	502	4	-	0/6/23/26	0/1/1/1
5	NAG	K	601	1,5	-	0/6/23/26	0/1/1/1
5	NAG	K	602	5	-	0/6/23/26	0/1/1/1
5	BMA	K	603	5	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	K	502	NAG	C1-C2	2.08	1.55	1.52
4	C	502	NAG	C1-C2	2.12	1.55	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	501	NAG	C4-C3-C2	-4.24	104.64	111.23
4	I	501	NAG	C4-C3-C2	-3.98	105.04	111.23
4	E	501	NAG	C4-C3-C2	-3.71	105.46	111.23
4	K	501	NAG	C4-C3-C2	-3.43	105.90	111.23
4	I	501	NAG	O4-C4-C3	2.02	114.89	110.34
5	C	603	BMA	C3-C4-C5	2.04	113.75	110.20
5	E	603	BMA	C1-C2-C3	2.05	111.97	109.54
4	E	501	NAG	O3-C3-C4	2.06	114.98	110.34
4	E	502	NAG	C1-O5-C5	2.24	115.08	112.25
5	G	601	NAG	C4-C3-C2	2.24	114.71	111.23
4	G	501	NAG	C3-C2-N2	2.32	116.12	110.56
4	K	502	NAG	C4-C3-C2	2.37	114.91	111.23
4	G	501	NAG	C2-N2-C7	2.58	126.35	123.04
5	K	601	NAG	C1-O5-C5	2.58	115.52	112.25
4	E	501	NAG	O4-C4-C3	2.62	116.24	110.34
5	I	602	NAG	C4-C3-C2	2.65	115.35	111.23
4	E	501	NAG	C1-O5-C5	2.83	115.84	112.25
5	G	603	BMA	C1-O5-C5	2.86	115.88	112.25
5	G	603	BMA	O5-C5-C6	2.91	113.66	107.35
4	E	502	NAG	C4-C3-C2	3.04	115.95	111.23
5	I	601	NAG	C1-O5-C5	3.04	116.11	112.25
5	A	601	NAG	C4-C3-C2	3.11	116.07	111.23
5	K	602	NAG	C1-O5-C5	3.18	116.29	112.25
4	G	502	NAG	C4-C3-C2	3.18	116.18	111.23
4	C	502	NAG	C1-O5-C5	3.30	116.44	112.25
4	K	502	NAG	C1-O5-C5	3.59	116.80	112.25
5	G	603	BMA	C1-C2-C3	3.89	114.15	109.54
5	I	603	BMA	C1-C2-C3	3.96	114.23	109.54
5	A	603	BMA	C1-C2-C3	4.01	114.28	109.54
4	I	501	NAG	C1-O5-C5	4.20	117.57	112.25
4	A	502	NAG	C1-O5-C5	4.66	118.16	112.25
4	K	501	NAG	C1-O5-C5	5.12	118.74	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	601	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	502	NAG	O7-C7-N2-C2
5	A	601	NAG	C8-C7-N2-C2

There are no ring outliers.

