



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:47 PM GMT

PDB ID : 4FQM  
Title : Structure of B/Brisbane/60/2008 Influenza Hemagglutinin  
Authors : Dreyfus, C.; Laursen, N.S.; Wilson, I.A.  
Deposited on : 2012-06-25  
Resolution : 3.45 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

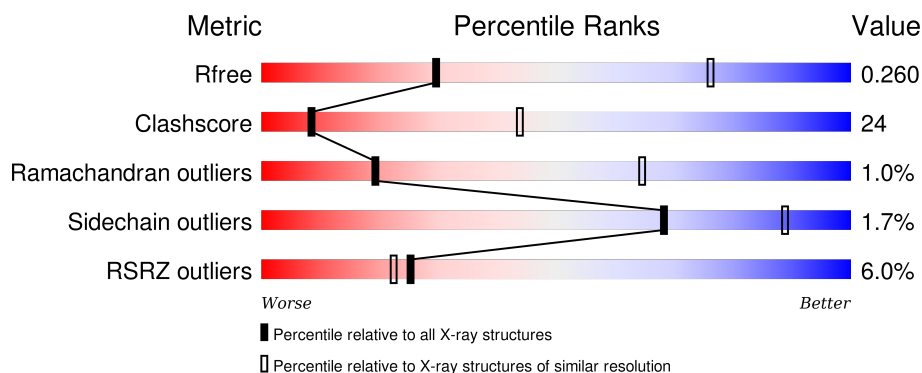
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.45 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	1000 (3.56-3.36)
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)

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	347	<div> <div>5%</div> <div>61%</div> <div>36%</div> <div>..</div> </div>
1	C	347	<div> <div>3%</div> <div>61%</div> <div>36%</div> <div>..</div> </div>
1	E	347	<div> <div>3%</div> <div>65%</div> <div>32%</div> <div>..</div> </div>
1	G	347	<div> <div>3%</div> <div>64%</div> <div>32%</div> <div>..</div> </div>
1	I	347	<div> <div>3%</div> <div>66%</div> <div>31%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	347	
2	B	179	
2	D	179	
2	F	179	
2	H	179	
2	J	179	
2	L	179	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	411	-	-	X	-
3	NAG	E	412	-	-	X	-
4	NAG	G	405	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24446 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	341	Total	C	N	O	S	0	0	0
			2588	1624	462	487	15			
1	C	341	Total	C	N	O	S	0	0	0
			2588	1624	462	487	15			
1	E	341	Total	C	N	O	S	0	0	0
			2588	1624	462	487	15			
1	G	341	Total	C	N	O	S	0	0	0
			2588	1624	462	487	15			
1	I	341	Total	C	N	O	S	0	0	0
			2588	1624	462	487	15			
1	K	341	Total	C	N	O	S	0	0	0
			2588	1624	462	487	15			

- Molecule 2 is a protein called Hemagglutinin HA2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	169	Total	C	N	O	S	0	0	0
			1282	801	218	257	6			
2	D	169	Total	C	N	O	S	0	0	0
			1282	801	218	257	6			
2	F	169	Total	C	N	O	S	0	0	0
			1282	801	218	257	6			
2	H	169	Total	C	N	O	S	0	0	0
			1282	801	218	257	6			
2	J	169	Total	C	N	O	S	0	0	0
			1282	801	218	257	6			
2	L	169	Total	C	N	O	S	0	0	0
			1282	801	218	257	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	524	SER	-	LINKER	UNP C0LT38

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Chain	Residue	Modelled	Actual	Comment	Reference
B	525	GLY	-	LINKER	UNP C0LT38
B	526	ARG	-	LINKER	UNP C0LT38
D	524	SER	-	LINKER	UNP C0LT38
D	525	GLY	-	LINKER	UNP C0LT38
D	526	ARG	-	LINKER	UNP C0LT38
F	524	SER	-	LINKER	UNP C0LT38
F	525	GLY	-	LINKER	UNP C0LT38
F	526	ARG	-	LINKER	UNP C0LT38
H	524	SER	-	LINKER	UNP C0LT38
H	525	GLY	-	LINKER	UNP C0LT38
H	526	ARG	-	LINKER	UNP C0LT38
J	524	SER	-	LINKER	UNP C0LT38
J	525	GLY	-	LINKER	UNP C0LT38
J	526	ARG	-	LINKER	UNP C0LT38
L	524	SER	-	LINKER	UNP C0LT38
L	525	GLY	-	LINKER	UNP C0LT38
L	526	ARG	-	LINKER	UNP C0LT38

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

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

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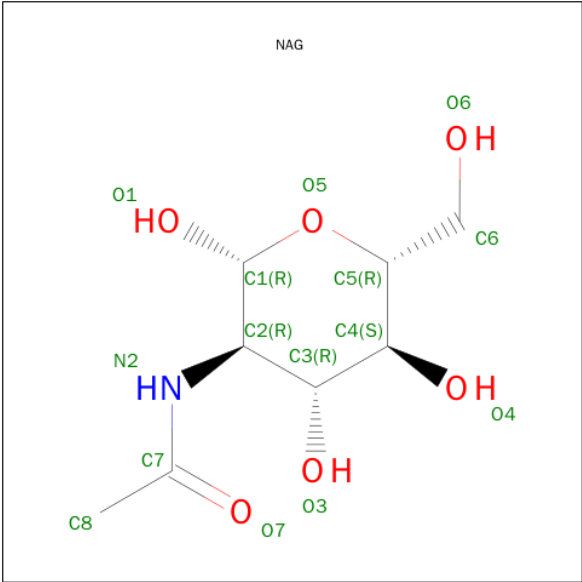
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	I	3	Total	C	N	O	0	0
			39	22	2	15		
3	I	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		

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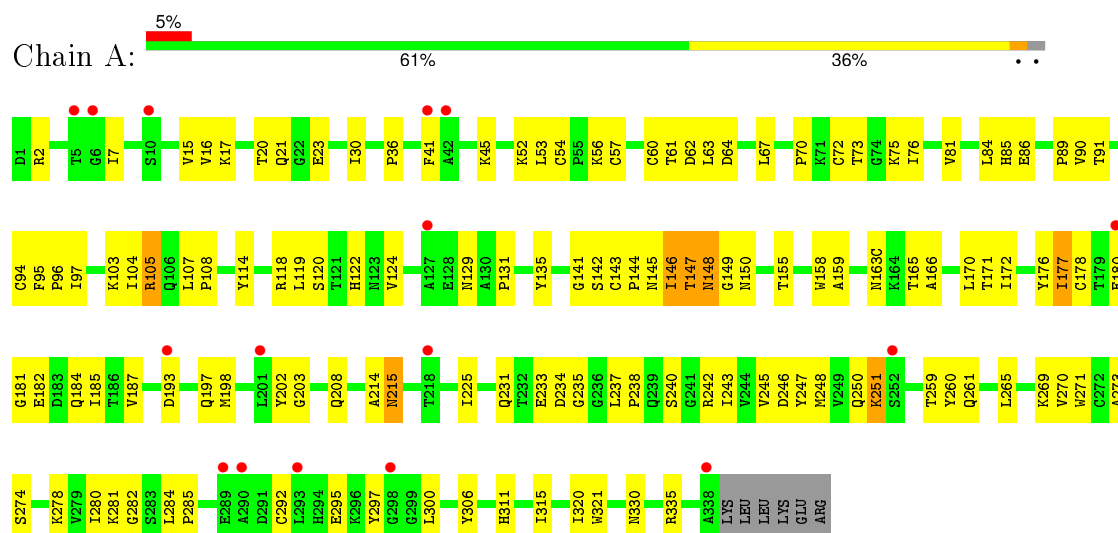
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		