7 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	501	NAG	2	0
4	C	502	NAG	2	0
4	E	502	NAG	1	0
5	G	601	NAG	2	0
5	G	602	NAG	2	0
4	K	501	NAG	1	0
4	K	502	NAG	1	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	323/338 (95%)	0.24	4 (1%) 81 69	64, 86, 103, 127	0
1	C	323/338 (95%)	0.07	2 (0%) 90 84	60, 85, 101, 122	0
1	E	323/338 (95%)	0.02	0 100 100	54, 86, 102, 135	0
1	G	323/338 (95%)	0.04	5 (1%) 76 63	66, 86, 101, 106	0
1	I	323/338 (95%)	0.02	5 (1%) 76 63	64, 84, 99, 113	0
1	K	323/338 (95%)	0.21	4 (1%) 81 69	64, 85, 98, 120	0
2	B	180/182 (98%)	0.42	5 (2%) 56 42	62, 82, 125, 138	0
2	D	180/182 (98%)	0.11	0 100 100	62, 82, 111, 141	0
2	F	180/182 (98%)	0.23	4 (2%) 65 50	61, 81, 121, 141	0
2	H	174/182 (95%)	0.50	19 (10%) 7 4	61, 92, 118, 147	0
2	J	174/182 (95%)	0.54	17 (9%) 10 5	65, 89, 118, 130	0
2	L	174/182 (95%)	0.59	20 (11%) 6 4	64, 90, 117, 132	0
3	S	233/280 (83%)	0.27	15 (6%) 23 13	86, 117, 134, 143	0
3	T	234/280 (83%)	0.36	14 (5%) 25 14	82, 113, 136, 147	0
3	U	234/280 (83%)	0.48	24 (10%) 9 5	88, 117, 134, 142	0
3	X	235/280 (83%)	-0.02	0 100 100	45, 64, 87, 94	0
3	Y	235/280 (83%)	0.10	1 (0%) 93 90	42, 61, 84, 100	0
3	Z	236/280 (84%)	0.02	0 100 100	43, 62, 88, 115	0
All	All	4407/4800 (91%)	0.20	139 (3%) 51 36	42, 86, 125, 147	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	6	GLN	8.2
2	B	63	PHE	5.2
2	H	134	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
2	F	63	PHE	4.8
2	H	132	GLU	4.5
2	L	2	LEU	4.4
2	J	171	GLU	4.4
1	K	326	GLN	4.4
3	S	248	VAL	4.4
3	T	48	LEU	4.4
3	U	48	LEU	4.2
1	A	66	LEU	4.1
2	L	3	PHE	4.0
2	J	161	GLN	4.0
3	S	120	VAL	3.9
2	H	131	LYS	3.8
3	T	104	CYS	3.8
2	H	138	PHE	3.7
1	G	7	ILE	3.7
2	L	66	VAL	3.7
1	I	7	ILE	3.7
2	B	62	GLN	3.6
2	H	136	GLY	3.6
2	J	9	PHE	3.6
2	L	138	PHE	3.5
1	K	321	LEU	3.5
2	J	138	PHE	3.5
2	L	1	GLY	3.4
2	L	126	LEU	3.4
2	L	36	ALA	3.4
2	B	7	ALA	3.4
2	H	160	PRO	3.3
3	U	18	VAL	3.3
1	G	8	CYS	3.3
2	H	171	GLU	3.3
2	J	5	ALA	3.3
3	S	249	LEU	3.3
2	J	168	LEU	3.3
3	U	235	LEU	3.3
3	T	213	LEU	3.3
2	F	65	ALA	3.2
1	I	9	ILE	3.2
3	T	111	PHE	3.2
2	B	61	THR	3.2
3	U	248	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
3	T	227	TYR	3.2
2	H	133	LEU	3.1
2	L	9	PHE	3.1
2	J	6	ILE	3.0
3	U	94	TYR	3.0
2	J	19	ASP	3.0
2	H	36	ALA	3.0
2	L	124	LEU	3.0
2	H	137	CYS	3.0
2	J	126	LEU	2.9
2	L	45	ILE	2.9
2	L	41	THR	2.9
3	U	155	GLN	2.9
1	C	151	VAL	2.9
3	T	94	TYR	2.8
2	H	9	PHE	2.8
2	L	7	ALA	2.8
3	S	27	VAL	2.8
3	U	37	VAL	2.8
2	J	142	HIS	2.8
2	H	27	SER	2.8
2	J	18	VAL	2.8
2	J	158	ASP	2.7
3	U	102	TYR	2.7
3	U	236	SER	2.7
2	J	143	LYS	2.7
2	H	153	ARG	2.7
1	K	33	ALA	2.7
3	T	11	VAL	2.7
2	B	64	GLU	2.6
2	H	3	PHE	2.6
2	L	38	LYS	2.6
3	U	83	LEU	2.6
1	I	291	SER	2.6