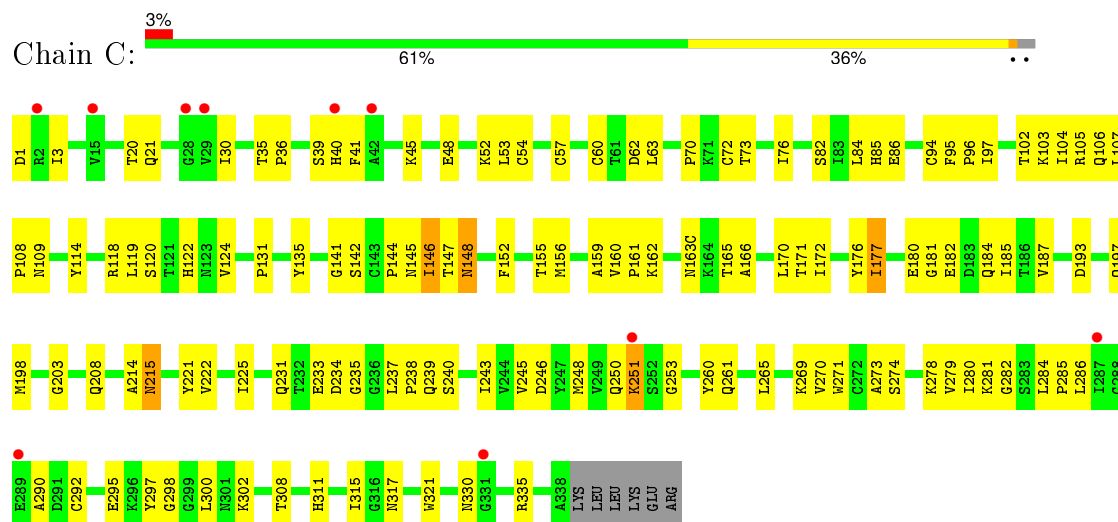
### 3 Residue-property plots

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

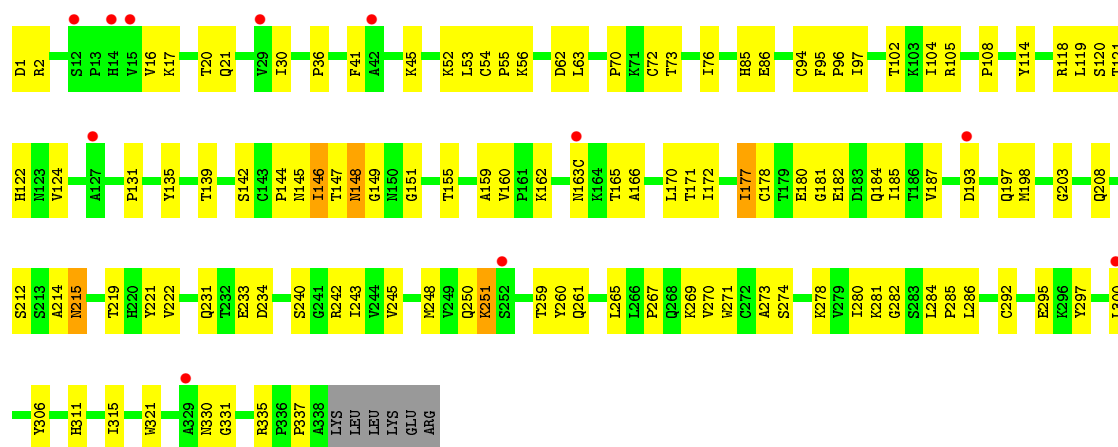


#### • Molecule 1: Hemagglutinin HA1

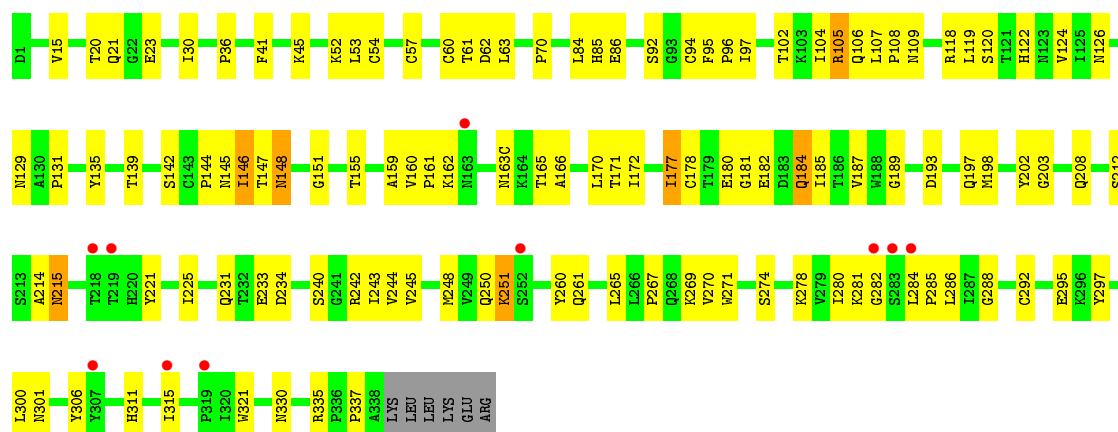


#### • Molecule 1: Hemagglutinin HA1

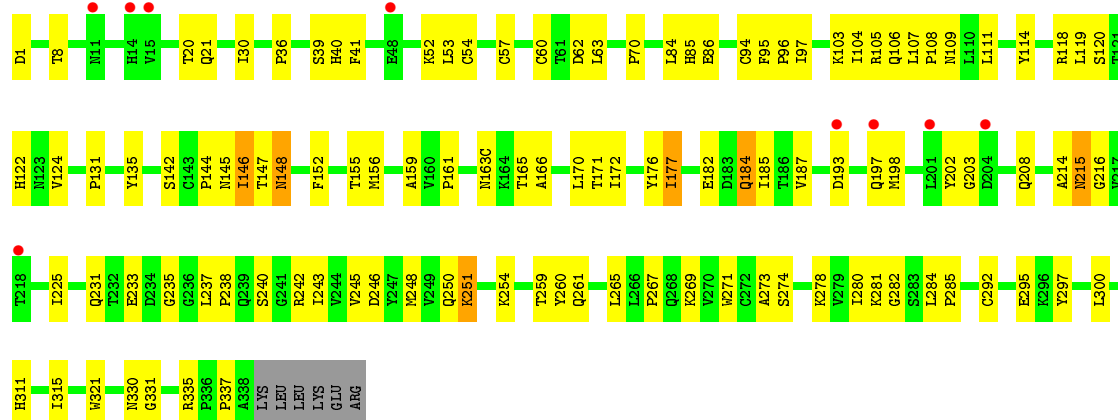




• Molecule 1: Hemagglutinin HA1

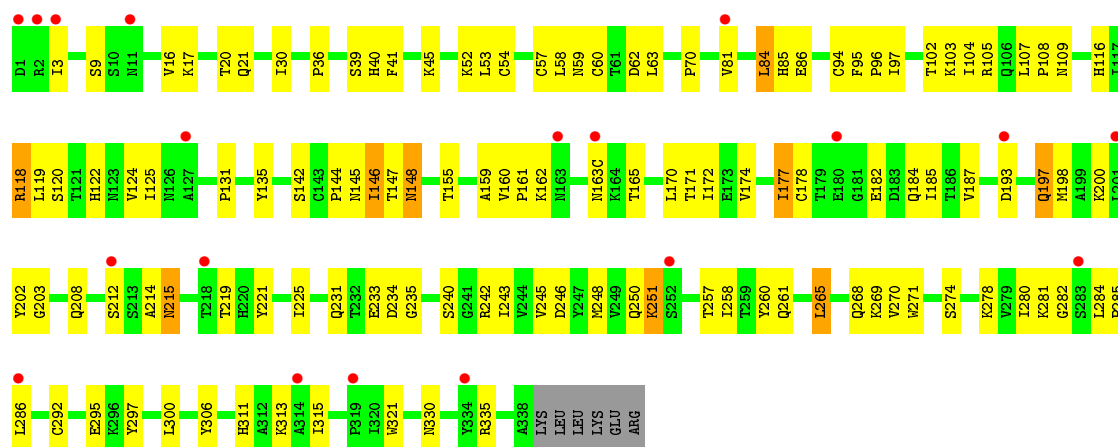


• Molecule 1: Hemagglutinin HA1



• Molecule 1: Hemagglutinin HA1





• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2

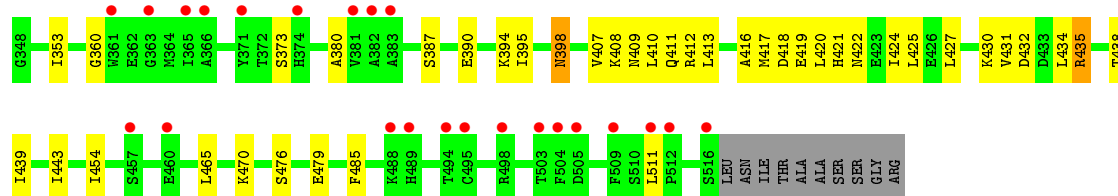


• Molecule 2: Hemagglutinin HA2

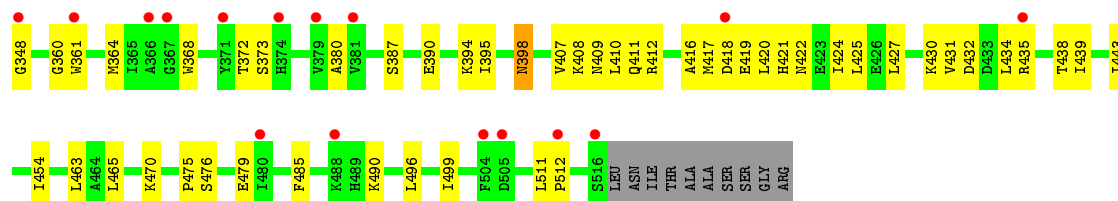


• Molecule 2: Hemagglutinin HA2

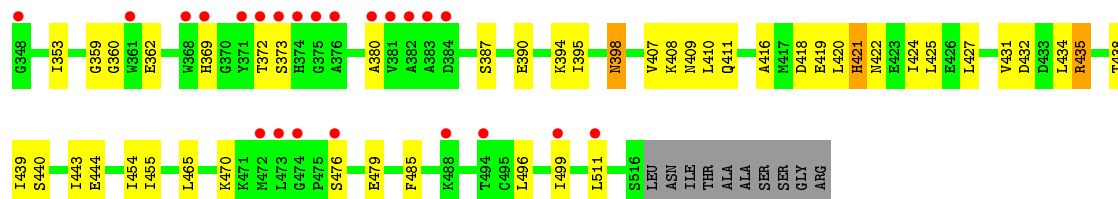




• Molecule 2: Hemagglutinin HA2



• Molecule 2: Hemagglutinin HA2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.69Å 242.54Å 135.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.07 – 3.45 49.07 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.07-3.45) 99.7 (49.07-3.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.23 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, $R_{free}$	0.257 , 0.268 0.249 , 0.260	Depositor DCC
$R_{free}$ test set	1922 reflections (3.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	82.4	Xtriage
Anisotropy	1.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 46.6	EDS
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 60738 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	24446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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 [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	0.64	0/2648	0.93	2/3598 (0.1%)
1	C	0.60	0/2648	0.79	0/3598
1	E	0.58	1/2648 (0.0%)	0.77	0/3598
1	G	0.55	0/2648	0.78	0/3598
1	I	0.56	1/2648 (0.0%)	0.75	0/3598
1	K	0.53	0/2648	0.75	1/3598 (0.0%)
2	B	0.43	0/1301	0.67	0/1753
2	D	0.44	0/1301	0.69	0/1753
2	F	0.44	0/1301	0.69	1/1753 (0.1%)
2	H	0.41	0/1301	0.66	1/1753 (0.1%)
2	J	0.40	0/1301	0.66	0/1753
2	L	0.40	0/1301	0.66	0/1753
All	All	0.53	2/23694 (0.0%)	0.76	5/32106 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	184	GLN	CD-NE2	-5.86	1.18	1.32
1	E	178	CYS	CB-SG	-5.04	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	84	LEU	CB-CG-CD2	-5.77	101.19	111.00
1	A	67	LEU	CB-CG-CD2	-5.74	101.25	111.00
2	H	413	LEU	CA-CB-CG	5.73	128.47	115.30
1	K	84	LEU	CA-CB-CG	5.63	128.25	115.30
2	F	413	LEU	CA-CB-CG	5.42	127.76	115.30

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	2588	0	2589	168	0
1	C	2588	0	2589	159	0
1	E	2588	0	2589	141	0
1	G	2588	0	2589	145	0
1	I	2588	0	2589	151	0
1	K	2588	0	2590	138	0
2	B	1282	0	1248	65	0
2	D	1282	0	1248	74	0
2	F	1282	0	1248	63	0
2	H	1282	0	1248	65	0
2	J	1282	0	1248	93	0
2	L	1282	0	1249	78	0
3	A	117	0	102	7	0
3	C	117	0	102	7	0
3	E	117	0	102	9	0
3	G	78	0	68	0	0
3	I	78	0	68	6	0
3	K	117	0	102	6	0
4	A	56	0	50	0	0
4	C	28	0	25	0	0
4	E	56	0	50	0	0
4	G	84	0	75	13	0
4	I	84	0	75	0	0
4	K	56	0	50	0	0
5	A	28	0	26	0	0
5	B	14	0	13	0	0
5	C	42	0	39	0	0
5	D	14	0	13	0	0
5	E	28	0	26	0	0
5	F	14	0	13	0	0
5	G	28	0	26	0	0
5	H	14	0	13	0	0
5	I	28	0	26	0	0
5	J	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	14	0	13	0	0
All	All	24446	0	24114	1165	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 24.

All (1165) 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:214:ALA:HB2	1:C:248:MET:CE	1.32	1.54
2:J:435:ARG:NH1	2:L:434:LEU:HD21	1.22	1.49
1:E:214:ALA:HB2	1:E:248:MET:CE	1.49	1.40
1:G:214:ALA:HB2	1:G:248:MET:CE	1.59	1.32
1:I:214:ALA:HB2	1:I:248:MET:CE	1.60	1.29
1:A:214:ALA:HB2	1:A:248:MET:CE	1.62	1.29
1:K:214:ALA:HB2	1:K:248:MET:CE	1.65	1.26
1:G:96:PRO:O	1:G:243:ILE:HG22	1.43	1.19
2:J:435:ARG:NH1	2:L:434:LEU:CD2	2.08	1.16
1:G:214:ALA:HB2	1:G:248:MET:HE3	1.25	1.14
1:C:280:ILE:HD11	1:C:315:ILE:HG23	1.22	1.14
1:C:214:ALA:CB	1:C:248:MET:CE	2.26	1.14
1:E:280:ILE:HD11	1:E:315:ILE:HG23	1.25	1.14
1:A:280:ILE:HD11	1:A:315:ILE:HG23	1.26	1.12
1:E:96:PRO:O	1:E:243:ILE:HG22	1.48	1.12
1:C:214:ALA:HB2	1:C:248:MET:HE2	1.32	1.11
2:J:407:VAL:HG12	2:J:435:ARG:HH21	1.00	1.11
1:K:214:ALA:HB2	1:K:248:MET:HE3	1.31	1.11
1:I:280:ILE:HD11	1:I:315:ILE:HG23	1.19	1.11
1:G:131:PRO:HG2	1:G:172:ILE:HD11	1.33	1.11
1:C:281:LYS:HD2	2:D:412:ARG:CZ	1.81	1.10
1:C:131:PRO:HG2	1:C:172:ILE:HD11	1.34	1.09
1:C:214:ALA:CB	1:C:248:MET:HE3	1.83	1.09
1:G:280:ILE:HD11	1:G:315:ILE:HG23	1.21	1.09
2:J:410:LEU:HD11	2:J:435:ARG:HD3	1.27	1.08
2:J:410:LEU:CD1	2:J:435:ARG:HD3	1.82	1.08
1:K:197:GLN:HE21	1:K:197:GLN:HA	1.19	1.07
1:C:214:ALA:HB2	1:C:248:MET:HE3	1.14	1.07
1:K:280:ILE:HD11	1:K:315:ILE:HG23	1.35	1.07
1:E:214:ALA:HB2	1:E:248:MET:HE3	1.12	1.07
1:C:240:SER:OG	3:C:411:NAG:H82	1.55	1.07
2:H:419:GLU:OE2	1:K:251:LYS:HG3	1.55	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:280:ILE:CD1	1:I:315:ILE:HG12	1.85	1.06
1:E:131:PRO:HG2	1:E:172:ILE:HD11	1.31	1.06
1:A:124:VAL:HG12	1:A:177:ILE:HG13	1.38	1.06
2:L:416:ALA:HB1	2:L:425:LEU:HD21	1.37	1.05
2:F:416:ALA:HB1	2:F:425:LEU:HD21	1.38	1.05
1:E:280:ILE:CD1	1:E:315:ILE:HG12	1.87	1.05
1:I:96:PRO:O	1:I:243:ILE:HG22	1.56	1.05
1:C:96:PRO:O	1:C:243:ILE:HG22	1.56	1.05
1:A:214:ALA:HB2	1:A:248:MET:HE3	1.40	1.04
1:K:131:PRO:HG2	1:K:172:ILE:HD11	1.38	1.04
1:A:280:ILE:CD1	1:A:315:ILE:HG12	1.88	1.04
1:K:280:ILE:CD1	1:K:315:ILE:HG12	1.87	1.04
1:K:96:PRO:O	1:K:243:ILE:HG22	1.54	1.04
1:A:56:LYS:NZ	1:A:75:LYS:HE3	1.72	1.04
2:J:416:ALA:HB1	2:J:425:LEU:HD21	1.36	1.03
1:A:214:ALA:HB2	1:A:248:MET:HE2	1.40	1.03
1:A:131:PRO:HG2	1:A:172:ILE:HD11	1.33	1.03
1:G:280:ILE:CD1	1:G:315:ILE:HG12	1.89	1.02
1:I:214:ALA:HB2	1:I:248:MET:HE3	1.41	1.02
1:A:96:PRO:O	1:A:243:ILE:HG22	1.59	1.02
1:I:251:LYS:HG3	2:L:419:GLU:OE2	1.59	1.02
1:I:131:PRO:HG2	1:I:172:ILE:HD11	1.42	1.01
1:I:124:VAL:HG12	1:I:177:ILE:HG13	1.40	1.01
1:I:280:ILE:HD12	1:I:315:ILE:HG12	1.43	1.01
1:K:240:SER:OG	3:K:411:NAG:H82	1.60	1.01
2:J:410:LEU:HD11	2:J:435:ARG:CD	1.91	1.01
2:J:407:VAL:HG12	2:J:435:ARG:NH2	1.76	1.01
1:I:281:LYS:HD2	2:J:412:ARG:CZ	1.91	1.00
2:B:416:ALA:HB1	2:B:425:LEU:HD21	1.42	1.00
2:H:416:ALA:HB1	2:H:425:LEU:HD21	1.43	1.00
1:E:214:ALA:CB	1:E:248:MET:HE3	1.91	1.00
1:E:171:THR:O	1:E:172:ILE:HD13	1.60	1.00
1:A:131:PRO:HG2	1:A:172:ILE:CD1	1.91	1.00
1:A:119:LEU:HD21	1:A:269:LYS:HB3	1.43	1.00
1:G:171:THR:O	1:G:172:ILE:HD13	1.62	0.99
1:G:215:ASN:OD1	1:G:251:LYS:HG2	1.62	0.98
2:D:416:ALA:HB1	2:D:425:LEU:HD21	1.42	0.98
1:I:281:LYS:HD2	2:J:412:ARG:NH2	1.78	0.98
1:K:280:ILE:HD12	1:K:315:ILE:HG12	1.44	0.98
1:E:124:VAL:HG12	1:E:177:ILE:HG13	1.43	0.98
1:C:280:ILE:CD1	1:C:315:ILE:HG12	1.91	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:PRO:O	1:E:56:LYS:HG2	1.63	0.97
1:I:214:ALA:HB2	1:I:248:MET:HE2	1.42	0.97
1:E:215:ASN:OD1	1:E:251:LYS:HG2	1.65	0.97
1:E:280:ILE:HD12	1:E:315:ILE:HG12	1.44	0.97
1:C:171:THR:O	1:C:172:ILE:HD13	1.65	0.97
1:A:215:ASN:OD1	1:A:251:LYS:HG2	1.65	0.97
1:A:281:LYS:HD2	2:B:412:ARG:NH2	1.80	0.97
1:G:280:ILE:HD12	1:G:315:ILE:HG12	1.44	0.97
1:G:280:ILE:HD11	1:G:315:ILE:CG2	1.94	0.96
1:C:215:ASN:OD1	1:C:251:LYS:HG2	1.65	0.96
1:I:215:ASN:OD1	1:I:251:LYS:HG2	1.63	0.96
1:I:280:ILE:HD11	1:I:315:ILE:CG2	1.94	0.96
1:G:124:VAL:HG12	1:G:177:ILE:HG13	1.44	0.96
1:G:240:SER:OG	4:G:412:NAG:H82	1.64	0.96
1:G:281:LYS:HD2	2:H:412:ARG:CZ	1.94	0.96
1:E:240:SER:OG	3:E:412:NAG:H82	1.65	0.96
1:I:240:SER:OG	3:I:411:NAG:H82	1.63	0.95
1:G:131:PRO:HG2	1:G:172:ILE:CD1	1.96	0.95
2:J:435:ARG:HD2	2:L:434:LEU:HD22	1.48	0.95
2:J:435:ARG:CZ	2:L:434:LEU:CD2	2.44	0.95
1:K:124:VAL:HG12	1:K:177:ILE:HG13	1.50	0.94
1:C:131:PRO:HG2	1:C:172:ILE:CD1	1.96	0.94
1:I:131:PRO:HG2	1:I:172:ILE:CD1	1.98	0.94
1:K:215:ASN:OD1	1:K:251:LYS:HG2	1.67	0.94
1:A:280:ILE:HD12	1:A:315:ILE:HG12	1.48	0.94
1:C:197:GLN:HE21	3:C:411:NAG:H81	1.30	0.94
1:A:320:ILE:CD1	2:B:405:LEU:HD22	1.98	0.94
1:C:281:LYS:HD2	2:D:412:ARG:NH2	1.82	0.93
1:G:281:LYS:HD2	2:H:412:ARG:NH2	1.83	0.93
1:E:281:LYS:HD2	2:F:412:ARG:CZ	1.98	0.93
2:B:421:HIS:O	2:B:425:LEU:HG	1.68	0.93
1:A:281:LYS:HD2	2:B:412:ARG:CZ	1.97	0.93
1:E:280:ILE:HD11	1:E:315:ILE:CG2	1.97	0.93
1:E:281:LYS:HD2	2:F:412:ARG:NH2	1.84	0.93
1:E:131:PRO:HG2	1:E:172:ILE:CD1	1.99	0.93
1:E:197:GLN:HE21	3:E:412:NAG:H81	1.29	0.92
1:E:214:ALA:CB	1:E:248:MET:CE	2.45	0.92
1:C:280:ILE:HD12	1:C:315:ILE:HG12	1.48	0.92
1:K:131:PRO:HG2	1:K:172:ILE:CD1	1.98	0.92
2:B:419:GLU:OE2	1:C:251:LYS:HG3	1.67	0.92
1:E:214:ALA:HB2	1:E:248:MET:HE2	1.48	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:SER:OG	3:A:412:NAG:H82	1.69	0.92
1:C:124:VAL:HG12	1:C:177:ILE:HG13	1.52	0.92
1:A:280:ILE:HD11	1:A:315:ILE:CG2	1.99	0.91
1:A:197:GLN:HE21	3:A:412:NAG:H81	1.35	0.91
1:C:119:LEU:HD21	1:C:269:LYS:HB3	1.52	0.91
1:C:180:GLU:HG3	1:C:181:GLY:H	1.34	0.91
1:I:197:GLN:HE21	3:I:411:NAG:H81	1.34	0.91
1:C:280:ILE:HD11	1:C:315:ILE:CG2	1.99	0.91
1:A:171:THR:O	1:A:172:ILE:HD13	1.71	0.91
1:K:171:THR:O	1:K:172:ILE:HD13	1.71	0.90
1:I:171:THR:O	1:I:172:ILE:HD13	1.71	0.90
1:C:155:THR:CG2	1:C:187:VAL:HB	2.02	0.90
2:D:419:GLU:O	1:E:251:LYS:HE2	1.72	0.89
1:A:180:GLU:HG3	1:A:181:GLY:H	1.37	0.89
1:A:119:LEU:HD23	1:A:120:SER:N	1.87	0.89
1:A:131:PRO:CG	1:A:172:ILE:HD11	2.01	0.89
1:G:155:THR:CG2	1:G:187:VAL:HB	2.02	0.88
1:G:197:GLN:HE21	4:G:412:NAG:H81	1.36	0.88
2:J:435:ARG:CZ	2:L:434:LEU:HD21	2.01	0.88
1:K:214:ALA:HB2	1:K:248:MET:HE2	1.55	0.87
2:F:421:HIS:O	2:F:425:LEU:HG	1.74	0.87
2:J:435:ARG:HH11	2:L:434:LEU:HD21	1.06	0.87
2:L:421:HIS:O	2:L:425:LEU:HG	1.75	0.87
2:H:421:HIS:O	2:H:425:LEU:HG	1.74	0.87
1:G:214:ALA:HB2	1:G:248:MET:HE2	1.54	0.87
1:I:251:LYS:HE2	2:L:419:GLU:O	1.75	0.86
1:E:215:ASN:O	1:E:215:ASN:ND2	2.09	0.86
1:A:56:LYS:HZ3	1:A:75:LYS:HE3	1.38	0.86
1:C:215:ASN:ND2	1:C:215:ASN:O	2.09	0.86
1:G:288:GLY:HA3	4:G:405:NAG:H62	1.56	0.86
1:G:214:ALA:CB	1:G:248:MET:HE3	2.03	0.86
2:D:421:HIS:O	2:D:425:LEU:HG	1.75	0.86
1:C:131:PRO:CG	1:C:172:ILE:HD11	2.05	0.86
1:C:231:GLN:HE22	1:C:239:GLN:H	1.23	0.86
2:L:416:ALA:HB1	2:L:425:LEU:CD2	2.06	0.85