3	U	214	THR	2.6
3	S	110	VAL	2.5
2	L	19	ASP	2.5
3	U	159	LEU	2.5
3	U	246	LEU	2.5
3	U	49	GLY	2.5
3	S	94	TYR	2.5
2	J	124	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
3	U	111	PHE	2.4
3	S	19	LYS	2.4
3	T	8	GLY	2.4
3	S	45	LEU	2.4
2	J	3	PHE	2.4
3	T	212	SER	2.4
3	U	215	ILE	2.3
3	U	222	ASP	2.3
3	T	175	TRP	2.3
2	L	141	TYR	2.3
2	H	6	ILE	2.3
3	S	109	CYS	2.3
3	T	211	ALA	2.3
1	I	326	GLN	2.3
3	S	111	PHE	2.3
2	J	63	PHE	2.2
3	S	20	VAL	2.2
2	F	61	THR	2.2
1	I	321	LEU	2.2
2	L	132	GLU	2.2
1	K	320	GLY	2.2
2	L	143	LYS	2.2
2	H	33	GLY	2.2
2	H	126	LEU	2.2
3	U	139	ILE	2.2
1	G	4	GLU	2.2
3	U	50	GLY	2.2
2	F	62	GLN	2.2
3	T	214	THR	2.2
2	J	45	ILE	2.2
1	A	65	LEU	2.1
3	U	176	LEU	2.1
3	U	202	PHE	2.1
3	T	34	ILE	2.1
2	L	171	GLU	2.1
2	H	19	ASP	2.1
1	A	148	PHE	2.1
1	C	152	VAL	2.1
2	L	127	ARG	2.1
1	A	185	PRO	2.1
3	S	102	TYR	2.1
3	S	176	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	S	93	VAL	2.1
1	G	9	ILE	2.0
3	T	159	LEU	2.0
3	S	9	ALA	2.0
3	U	187	LEU	2.0
3	Y	124	SER	2.0
3	U	38	ARG	2.0
2	L	168	LEU	2.0
2	H	35	ALA	2.0
3	U	244	THR	2.0

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NAG	C	601	14/15	0.94	0.14	-1.23	101,110,119,120	0
5	NAG	E	601	14/15	0.95	0.13	-1.60	93,105,110,114	0
5	NAG	I	601	14/15	0.96	0.12	-2.09	100,107,127,132	0
5	NAG	A	601	14/15	0.95	0.11	-3.01	100,109,112,119	0
4	NAG	E	501	14/15	0.91	0.11	-	93,112,126,138	0
5	NAG	G	602	14/15	0.87	0.14	-	110,123,130,139	0
5	NAG	I	602	14/15	0.80	0.17	-	142,147,153,161	0
5	BMA	I	603	11/12	0.69	0.20	-	161,168,170,172	0
5	NAG	K	601	14/15	0.94	0.14	-	76,84,97,110	0
4	NAG	G	501	14/15	0.86	0.17	-	120,133,141,143	0
4	NAG	I	501	14/15	0.86	0.16	-	109,123,133,140	0
5	NAG	A	602	14/15	0.94	0.12	-	99,110,116,124	0
5	BMA	C	603	11/12	0.83	0.14	-	142,144,147,151	0
4	NAG	A	501	14/15	0.91	0.12	-	89,107,123,135	0
4	NAG	C	501	14/15	0.91	0.14	-	85,102,113,126	0
5	BMA	A	603	11/12	0.86	0.16	-	118,130,133,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	BMA	E	603	11/12	0.83	0.14	-	125,131,135,138	0
5	NAG	C	602	14/15	0.88	0.23	-	111,122,132,139	0
5	NAG	E	602	14/15	0.91	0.16	-	96,110,123,131	0
5	NAG	G	601	14/15	0.95	0.13	-	76,98,109,116	0
5	NAG	K	602	14/15	0.86	0.18	-	111,125,129,133	0
4	NAG	I	502	14/15	0.85	0.20	-	139,149,154,154	0
4	NAG	G	502	14/15	0.76	0.27	-	143,147,157,159	0
4	NAG	C	502	14/15	0.84	0.15	-	121,134,139,140	0
4	NAG	A	502	14/15	0.91	0.13	-	130,143,150,152	0
5	BMA	K	603	11/12	0.78	0.16	-	130,132,134,135	0
4	NAG	K	502	14/15	0.76	0.19	-	140,152,156,157	0
4	NAG	E	502	14/15	0.82	0.30	-	150,157,163,163	0
5	BMA	G	603	11/12	0.86	0.16	-	135,143,146,147	0
4	NAG	K	501	14/15	0.90	0.13	-	108,125,132,136	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.