1:A:251:LYS:HG3	2:F:419:GLU:OE2	1.75	0.85
1:C:119:LEU:HD23	1:C:120:SER:N	1.91	0.85
1:C:84:LEU:CD1	1:C:109:ASN:OD1	2.24	0.85
1:E:131:PRO:CG	1:E:172:ILE:HD11	2.06	0.85
1:A:155:THR:CG2	1:A:187:VAL:HB	2.05	0.85
1:I:215:ASN:O	1:I:215:ASN:ND2	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:131:PRO:CG	1:G:172:ILE:HD11	2.06	0.85
1:C:180:GLU:HG3	1:C:181:GLY:N	1.90	0.85
1:I:119:LEU:HD21	1:I:269:LYS:HB3	1.57	0.85
1:E:155:THR:CG2	1:E:187:VAL:HB	2.06	0.85
1:A:56:LYS:NZ	1:A:75:LYS:CE	2.40	0.85
1:K:280:ILE:HD11	1:K:315:ILE:CG2	2.06	0.84
1:A:215:ASN:O	1:A:215:ASN:ND2	2.09	0.84
1:K:214:ALA:CB	1:K:248:MET:HE3	2.08	0.84
1:K:131:PRO:CG	1:K:172:ILE:HD11	2.08	0.84
1:I:84:LEU:CD1	1:I:109:ASN:OD1	2.25	0.84
1:I:1:ASP:OD1	2:J:490:LYS:HG2	1.78	0.84
1:I:155:THR:CG2	1:I:187:VAL:HB	2.07	0.83
1:G:193:ASP:OD1	1:G:198:MET:SD	2.36	0.83
1:K:215:ASN:ND2	1:K:215:ASN:O	2.11	0.83
2:J:407:VAL:CG1	2:J:435:ARG:HH21	1.87	0.83
1:G:251:LYS:HG3	2:J:419:GLU:OE2	1.77	0.83
1:G:215:ASN:ND2	1:G:215:ASN:O	2.10	0.82
2:B:416:ALA:HB1	2:B:425:LEU:CD2	2.09	0.82
2:D:416:ALA:HB1	2:D:425:LEU:CD2	2.10	0.82
1:E:55:PRO:O	1:E:56:LYS:CG	2.27	0.81
1:A:180:GLU:HG3	1:A:181:GLY:N	1.94	0.81
1:I:131:PRO:CG	1:I:172:ILE:HD11	2.10	0.81
1:K:155:THR:CG2	1:K:187:VAL:HB	2.10	0.80
2:J:410:LEU:CD1	2:J:435:ARG:HH11	1.94	0.80
1:K:119:LEU:HD21	1:K:269:LYS:HB3	1.63	0.80
1:G:84:LEU:CD1	1:G:109:ASN:OD1	2.30	0.80
2:J:421:HIS:O	2:J:425:LEU:HG	1.82	0.79
2:D:422:ASN:OD1	1:E:251:LYS:HE3	1.81	0.79
1:I:251:LYS:HE3	2:L:422:ASN:OD1	1.83	0.79
1:C:214:ALA:HB2	1:C:248:MET:HE1	1.61	0.79
2:J:435:ARG:CD	2:L:434:LEU:HD22	2.14	0.78
1:I:335:ARG:HB3	2:J:360:GLY:H	1.46	0.78
1:C:292:CYS:HB3	1:C:300:LEU:HB3	1.64	0.78
1:E:149:GLY:HA3	3:E:401:NAG:O6	1.84	0.78
1:G:119:LEU:HD21	1:G:269:LYS:HB3	1.66	0.78
1:I:119:LEU:HD23	1:I:120:SER:N	1.99	0.77
2:L:479:GLU:OE1	2:L:485:PHE:CE2	2.37	0.77
2:H:416:ALA:HB1	2:H:425:LEU:CD2	2.14	0.77
1:I:214:ALA:CB	1:I:248:MET:CE	2.53	0.77
1:K:197:GLN:NE2	1:K:197:GLN:HA	1.99	0.77
1:E:171:THR:O	1:E:172:ILE:CD1	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:284:LEU:HB3	1:G:285:PRO:HA	1.67	0.76
1:E:284:LEU:HB3	1:E:285:PRO:HA	1.67	0.76
1:I:280:ILE:HG23	1:I:295:GLU:HG3	1.67	0.76
1:E:292:CYS:HB3	1:E:300:LEU:HB3	1.66	0.76
1:C:284:LEU:HB3	1:C:285:PRO:HA	1.67	0.76
1:A:129:ASN:ND2	3:K:403:BMA:H3	2.00	0.76
1:G:171:THR:O	1:G:172:ILE:CD1	2.34	0.76
1:A:284:LEU:HB3	1:A:285:PRO:HA	1.67	0.76
1:K:292:CYS:HB3	1:K:300:LEU:HB3	1.68	0.75
2:J:435:ARG:HD2	2:L:434:LEU:CD2	2.17	0.75
2:J:410:LEU:CD1	2:J:435:ARG:CD	2.56	0.75
1:I:284:LEU:HB3	1:I:285:PRO:HA	1.67	0.75
1:C:280:ILE:HG23	1:C:295:GLU:HG3	1.68	0.75
1:C:281:LYS:CD	2:D:412:ARG:NH2	2.49	0.75
1:K:284:LEU:HB3	1:K:285:PRO:HA	1.67	0.74
1:E:119:LEU:HD21	1:E:269:LYS:HB3	1.68	0.74
1:I:172:ILE:HG13	1:I:260:TYR:HE2	1.53	0.74
1:A:119:LEU:HD21	1:A:269:LYS:CB	2.18	0.74
2:L:479:GLU:OE1	2:L:485:PHE:CZ	2.40	0.74
1:A:193:ASP:OD1	1:A:198:MET:SD	2.46	0.74
1:A:214:ALA:CB	1:A:248:MET:CE	2.57	0.74
1:A:214:ALA:CB	1:A:248:MET:HE3	2.17	0.74
1:I:193:ASP:OD1	1:I:198:MET:SD	2.46	0.73
1:I:281:LYS:CD	2:J:412:ARG:NH2	2.51	0.73
1:G:288:GLY:HA3	4:G:405:NAG:C6	2.17	0.73
1:A:36:PRO:HB2	1:A:297:TYR:CD1	2.24	0.73
1:K:215:ASN:HD22	1:K:215:ASN:C	1.90	0.73
2:D:479:GLU:OE1	2:D:485:PHE:CE2	2.41	0.73
1:I:292:CYS:HB3	1:I:300:LEU:HB3	1.70	0.73
2:F:416:ALA:HB1	2:F:425:LEU:CD2	2.16	0.73
1:G:215:ASN:C	1:G:215:ASN:HD22	1.91	0.73
1:G:84:LEU:CD1	1:G:109:ASN:CG	2.57	0.73
1:K:84:LEU:CD1	1:K:109:ASN:OD1	2.36	0.73
1:G:288:GLY:HA2	4:G:405:NAG:O6	1.89	0.72
1:G:288:GLY:CA	4:G:405:NAG:C6	2.66	0.72
1:K:193:ASP:OD1	1:K:198:MET:SD	2.47	0.72
1:I:215:ASN:C	1:I:215:ASN:HD22	1.91	0.72
1:A:280:ILE:HG23	1:A:295:GLU:HG3	1.71	0.72
2:J:479:GLU:OE1	2:J:485:PHE:CE2	2.42	0.72
2:H:479:GLU:OE1	2:H:485:PHE:CE2	2.42	0.72
1:C:84:LEU:HD12	1:C:109:ASN:OD1	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:119:LEU:HD23	1:G:120:SER:N	2.04	0.72
1:A:158:TRP:HA	1:A:265:LEU:HD23	1.70	0.72
2:J:408:LYS:HB2	2:J:435:ARG:HH22	1.55	0.72
1:C:215:ASN:C	1:C:215:ASN:HD22	1.90	0.72
1:A:215:ASN:C	1:A:215:ASN:HD22	1.91	0.72
1:E:193:ASP:OD1	1:E:198:MET:SD	2.48	0.72
1:I:172:ILE:CG1	1:I:260:TYR:HE2	2.03	0.72
2:J:410:LEU:HD12	2:J:435:ARG:HH11	1.53	0.72
1:E:215:ASN:C	1:E:215:ASN:HD22	1.91	0.72
1:A:281:LYS:CD	2:B:412:ARG:NH2	2.53	0.72
2:J:416:ALA:HB1	2:J:425:LEU:CD2	2.16	0.71
1:A:292:CYS:HB3	1:A:300:LEU:HB3	1.72	0.71
2:F:479:GLU:OE1	2:F:485:PHE:CE2	2.42	0.71
1:C:106:GLN:HB3	2:D:417:MET:SD	2.31	0.71
1:I:214:ALA:CB	1:I:248:MET:HE3	2.16	0.71
1:K:84:LEU:CD1	1:K:109:ASN:CG	2.59	0.71
1:E:335:ARG:HB3	2:F:360:GLY:H	1.56	0.71
1:G:281:LYS:CD	2:H:412:ARG:NH2	2.54	0.71
1:C:214:ALA:CB	1:C:248:MET:HE2	2.09	0.71
1:G:292:CYS:HB3	1:G:300:LEU:HB3	1.73	0.71
1:G:280:ILE:HG23	1:G:295:GLU:HG3	1.72	0.71
2:H:479:GLU:OE1	2:H:485:PHE:CZ	2.43	0.71
1:C:231:GLN:HB3	1:C:234:ASP:OD2	1.90	0.70
2:B:479:GLU:OE1	2:B:485:PHE:CE2	2.44	0.70
1:C:240:SER:OG	3:C:411:NAG:C8	2.38	0.70
1:A:119:LEU:HD23	1:A:120:SER:H	1.54	0.70
1:A:129:ASN:HD21	3:K:403:BMA:H3	1.55	0.70
2:J:479:GLU:OE1	2:J:485:PHE:CZ	2.45	0.70
1:I:147:THR:O	1:I:148:ASN:CG	2.30	0.70
1:G:84:LEU:HD12	1:G:109:ASN:OD1	1.91	0.70
2:B:439:ILE:CD1	2:F:438:THR:HG23	2.22	0.70
1:G:147:THR:O	1:G:148:ASN:CG	2.30	0.70
1:A:243:ILE:HD11	1:A:265:LEU:HD11	1.73	0.70
2:F:398:ASN:HD22	2:F:398:ASN:C	1.95	0.70
1:E:280:ILE:HG23	1:E:295:GLU:HG3	1.73	0.69
1:K:280:ILE:HG23	1:K:295:GLU:HG3	1.73	0.69
1:G:84:LEU:HD11	1:G:109:ASN:CG	2.13	0.69
2:D:479:GLU:OE1	2:D:485:PHE:CZ	2.44	0.69
1:A:335:ARG:HB3	2:B:360:GLY:H	1.56	0.69
1:C:119:LEU:HD21	1:C:269:LYS:CB	2.22	0.69
1:I:84:LEU:HD12	1:I:109:ASN:OD1	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:479:GLU:OE1	2:B:485:PHE:CZ	2.45	0.69
2:D:419:GLU:OE2	1:E:251:LYS:HG3	1.92	0.69
1:A:280:ILE:HD11	1:A:315:ILE:HG12	1.73	0.69
1:E:281:LYS:CD	2:F:412:ARG:NH2	2.56	0.69
2:H:438:THR:HG23	2:L:439:ILE:CD1	2.23	0.69
2:L:398:ASN:HD22	2:L:398:ASN:C	1.92	0.69
1:K:280:ILE:HD11	1:K:315:ILE:HG12	1.75	0.69
1:A:172:ILE:HG13	1:A:260:TYR:HE2	1.56	0.69
1:C:193:ASP:OD1	1:C:198:MET:SD	2.51	0.69
1:G:280:ILE:HD12	1:G:315:ILE:CG1	2.23	0.68
1:G:172:ILE:HG13	1:G:260:TYR:HE2	1.57	0.68
2:J:408:LYS:N	2:J:435:ARG:HH22	1.91	0.68
2:F:479:GLU:OE1	2:F:485:PHE:CZ	2.46	0.68
2:H:398:ASN:HD22	2:H:398:ASN:C	1.96	0.68
2:D:398:ASN:C	2:D:398:ASN:HD22	1.97	0.68
1:I:280:ILE:HD12	1:I:315:ILE:CG1	2.22	0.68
2:J:408:LYS:CA	2:J:435:ARG:HH22	2.07	0.68
2:F:427:LEU:O	2:F:431:VAL:HG23	1.94	0.68
1:E:280:ILE:HD12	1:E:315:ILE:CG1	2.23	0.67
1:G:119:LEU:HD21	1:G:269:LYS:CB	2.22	0.67
1:G:97:ILE:HA	1:G:243:ILE:HG23	1.77	0.67
1:E:119:LEU:HD23	1:E:120:SER:N	2.10	0.67
1:I:84:LEU:CD1	1:I:109:ASN:CG	2.63	0.67
1:G:335:ARG:HB3	2:H:360:GLY:H	1.59	0.67
2:J:373:SER:HB2	2:J:380:ALA:HB3	1.76	0.67
1:A:53:LEU:CD1	1:A:62:ASP:HB3	2.25	0.67
1:E:280:ILE:CD1	1:E:315:ILE:CG1	2.70	0.67
1:K:84:LEU:HD12	1:K:109:ASN:OD1	1.93	0.67
1:E:172:ILE:HG13	1:E:260:TYR:HE2	1.58	0.67
1:A:56:LYS:HZ3	1:A:75:LYS:CE	2.04	0.67
1:A:36:PRO:HB2	1:A:297:TYR:HD1	1.58	0.67
2:F:373:SER:HB2	2:F:380:ALA:HB3	1.77	0.67
1:E:119:LEU:HD21	1:E:269:LYS:CB	2.25	0.66
1:K:172:ILE:HG13	1:K:260:TYR:HE2	1.58	0.66
1:C:231:GLN:NE2	1:C:239:GLN:H	1.91	0.66
1:E:147:THR:O	1:E:148:ASN:CG	2.33	0.66
1:E:180:GLU:HG3	1:E:181:GLY:H	1.60	0.66
1:C:171:THR:O	1:C:172:ILE:CD1	2.41	0.66
1:G:214:ALA:O	1:G:215:ASN:ND2	2.28	0.66
1:A:180:GLU:CG	1:A:181:GLY:H	2.00	0.66
1:G:280:ILE:CD1	1:G:315:ILE:CG1	2.72	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LYS:NZ	1:A:75:LYS:NZ	2.44	0.66
2:B:373:SER:HB2	2:B:380:ALA:HB3	1.78	0.66
1:A:89:PRO:HG2	1:A:105:ARG:O	1.96	0.66
2:B:438:THR:HG23	2:D:439:ILE:CD1	2.26	0.66
2:H:373:SER:HB2	2:H:380:ALA:HB3	1.77	0.66
1:I:251:LYS:CE	2:L:419:GLU:O	2.44	0.66
1:K:119:LEU:HD23	1:K:120:SER:N	2.10	0.66
2:B:479:GLU:HG2	2:D:470:LYS:NZ	2.11	0.66
1:A:20:THR:HG23	1:A:21:GLN:HG2	1.77	0.66
2:J:410:LEU:HD13	2:J:435:ARG:HD3	1.72	0.65
1:I:119:LEU:HD21	1:I:269:LYS:CB	2.26	0.65
1:C:172:ILE:CG1	1:C:260:TYR:HE2	2.09	0.65
1:C:84:LEU:CD1	1:C:109:ASN:CG	2.65	0.65
1:C:335:ARG:HB3	2:D:360:GLY:H	1.60	0.65
1:A:85:HIS:HD2	1:A:86:GLU:HG3	1.61	0.65
1:K:278:LYS:NZ	2:L:409:ASN:OD1	2.29	0.65
1:I:106:GLN:HB3	2:J:417:MET:SD	2.36	0.65
2:D:373:SER:HB2	2:D:380:ALA:HB3	1.79	0.65
1:A:251:LYS:HE3	2:F:422:ASN:OD1	1.97	0.65
2:L:418:ASP:O	2:L:422:ASN:ND2	2.29	0.65
1:C:119:LEU:HD23	1:C:120:SER:H	1.62	0.65
1:C:180:GLU:CG	1:C:181:GLY:H	2.00	0.65
2:H:421:HIS:HB3	2:H:424:ILE:HD12	1.79	0.65
2:J:427:LEU:O	2:J:431:VAL:HG23	1.97	0.65
2:J:398:ASN:HD22	2:J:398:ASN:C	2.00	0.65
1:I:251:LYS:CG	2:L:419:GLU:OE2	2.41	0.65
1:A:214:ALA:O	1:A:215:ASN:ND2	2.30	0.65
1:C:94:CYS:HA	1:C:142:SER:O	1.97	0.65
2:L:373:SER:HB2	2:L:380:ALA:HB3	1.78	0.65
2:H:417:MET:HB2	2:H:421:HIS:HD1	1.62	0.64
1:C:280:ILE:HD11	1:C:315:ILE:HG12	1.79	0.64
1:C:172:ILE:HG13	1:C:260:TYR:HE2	1.62	0.64
1:G:292:CYS:HB3	1:G:300:LEU:HD22	1.79	0.64
1:A:278:LYS:NZ	2:B:409:ASN:OD1	2.30	0.64
1:I:36:PRO:HB2	1:I:297:TYR:CD1	2.31	0.64
1:K:119:LEU:HD21	1:K:269:LYS:CB	2.26	0.64
1:G:147:THR:O	1:G:148:ASN:OD1	2.15	0.64
1:I:36:PRO:HB2	1:I:297:TYR:HD1	1.62	0.64
2:F:421:HIS:O	2:F:425:LEU:CG	2.46	0.64
1:G:172:ILE:CG1	1:G:260:TYR:HE2	2.10	0.64
2:H:427:LEU:O	2:H:431:VAL:HG23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:THR:HG21	1:C:187:VAL:HB	1.80	0.64
1:E:121:THR:HG22	1:E:122:HIS:N	2.12	0.64
1:G:57:CYS:O	1:G:60:CYS:HB2	1.98	0.64
1:A:56:LYS:HZ2	1:A:75:LYS:NZ	1.95	0.64
1:G:214:ALA:CB	1:G:248:MET:CE	2.54	0.64
1:K:172:ILE:CG1	1:K:260:TYR:HE2	2.10	0.64
1:E:311:HIS:HB2	1:E:321:TRP:CD1	2.33	0.64
1:A:320:ILE:CD1	2:B:405:LEU:CD2	2.75	0.64
1:C:85:HIS:HD2	1:C:86:GLU:HG3	1.63	0.64
1:G:180:GLU:HG3	1:G:181:GLY:H	1.62	0.64
1:K:147:THR:O	1:K:148:ASN:CG	2.36	0.64
2:J:410:LEU:CD1	2:J:435:ARG:NH1	2.60	0.64
1:E:36:PRO:HB2	1:E:297:TYR:CD1	2.33	0.63
2:B:427:LEU:O	2:B:431:VAL:HG23	1.97	0.63
1:C:147:THR:O	1:C:148:ASN:CG	2.37	0.63
1:K:243:ILE:HD11	1:K:265:LEU:HD11	1.80	0.63
2:H:435:ARG:HD3	2:H:439:ILE:CG1	2.28	0.63
1:A:94:CYS:HA	1:A:142:SER:O	1.99	0.63
1:I:280:ILE:CD1	1:I:315:ILE:CG1	2.70	0.63
1:K:20:THR:HG23	1:K:21:GLN:HG2	1.80	0.63
2:D:417:MET:HB2	2:D:421:HIS:HD1	1.64	0.63
1:E:148:ASN:O	3:E:401:NAG:O6	2.17	0.63
1:K:280:ILE:CD1	1:K:315:ILE:CG1	2.73	0.63
1:A:172:ILE:CG1	1:A:260:TYR:HE2	2.11	0.63
2:D:435:ARG:HD3	2:D:439:ILE:CG1	2.29	0.63
1:A:147:THR:O	1:A:148:ASN:CG	2.37	0.63
1:K:240:SER:OG	3:K:411:NAG:C8	2.43	0.63
1:C:1:ASP:OD1	2:D:490:LYS:HG2	1.98	0.63
1:K:335:ARG:HB3	2:L:360:GLY:H	1.63	0.63
1:A:214:ALA:CB	1:A:248:MET:HE2	2.25	0.62
2:D:419:GLU:O	1:E:251:LYS:CE	2.47	0.62
2:J:408:LYS:CB	2:J:435:ARG:HH22	2.11	0.62
1:I:214:ALA:CB	1:I:248:MET:HE2	2.22	0.62
1:A:131:PRO:CG	1:A:172:ILE:CD1	2.72	0.62
1:I:335:ARG:HB3	2:J:360:GLY:N	2.12	0.62
1:C:180:GLU:CG	1:C:181:GLY:N	2.59	0.62
1:C:147:THR:O	1:C:148:ASN:OD1	2.18	0.62
2:B:479:GLU:HG2	2:D:470:LYS:HZ3	1.65	0.62
1:I:20:THR:HG23	1:I:21:GLN:HG2	1.82	0.62
1:I:94:CYS:HA	1:I:142:SER:O	2.00	0.62
1:I:280:ILE:HD11	1:I:315:ILE:HG12	1.78	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:147:THR:O	1:I:148:ASN:OD1	2.18	0.61
1:E:36:PRO:HB2	1:E:297:TYR:HD1	1.65	0.61
1:I:53:LEU:CD1	1:I:62:ASP:HB3	2.31	0.61
1:E:335:ARG:HB3	2:F:360:GLY:N	2.15	0.61
1:I:41:PHE:CZ	1:I:282:GLY:HA2	2.36	0.61
2:J:476:SER:HB3	2:J:511:LEU:HD13	1.82	0.61
1:G:36:PRO:HB2	1:G:297:TYR:HD1	1.66	0.61
1:E:1:ASP:OD1	2:F:490:LYS:HG2	2.01	0.61
2:J:439:ILE:CD1	2:L:438:THR:HG23	2.29	0.61
1:A:311:HIS:HB2	1:A:321:TRP:CD1	2.36	0.61
1:E:240:SER:OG	3:E:412:NAG:C8	2.46	0.61
1:G:288:GLY:HA2	4:G:405:NAG:C6	2.29	0.61
2:D:435:ARG:HD3	2:D:439:ILE:HG13	1.81	0.61
1:C:41:PHE:CZ	1:C:282:GLY:HA2	2.36	0.61
1:C:36:PRO:HB2	1:C:297:TYR:CD1	2.36	0.61
2:J:421:HIS:HB3	2:J:424:ILE:HD12	1.83	0.61
1:C:36:PRO:HB2	1:C:297:TYR:HD1	1.66	0.61
1:E:94:CYS:HA	1:E:142:SER:O	2.00	0.61
2:F:418:ASP:O	2:F:422:ASN:ND2	2.34	0.60
2:H:394:LYS:HD3	1:I:20:THR:OG1	2.02	0.60
1:K:103:LYS:NZ	1:K:246:ASP:OD1	2.33	0.60
1:G:20:THR:HG23	1:G:21:GLN:HG2	1.83	0.60
1:G:41:PHE:CZ	1:G:282:GLY:HA2	2.36	0.60
1:I:84:LEU:HD11	1:I:109:ASN:CG	2.22	0.60
2:H:479:GLU:HG2	2:L:470:LYS:NZ	2.16	0.60
1:E:20:THR:HG23	1:E:21:GLN:HG2	1.83	0.60
1:G:106:GLN:HB3	2:H:417:MET:SD	2.41	0.60
1:K:147:THR:O	1:K:148:ASN:OD1	2.19	0.60
1:A:70:PRO:HB2	1:A:144:PRO:O	2.01	0.60
1:G:97:ILE:HA	1:G:243:ILE:CG2	2.30	0.60
2:B:435:ARG:HD3	2:B:439:ILE:CG1	2.31	0.60
2:B:353:ILE:HG21	2:D:465:LEU:HD12	1.83	0.60
1:G:36:PRO:HB2	1:G:297:TYR:CD1	2.36	0.60
1:G:70:PRO:HB2	1:G:144:PRO:O	2.01	0.60
2:B:421:HIS:HB3	2:B:424:ILE:HD12	1.84	0.60
1:G:184:GLN:NE2	1:G:250:GLN:OE1	2.35	0.60
1:K:36:PRO:HB2	1:K:297:TYR:CD1	2.37	0.60
1:E:172:ILE:CG1	1:E:260:TYR:HE2	2.14	0.60
1:K:36:PRO:HB2	1:K:297:TYR:HD1	1.66	0.60
1:E:280:ILE:HD11	1:E:315:ILE:HG12	1.81	0.60
1:K:280:ILE:HD12	1:K:315:ILE:CG1	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:GLN:HE22	1:C:239:GLN:N	1.97	0.60
1:A:41:PHE:CZ	1:A:282:GLY:HA2	2.37	0.60
2:B:398:ASN:HD21	2:B:450:SER:HB3	1.66	0.60
2:D:427:LEU:O	2:D:431:VAL:HG23	2.02	0.60
1:I:278:LYS:NZ	2:J:409:ASN:OD1	2.32	0.60
1:G:94:CYS:HA	1:G:142:SER:O	2.02	0.60
2:B:418:ASP:O	2:B:422:ASN:ND2	2.35	0.59
1:C:84:LEU:HD11	1:C:109:ASN:CG	2.21	0.59
2:F:408:LYS:O	2:F:435:ARG:NH2	2.35	0.59
2:D:418:ASP:O	2:D:422:ASN:ND2	2.35	0.59
1:E:214:ALA:O	1:E:215:ASN:ND2	2.35	0.59
1:E:337:PRO:HA	2:F:360:GLY:O	2.02	0.59
2:D:408:LYS:O	2:D:435:ARG:NH2	2.35	0.59
1:A:56:LYS:HZ1	1:A:75:LYS:HE3	1.67	0.59
2:L:427:LEU:O	2:L:431:VAL:HG23	2.01	0.59
1:C:281:LYS:CD	2:D:412:ARG:CZ	2.70	0.59
1:E:197:GLN:NE2	3:E:412:NAG:O7	2.36	0.59
1:K:94:CYS:HA	1:K:142:SER:O	2.02	0.59
2:H:421:HIS:O	2:H:425:LEU:CG	2.49	0.59
1:K:84:LEU:HD11	1:K:109:ASN:CG	2.22	0.59
2:F:421:HIS:HB3	2:F:424:ILE:HD12	1.85	0.59
1:A:171:THR:O	1:A:172:ILE:CD1	2.46	0.59
1:E:155:THR:HG23	1:E:187:VAL:HB	1.82	0.59
1:E:147:THR:O	1:E:148:ASN:OD1	2.19	0.59
1:K:214:ALA:O	1:K:215:ASN:ND2	2.35	0.59
1:A:278:LYS:HB3	2:B:411:GLN:HG3	1.85	0.59
1:C:70:PRO:HB2	1:C:144:PRO:O	2.02	0.59
1:E:41:PHE:CZ	1:E:282:GLY:HA2	2.38	0.59
2:B:421:HIS:O	2:B:425:LEU:CG	2.48	0.58
1:G:53:LEU:HG	1:G:62:ASP:CG	2.23	0.58
1:K:131:PRO:O	1:K:170:LEU:HD13	2.03	0.58
1:A:119:LEU:CD2	1:A:269:LYS:HB3	2.27	0.58
1:A:320:ILE:HD11	2:B:405:LEU:HD22	1.83	0.58
1:I:214:ALA:O	1:I:215:ASN:ND2	2.35	0.58
2:J:417:MET:HB2	2:J:421:HIS:HD1	1.69	0.58
1:G:240:SER:OG	4:G:412:NAG:C8	2.46	0.58
1:K:70:PRO:HB2	1:K:144:PRO:O	2.03	0.58
2:D:476:SER:HB3	2:D:511:LEU:HD13	1.85	0.58
2:B:479:GLU:CG	2:D:470:LYS:NZ	2.67	0.58
1:A:20:THR:OG1	2:D:394:LYS:HD3	2.04	0.58
1:K:184:GLN:NE2	1:K:270:VAL:HG11	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:GLN:NE2	3:E:412:NAG:H81	2.10	0.58
2:L:435:ARG:HD3	2:L:439:ILE:CG1	2.33	0.58
2:L:476:SER:HB3	2:L:511:LEU:HD13	1.84	0.58
2:F:422:ASN:HA	2:F:425:LEU:HD12	1.84	0.58
1:E:97:ILE:HA	1:E:243:ILE:HG23	1.84	0.58
1:A:155:THR:HG23	1:A:187:VAL:HB	1.84	0.58
1:G:278:LYS:NZ	2:H:409:ASN:OD1	2.37	0.58
1:C:20:THR:HG23	1:C:21:GLN:HG2	1.84	0.58
1:I:124:VAL:HG12	1:I:177:ILE:CG1	2.24	0.58
1:I:311:HIS:HB2	1:I:321:TRP:CD1	2.39	0.58
2:F:476:SER:HB3	2:F:511:LEU:HD13	1.86	0.58
2:L:421:HIS:O	2:L:425:LEU:CG	2.52	0.57
2:H:435:ARG:HD3	2:H:439:ILE:HG13	1.86	0.57
2:H:416:ALA:O	2:H:417:MET:HB2	2.04	0.57
1:A:292:CYS:SG	1:A:300:LEU:HD23	2.44	0.57
1:K:41:PHE:CZ	1:K:282:GLY:HA2	2.39	0.57
1:C:311:HIS:HB2	1:C:321:TRP:CD1	2.39	0.57
2:H:408:LYS:O	2:H:435:ARG:NH2	2.38	0.57
1:I:240:SER:OG	3:I:411:NAG:C8	2.46	0.57
1:A:131:PRO:CD	1:A:172:ILE:HD11	2.35	0.57
2:H:419:GLU:HG3	1:K:215:ASN:HB2	1.85	0.57
2:J:408:LYS:N	2:J:435:ARG:NH2	2.52	0.57
2:F:435:ARG:HD3	2:F:439:ILE:CG1	2.34	0.57
1:A:104:ILE:HD13	1:A:245:VAL:HG12	1.87	0.57
1:C:197:GLN:NE2	3:C:411:NAG:H81	2.10	0.56
1:K:171:THR:O	1:K:172:ILE:CD1	2.47	0.56
1:G:311:HIS:HB2	1:G:321:TRP:CD1	2.40	0.56
1:A:280:ILE:CD1	1:A:315:ILE:CG1	2.73	0.56
1:E:292:CYS:HB3	1:E:300:LEU:HD22	1.86	0.56
2:D:421:HIS:O	2:D:425:LEU:CG	2.50	0.56
2:D:421:HIS:HB3	2:D:424:ILE:HD12	1.85	0.56
1:I:171:THR:O	1:I:172:ILE:CD1	2.50	0.56
1:E:180:GLU:HG3	1:E:181:GLY:N	2.20	0.56
2:J:470:LYS:NZ	2:L:479:GLU:HG2	2.20	0.56
2:H:435:ARG:HG3	2:J:434:LEU:HD22	1.88	0.56
1:C:185:ILE:HB	1:C:271:TRP:HB2	1.87	0.56
1:K:197:GLN:HE22	1:K:200:LYS:HD3	1.70	0.56
1:E:121:THR:HG22	1:E:122:HIS:H	1.70	0.56
2:H:439:ILE:CD1	2:J:438:THR:HG23	2.36	0.56
1:K:53:LEU:HG	1:K:62:ASP:CG	2.25	0.56
1:G:251:LYS:HE3	2:J:422:ASN:OD1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:439:ILE:HD11	2:F:438:THR:HG23	1.87	0.56
1:A:251:LYS:HE2	2:F:419:GLU:O	2.06	0.55
1:I:97:ILE:HA	1:I:243:ILE:HG23	1.88	0.55
2:J:410:LEU:HD11	2:J:435:ARG:HD2	1.83	0.55
2:H:417:MET:HB2	2:H:421:HIS:ND1	2.20	0.55
2:B:435:ARG:HD3	2:B:439:ILE:HG13	1.89	0.55
2:H:422:ASN:OD1	1:K:251:LYS:HE3	2.05	0.55
1:E:97:ILE:HA	1:E:243:ILE:CG2	2.37	0.55
1:C:97:ILE:HA	1:C:243:ILE:CG2	2.36	0.55
1:G:335:ARG:HB3	2:H:360:GLY:N	2.21	0.55
1:K:53:LEU:CD1	1:K:62:ASP:HB3	2.36	0.55
1:A:124:VAL:HG12	1:A:177:ILE:CG1	2.26	0.55
1:C:97:ILE:HA	1:C:243:ILE:HG23	1.88	0.55
1:A:129:ASN:HD21	3:K:403:BMA:C3	2.19	0.55
1:E:70:PRO:HB2	1:E:144:PRO:O	2.06	0.55
1:G:96:PRO:O	1:G:243:ILE:CG2	2.37	0.55
1:I:197:GLN:NE2	3:I:411:NAG:H81	2.14	0.55
1:E:278:LYS:HB3	2:F:411:GLN:HG3	1.89	0.55
2:D:416:ALA:CB	2:D:425:LEU:HD21	2.27	0.55
2:J:390:GLU:O	2:J:394:LYS:HG2	2.07	0.55
1:I:97:ILE:HA	1:I:243:ILE:CG2	2.37	0.55
1:E:180:GLU:CG	1:E:181:GLY:H	2.18	0.55
1:C:214:ALA:O	1:C:215:ASN:ND2	2.39	0.54
2:H:438:THR:HG23	2:L:439:ILE:HD11	1.88	0.54
1:K:284:LEU:CB	1:K:285:PRO:HA	2.36	0.54
1:C:222:VAL:HG13	1:E:259:THR:HG21	1.88	0.54
1:E:292:CYS:CB	1:E:300:LEU:HD22	2.37	0.54
1:K:311:HIS:HB2	1:K:321:TRP:CD1	2.42	0.54
1:I:176:TYR:HA	1:I:184:GLN:HE22	1.70	0.54
2:B:410:LEU:HG	2:B:432:ASP:OD2	2.08	0.54
1:C:131:PRO:CD	1:C:172:ILE:HD11	2.38	0.54
2:L:390:GLU:O	2:L:394:LYS:HG2	2.07	0.54
1:G:84:LEU:HD11	1:G:109:ASN:ND2	2.23	0.54
1:I:70:PRO:HB2	1:I:144:PRO:O	2.07	0.54
2:D:410:LEU:HG	2:D:432:ASP:OD2	2.08	0.54
1:E:243:ILE:HD11	1:E:265:LEU:HD11	1.89	0.54
1:A:75:LYS:HB3	1:K:118:ARG:HD2	1.89	0.54
1:I:131:PRO:O	1:I:170:LEU:HD13	2.08	0.54
1:G:197:GLN:NE2	4:G:412:NAG:H81	2.14	0.54
1:A:85:HIS:CD2	1:A:86:GLU:HG3	2.42	0.54
2:B:470:LYS:NZ	2:F:479:GLU:HG2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:331:GLY:HA2	2:J:368:TRP:CZ2	2.43	0.54
1:C:292:CYS:CB	1:C:300:LEU:HD22	2.37	0.54
1:G:119:LEU:HD23	1:G:120:SER:H	1.73	0.54
2:B:476:SER:HB3	2:B:511:LEU:HD13	1.89	0.54
1:G:292:CYS:CB	1:G:300:LEU:HD22	2.37	0.53
1:A:259:THR:HG21	1:E:222:VAL:HG13	1.90	0.53
2:J:408:LYS:HB2	2:J:435:ARG:NH2	2.22	0.53
1:I:215:ASN:HB2	2:L:419:GLU:HG3	1.90	0.53
1:E:119:LEU:CD2	1:E:269:LYS:HB3	2.38	0.53
1:C:41:PHE:CE1	1:C:282:GLY:HA2	2.44	0.53
2:D:438:THR:HG23	2:F:439:ILE:CD1	2.39	0.53
1:C:184:GLN:NE2	1:C:270:VAL:HG11	2.23	0.53
2:D:416:ALA:O	2:D:417:MET:HB2	2.09	0.53
1:I:1:ASP:CG	2:J:490:LYS:HG2	2.29	0.53
2:L:416:ALA:O	2:L:421:HIS:ND1	2.41	0.53
1:G:155:THR:HG23	1:G:187:VAL:HB	1.88	0.53
1:C:280:ILE:HD12	1:C:315:ILE:CG1	2.31	0.53
2:D:417:MET:HB2	2:D:421:HIS:ND1	2.23	0.53
2:H:416:ALA:O	2:H:421:HIS:ND1	2.42	0.53
1:A:197:GLN:NE2	3:A:412:NAG:H81	2.13	0.53
2:B:434:LEU:HD22	2:D:435:ARG:HG3	1.91	0.53
2:H:390:GLU:O	2:H:394:LYS:HG2	2.09	0.53
1:C:292:CYS:HB3	1:C:300:LEU:HD22	1.90	0.53
1:C:280:ILE:CD1	1:C:315:ILE:CG1	2.77	0.52
1:A:280:ILE:HD11	1:A:315:ILE:CG1	2.37	0.52
1:C:197:GLN:NE2	3:C:411:NAG:O7	2.42	0.52
1:K:119:LEU:CD2	1:K:269:LYS:HB3	2.35	0.52
2:B:408:LYS:O	2:B:435:ARG:NH2	2.42	0.52
1:I:122:HIS:O	1:I:269:LYS:HD3	2.09	0.52
1:G:180:GLU:HG3	1:G:181:GLY:N	2.23	0.52
1:I:41:PHE:CE1	1:I:282:GLY:HA2	2.44	0.52
1:C:208:GLN:HB3	1:C:261:GLN:HB2	1.91	0.52
1:A:280:ILE:HD12	1:A:315:ILE:CG1	2.30	0.52
2:J:421:HIS:O	2:J:425:LEU:CG	2.55	0.52
2:B:470:LYS:HZ3	2:F:479:GLU:HG2	1.75	0.52
1:G:208:GLN:HB3	1:G:261:GLN:HB2	1.92	0.52
1:K:163(C):ASN:O	1:K:165:THR:HG22	2.09	0.52
2:H:476:SER:HB3	2:H:511:LEU:HD13	1.92	0.52
1:C:182:GLU:HG2	1:C:274:SER:HB3	1.92	0.52
2:B:422:ASN:HA	2:B:425:LEU:HD12	1.90	0.52
1:K:97:ILE:HA	1:K:243:ILE:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:122:HIS:O	1:G:269:LYS:HD3	2.10	0.52
1:I:145:ASN:O	1:I:147:THR:N	2.43	0.52
1:A:208:GLN:HB3	1:A:261:GLN:HB2	1.92	0.52
2:L:422:ASN:HA	2:L:425:LEU:HD12	1.91	0.52
1:K:97:ILE:HA	1:K:243:ILE:HG23	1.90	0.52
1:I:197:GLN:NE2	3:I:411:NAG:O7	2.43	0.52
2:L:408:LYS:O	2:L:435:ARG:NH2	2.42	0.52
2:L:435:ARG:HD3	2:L:439:ILE:HG13	1.91	0.52
1:G:306:TYR:CE2	2:H:443:ILE:HD13	2.45	0.52
1:G:41:PHE:CE1	1:G:282:GLY:HA2	2.43	0.52
1:C:103:LYS:NZ	1:C:246:ASP:OD1	2.36	0.52
1:I:216:GLY:HA3	2:L:420:LEU:HD23	1.91	0.52
1:A:180:GLU:CG	1:A:181:GLY:N	2.61	0.52
1:A:335:ARG:HB3	2:B:360:GLY:N	2.25	0.52
2:J:435:ARG:CD	2:L:434:LEU:CD2	2.84	0.51
2:J:435:ARG:NE	2:L:434:LEU:HD22	2.25	0.51
1:E:119:LEU:HD23	1:E:120:SER:H	1.74	0.51
1:A:53:LEU:HD11	1:A:62:ASP:HB3	1.91	0.51
2:J:410:LEU:HG	2:J:432:ASP:OD2	2.10	0.51
1:K:131:PRO:CD	1:K:172:ILE:HD11	2.40	0.51
2:J:416:ALA:O	2:J:421:HIS:ND1	2.43	0.51
1:G:119:LEU:CD2	1:G:269:LYS:HB3	2.39	0.51
2:L:398:ASN:ND2	2:L:398:ASN:C	2.62	0.51
2:D:390:GLU:O	2:D:394:LYS:HG2	2.10	0.51
2:L:439:ILE:O	2:L:443:ILE:HG13	2.10	0.51
1:G:41:PHE:O	1:G:286:LEU:HA	2.10	0.51
1:E:184:GLN:NE2	1:E:270:VAL:HG11	2.25	0.51
1:A:172:ILE:HG13	1:A:260:TYR:CE2	2.44	0.51
1:G:288:GLY:CA	4:G:405:NAG:H62	2.30	0.51
1:C:141:GLY:O	1:C:142:SER:OG	2.24	0.51
2:B:416:ALA:O	2:B:421:HIS:ND1	2.43	0.51
1:G:131:PRO:O	1:G:170:LEU:HD13	2.10	0.51
2:B:439:ILE:O	2:B:443:ILE:HG13	2.10	0.51
2:H:435:ARG:HD3	2:H:439:ILE:HG12	1.92	0.51
1:A:280:ILE:CG2	1:A:295:GLU:HG3	2.39	0.51
1:C:278:LYS:NZ	2:D:409:ASN:OD1	2.44	0.51
1:K:280:ILE:HD11	1:K:315:ILE:CG1	2.40	0.51
1:I:131:PRO:CD	1:I:172:ILE:HD11	2.40	0.51
1:I:152:PHE:CZ	1:I:265:LEU:HD21	2.46	0.51
1:A:75:LYS:HE2	1:K:116:HIS:CG	2.46	0.51
2:J:416:ALA:CB	2:J:425:LEU:HD21	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:GLN:NE2	3:A:412:NAG:O7	2.44	0.51
1:E:145:ASN:O	1:E:147:THR:N	2.44	0.51
1:E:121:THR:CG2	1:E:122:HIS:N	2.74	0.51
1:A:105:ARG:NH2	1:A:233:GLU:OE1	2.44	0.51
2:B:438:THR:HG23	2:D:439:ILE:HD13	1.93	0.51
1:I:53:LEU:HG	1:I:62:ASP:CG	2.30	0.51
1:K:84:LEU:HD11	1:K:109:ASN:ND2	2.25	0.50
1:E:163(C):ASN:O	1:E:165:THR:HG22	2.11	0.50
2:H:419:GLU:O	1:K:251:LYS:HE2	2.10	0.50
2:J:439:ILE:HD11	2:L:438:THR:HG23	1.94	0.50
1:E:197:GLN:HE21	3:E:412:NAG:C8	2.14	0.50
1:C:122:HIS:O	1:C:269:LYS:HD3	2.12	0.50
1:C:145:ASN:O	1:C:146:ILE:C	2.50	0.50
1:A:145:ASN:O	1:A:146:ILE:C	2.50	0.50
1:E:306:TYR:CE2	2:F:443:ILE:HD13	2.47	0.50
1:K:53:LEU:HD11	1:K:62:ASP:HB3	1.94	0.50
1:E:278:LYS:NZ	2:F:409:ASN:OD1	2.45	0.50
1:A:131:PRO:O	1:A:170:LEU:HD13	2.11	0.50
1:I:145:ASN:O	1:I:146:ILE:C	2.50	0.50
2:H:438:THR:HG23	2:L:439:ILE:HD13	1.92	0.50
2:J:418:ASP:O	2:J:422:ASN:ND2	2.45	0.50
1:E:145:ASN:O	1:E:146:ILE:C	2.50	0.50
1:G:185:ILE:HB	1:G:271:TRP:HB2	1.94	0.50
1:A:149:GLY:HA3	3:A:401:NAG:O6	2.11	0.50
1:I:119:LEU:HD23	1:I:120:SER:H	1.72	0.50
1:E:122:HIS:O	1:E:269:LYS:HD3	2.12	0.50
1:G:105:ARG:NH2	1:G:233:GLU:OE1	2.43	0.50
1:E:131:PRO:O	1:E:170:LEU:HD13	2.10	0.50
1:G:124:VAL:HG12	1:G:177:ILE:CG1	2.31	0.50
1:A:131:PRO:HD2	1:A:172:ILE:HD11	1.94	0.50
1:A:320:ILE:HD11	2:B:405:LEU:CD2	2.39	0.50
1:E:121:THR:CG2	1:E:122:HIS:H	2.24	0.50
1:K:145:ASN:O	1:K:146:ILE:C	2.50	0.50
1:A:94:CYS:O	1:A:235:GLY:N	2.43	0.50
1:K:208:GLN:HB3	1:K:261:GLN:HB2	1.93	0.50
1:I:152:PHE:CE2	1:I:265:LEU:HD21	2.47	0.50
2:H:422:ASN:HA	2:H:425:LEU:HD12	1.93	0.49
2:B:479:GLU:CG	2:D:470:LYS:HZ3	2.22	0.49
2:D:439:ILE:O	2:D:443:ILE:HG13	2.12	0.49
1:E:41:PHE:CE1	1:E:282:GLY:HA2	2.47	0.49
1:K:102:THR:HG22	1:K:221:TYR:CE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LYS:NZ	1:A:246:ASP:OD1	2.38	0.49
1:E:105:ARG:NH2	1:E:233:GLU:OE1	2.45	0.49
1:G:280:ILE:HD11	1:G:315:ILE:HG12	1.85	0.49
1:C:155:THR:HG21	1:C:187:VAL:CB	2.42	0.49
1:G:155:THR:HG21	1:G:187:VAL:HB	1.90	0.49
1:A:97:ILE:HA	1:A:243:ILE:HG23	1.93	0.49
2:B:390:GLU:O	2:B:394:LYS:HG2	2.11	0.49
1:E:331:GLY:HA2	2:F:368:TRP:CZ2	2.47	0.49
2:F:416:ALA:O	2:F:421:HIS:ND1	2.44	0.49
2:J:439:ILE:O	2:J:443:ILE:HG13	2.12	0.49
2:F:435:ARG:HD3	2:F:439:ILE:HG13	1.94	0.49
2:F:390:GLU:O	2:F:394:LYS:HG2	2.12	0.49
1:G:126:ASN:ND2	1:G:129:ASN:ND2	2.60	0.49
1:G:107:LEU:HB3	1:G:108:PRO:HD3	1.95	0.49
1:G:145:ASN:O	1:G:146:ILE:C	2.50	0.49
2:D:416:ALA:O	2:D:421:HIS:ND1	2.45	0.49
1:C:119:LEU:CD2	1:C:269:LYS:HB3	2.34	0.49
1:G:288:GLY:CA	4:G:405:NAG:O6	2.56	0.49
2:J:435:ARG:HH11	2:L:434:LEU:CD2	1.98	0.49
2:L:421:HIS:HB3	2:L:424:ILE:HD12	1.94	0.49
2:B:438:THR:HG23	2:D:439:ILE:HD11	1.93	0.49
1:E:197:GLN:CD	3:E:412:NAG:O7	2.51	0.49
1:A:320:ILE:HD13	2:B:405:LEU:HD22	1.91	0.49
1:I:52:LYS:HD3	1:I:62:ASP:OD1	2.12	0.49
1:I:278:LYS:HB3	2:J:411:GLN:HG3	1.94	0.49
1:E:185:ILE:HB	1:E:271:TRP:HB2	1.95	0.49
1:K:58:LEU:O	1:K:59:ASN:HB2	2.13	0.49
1:C:163(C):ASN:O	1:C:165:THR:HG22	2.13	0.49
1:K:105:ARG:NH2	1:K:233:GLU:OE1	2.46	0.49
1:I:187:VAL:O	1:I:267:PRO:HB3	2.13	0.49
2:B:439:ILE:HD13	2:F:438:THR:HG23	1.94	0.49
1:I:103:LYS:NZ	1:I:246:ASP:OD1	2.38	0.49
2:H:398:ASN:ND2	2:H:398:ASN:C	2.66	0.48
1:K:145:ASN:O	1:K:147:THR:N	2.46	0.48
1:E:53:LEU:HG	1:E:62:ASP:CG	2.33	0.48
1:I:163(C):ASN:O	1:I:165:THR:HG22	2.12	0.48
1:C:85:HIS:CD2	1:C:86:GLU:HG3	2.47	0.48
1:C:20:THR:HB	2:D:452:GLU:OE2	2.12	0.48
2:J:465:LEU:HD12	2:L:353:ILE:HG21	1.96	0.48
1:I:170:LEU:HD12	1:I:260:TYR:CE1	2.48	0.48
1:K:125:ILE:O	1:K:268:GLN:NE2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:479:GLU:HG2	2:L:470:LYS:HZ3	1.77	0.48
2:B:435:ARG:HG3	2:F:434:LEU:HD22	1.95	0.48
2:F:407:VAL:HG12	2:F:435:ARG:HH21	1.79	0.48
1:K:41:PHE:CE1	1:K:282:GLY:HA2	2.48	0.48
1:C:176:TYR:CE1	1:C:253:GLY:N	2.73	0.48
2:H:418:ASP:O	2:H:422:ASN:ND2	2.46	0.48
1:E:155:THR:CG2	1:E:187:VAL:CB	2.88	0.48
2:J:395:ILE:HG12	2:J:454:ILE:HD13	1.94	0.48
1:C:53:LEU:O	1:C:76:ILE:HG23	2.13	0.48
1:G:178:CYS:SG	1:G:184:GLN:HG3	2.53	0.48
2:J:470:LYS:HZ3	2:L:479:GLU:HG2	1.78	0.48
1:A:36:PRO:HB2	1:A:297:TYR:CE1	2.48	0.48
1:K:52:LYS:HD3	1:K:62:ASP:OD1	2.13	0.48
1:G:63:LEU:HA	1:G:108:PRO:HG3	1.95	0.48
1:E:63:LEU:HA	1:E:108:PRO:HG3	1.96	0.48
1:C:145:ASN:O	1:C:147:THR:N	2.47	0.48
1:E:41:PHE:O	1:E:286:LEU:HA	2.14	0.48
1:E:208:GLN:HB3	1:E:261:GLN:HB2	1.96	0.48
1:C:107:LEU:HB3	1:C:108:PRO:HD3	1.94	0.48
1:C:119:LEU:HD23	1:C:120:SER:O	2.13	0.48
1:I:155:THR:HG21	1:I:187:VAL:HB	1.93	0.48
1:K:122:HIS:O	1:K:269:LYS:HD3	2.13	0.48
1:G:126:ASN:HD22	1:G:129:ASN:ND2	2.12	0.48
1:K:135:TYR:CD1	1:K:159:ALA:HB1	2.49	0.48
1:A:163(C):ASN:O	1:A:165:THR:HG22	2.14	0.48
1:E:214:ALA:CB	1:E:248:MET:HE2	2.31	0.48
1:A:75:LYS:HB3	1:K:118:ARG:CD	2.43	0.48
1:I:119:LEU:CD2	1:I:269:LYS:HB3	2.37	0.48
1:K:119:LEU:HD23	1:K:120:SER:H	1.78	0.48
1:G:145:ASN:O	1:G:147:THR:N	2.47	0.48
1:G:53:LEU:CD1	1:G:62:ASP:HB3	2.44	0.48
1:G:172:ILE:HG13	1:G:260:TYR:CE2	2.44	0.48
1:K:212:SER:HG	1:K:219:THR:HG1	1.60	0.48
2:H:419:GLU:OE2	1:K:251:LYS:CG	2.45	0.47
1:C:280:ILE:CG2	1:C:295:GLU:HG3	2.41	0.47
1:C:172:ILE:HG12	1:C:260:TYR:HE2	1.79	0.47
1:E:52:LYS:HD3	1:E:62:ASP:OD1	2.14	0.47
1:E:182:GLU:HG2	1:E:274:SER:HB3	1.96	0.47
1:I:337:PRO:HA	2:J:360:GLY:O	2.15	0.47
1:A:193:ASP:OD1	1:A:198:MET:HB2	2.14	0.47
2:B:419:GLU:O	1:C:251:LYS:HE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:250:GLN:O	1:I:251:LYS:O	2.33	0.47
1:I:131:PRO:HD2	1:I:172:ILE:HD11	1.96	0.47
2:F:435:ARG:HD3	2:F:439:ILE:HG12	1.95	0.47
2:F:410:LEU:HG	2:F:432:ASP:OD2	2.14	0.47
1:G:131:PRO:CD	1:G:172:ILE:HD11	2.44	0.47
1:A:52:LYS:HD3	1:A:62:ASP:OD1	2.14	0.47
1:K:335:ARG:HD2	2:L:359:GLY:HA2	1.97	0.47
2:D:427:LEU:O	2:D:430:LYS:HB3	2.14	0.47
2:D:353:ILE:HG21	2:F:465:LEU:HD12	1.95	0.47
1:A:63:LEU:HA	1:A:108:PRO:HG3	1.95	0.47
1:G:184:GLN:HE21	1:G:184:GLN:HB3	1.53	0.47
1:K:250:GLN:O	1:K:251:LYS:O	2.33	0.47
1:A:97:ILE:HA	1:A:243:ILE:CG2	2.44	0.47
1:A:240:SER:OG	3:A:412:NAG:C8	2.51	0.47
1:I:119:LEU:HD23	1:I:120:SER:O	2.14	0.47
2:B:435:ARG:HD3	2:B:439:ILE:HG12	1.96	0.47
1:I:53:LEU:HD11	1:I:62:ASP:HB3	1.96	0.47
2:D:481:GLY:HA2	2:F:467:ARG:HH21	1.80	0.47
2:F:421:HIS:O	2:F:425:LEU:CD1	2.63	0.47
1:K:81:VAL:CG1	1:K:315:ILE:HD11	2.45	0.47
1:C:197:GLN:HE21	3:C:411:NAG:C8	2.16	0.47
1:K:155:THR:HG23	1:K:187:VAL:HB	1.96	0.47
1:K:193:ASP:OD1	1:K:198:MET:HB2	2.15	0.47
1:C:52:LYS:HD3	1:C:62:ASP:OD1	2.15	0.47
2:J:416:ALA:O	2:J:417:MET:HB2	2.14	0.47
1:A:122:HIS:O	1:A:269:LYS:HD3	2.15	0.47
1:G:337:PRO:HA	2:H:360:GLY:O	2.14	0.47
2:D:434:LEU:HD22	2:F:435:ARG:HG3	1.97	0.47
1:G:278:LYS:HB3	2:H:411:GLN:HG3	1.96	0.47
1:E:102:THR:HG22	1:E:221:TYR:CE2	2.50	0.47
1:I:208:GLN:HB3	1:I:261:GLN:HB2	1.96	0.47
1:E:131:PRO:CD	1:E:172:ILE:HD11	2.44	0.47
1:K:172:ILE:HG13	1:K:260:TYR:CE2	2.45	0.47
1:I:172:ILE:CG1	1:I:260:TYR:CE2	2.92	0.47
1:C:53:LEU:HG	1:C:62:ASP:CG	2.35	0.47
1:G:250:GLN:O	1:G:251:LYS:O	2.33	0.47
2:H:470:LYS:NZ	2:J:479:GLU:HG2	2.29	0.47
1:A:250:GLN:O	1:A:251:LYS:O	2.33	0.47
1:A:81:VAL:CG1	1:A:315:ILE:HD11	2.45	0.47
2:J:417:MET:HB2	2:J:421:HIS:ND1	2.29	0.47
2:D:479:GLU:HG2	2:F:470:LYS:NZ	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLU:HG2	1:A:274:SER:HB3	1.96	0.47
1:A:225:ILE:HA	1:A:225:ILE:HD13	1.72	0.47
1:E:124:VAL:HG11	1:E:270:VAL:HG21	1.97	0.46
2:H:420:LEU:HD12	2:H:421:HIS:CE1	2.50	0.46
1:I:280:ILE:HD11	1:I:315:ILE:CG1	2.40	0.46
1:C:278:LYS:HB3	2:D:411:GLN:HG3	1.97	0.46
1:E:250:GLN:O	1:E:251:LYS:O	2.33	0.46
1:I:165:THR:OG1	1:I:166:ALA:N	2.48	0.46
1:C:63:LEU:HA	1:C:108:PRO:HG3	1.97	0.46
1:I:185:ILE:HB	1:I:271:TRP:HB2	1.96	0.46
1:C:250:GLN:O	1:C:251:LYS:O	2.33	0.46
2:J:394:LYS:HD3	1:K:20:THR:OG1	2.14	0.46
2:B:465:LEU:HD12	2:F:353:ILE:HG21	1.98	0.46
1:K:131:PRO:C	1:K:170:LEU:HD13	2.36	0.46
1:K:278:LYS:HB3	2:L:411:GLN:HG3	1.98	0.46
1:K:107:LEU:HB3	1:K:108:PRO:HD3	1.96	0.46
1:E:104:ILE:HD13	1:E:245:VAL:HG12	1.97	0.46
1:E:231:GLN:HG2	1:E:242:ARG:NH2	2.30	0.46
2:B:422:ASN:OD1	1:C:251:LYS:HE3	2.16	0.46
1:E:172:ILE:HG13	1:E:260:TYR:CE2	2.45	0.46
1:I:171:THR:HG23	1:I:259:THR:HG22	1.97	0.46
1:E:193:ASP:OD1	1:E:198:MET:HB2	2.16	0.46
2:J:439:ILE:HD13	2:L:438:THR:HG23	1.96	0.46
2:L:440:SER:O	2:L:444:GLU:HG3	2.16	0.46
1:E:72:CYS:O	1:E:73:THR:HG23	2.16	0.46
1:C:95:PHE:CG	1:C:96:PRO:HD2	2.50	0.46
1:G:284:LEU:CB	1:G:285:PRO:HA	2.36	0.46
1:A:292:CYS:HB3	1:A:300:LEU:HD23	1.98	0.46
1:A:30:ILE:HG13	1:A:330:ASN:HB2	1.97	0.46
1:I:182:GLU:HG2	1:I:274:SER:HB3	1.96	0.46
2:D:422:ASN:HA	2:D:425:LEU:HD12	1.97	0.46
1:K:155:THR:HG21	1:K:187:VAL:HB	1.95	0.46
1:G:20:THR:OG1	2:L:394:LYS:HD3	2.15	0.46
1:K:41:PHE:O	1:K:286:LEU:HA	2.16	0.46
1:A:103:LYS:HG3	1:A:247:TYR:CE1	2.50	0.46
1:C:165:THR:HA	1:C:203:GLY:HA3	1.97	0.46
1:I:30:ILE:HG13	1:I:330:ASN:HB2	1.98	0.46
1:A:114:TYR:CG	1:A:273:ALA:HB1	2.51	0.46
1:K:197:GLN:CA	1:K:197:GLN:HE21	1.98	0.46
1:E:55:PRO:C	1:E:56:LYS:HG2	2.32	0.46
1:G:197:GLN:NE2	4:G:412:NAG:O7	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:155:THR:CG2	1:G:187:VAL:CB	2.86	0.46
2:L:407:VAL:HG12	2:L:435:ARG:HH21	1.81	0.46
2:L:420:LEU:HD12	2:L:421:HIS:CE1	2.51	0.46
1:C:131:PRO:HD2	1:C:172:ILE:HD11	1.97	0.46
1:K:131:PRO:HD2	1:K:172:ILE:HD11	1.98	0.46
2:L:435:ARG:HD3	2:L:439:ILE:HG12	1.98	0.46
1:G:251:LYS:HE2	2:J:419:GLU:O	2.16	0.46
1:E:165:THR:HA	1:E:203:GLY:HA3	1.97	0.46
1:K:3:ILE:HA	2:L:372:THR:O	2.16	0.46
2:H:439:ILE:HD13	2:J:438:THR:HG23	1.97	0.45
1:G:231:GLN:HB3	1:G:234:ASP:OD2	2.16	0.45
1:I:251:LYS:HE3	2:L:422:ASN:CG	2.36	0.45
1:I:193:ASP:OD1	1:I:198:MET:HB2	2.16	0.45
1:K:185:ILE:HB	1:K:271:TRP:HB2	1.98	0.45
1:G:280:ILE:CG2	1:G:295:GLU:HG3	2.44	0.45
1:G:180:GLU:CG	1:G:181:GLY:H	2.22	0.45
1:A:178:CYS:SG	1:A:184:GLN:HG3	2.55	0.45
1:G:301:ASN:ND2	4:G:404:NAG:C7	2.79	0.45
1:I:251:LYS:CE	2:L:422:ASN:OD1	2.58	0.45
1:K:280:ILE:CG2	1:K:295:GLU:HG3	2.42	0.45
1:K:97:ILE:HG12	1:K:243:ILE:HG23	1.98	0.45
1:A:131:PRO:CD	1:A:172:ILE:CD1	2.95	0.45
2:B:407:VAL:HG12	2:B:435:ARG:HH21	1.82	0.45
2:D:398:ASN:ND2	2:D:398:ASN:C	2.66	0.45
1:I:94:CYS:O	1:I:235:GLY:N	2.47	0.45
1:I:165:THR:HA	1:I:203:GLY:HA3	1.97	0.45
2:D:481:GLY:HA2	2:F:467:ARG:NH2	2.32	0.45
1:I:114:TYR:CG	1:I:273:ALA:HB1	2.51	0.45
1:I:104:ILE:HB	1:I:245:VAL:O	2.15	0.45
2:B:470:LYS:NZ	2:F:479:GLU:CG	2.80	0.45
2:B:394:LYS:HD3	1:E:20:THR:OG1	2.17	0.45
1:C:225:ILE:HD13	1:C:225:ILE:HA	1.76	0.45
1:A:231:GLN:HG2	1:A:242:ARG:NH2	2.31	0.45
1:A:215:ASN:C	1:A:215:ASN:ND2	2.63	0.45
1:C:193:ASP:OD1	1:C:198:MET:HB2	2.16	0.45
2:H:410:LEU:HG	2:H:432:ASP:OD2	2.16	0.45
1:I:105:ARG:NH2	1:I:233:GLU:OE1	2.48	0.45
1:I:39:SER:OG	1:I:40:HIS:N	2.50	0.45
1:K:104:ILE:HB	1:K:245:VAL:O	2.17	0.45
1:A:135:TYR:CD1	1:A:159:ALA:HB1	2.50	0.45
2:H:417:MET:HB2	2:H:421:HIS:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:84:LEU:HD11	1:I:109:ASN:ND2	2.32	0.45
1:K:306:TYR:CE2	2:L:443:ILE:HD13	2.51	0.45
2:F:440:SER:O	2:F:444:GLU:HG3	2.16	0.45
2:H:420:LEU:CD1	2:H:421:HIS:CE1	3.00	0.45
1:K:170:LEU:HD12	1:K:260:TYR:CE1	2.51	0.45
2:D:435:ARG:HD3	2:D:439:ILE:HG12	1.99	0.45
1:C:41:PHE:O	1:C:286:LEU:HA	2.17	0.45
1:A:184:GLN:NE2	1:A:270:VAL:HG11	2.31	0.45
1:K:57:CYS:O	1:K:60:CYS:HB2	2.17	0.45
1:A:61:THR:O	1:A:64:ASP:HB2	2.16	0.45
1:K:281:LYS:HB2	1:K:295:GLU:HG2	1.98	0.45
2:H:434:LEU:HD22	2:L:435:ARG:HG3	1.98	0.45
1:K:178:CYS:SG	1:K:184:GLN:HG3	2.57	0.45
1:K:165:THR:HA	1:K:203:GLY:HA3	1.98	0.45
1:E:30:ILE:HG13	1:E:330:ASN:HB2	1.98	0.45
1:A:306:TYR:CE2	2:B:443:ILE:HD13	2.52	0.45
2:D:407:VAL:HG12	2:D:435:ARG:HH21	1.82	0.45
1:I:63:LEU:HA	1:I:108:PRO:HG3	1.98	0.45
1:E:184:GLN:OE1	1:E:250:GLN:OE1	2.35	0.44
1:C:280:ILE:HD11	1:C:315:ILE:CG1	2.44	0.44
1:E:104:ILE:HB	1:E:245:VAL:O	2.17	0.44
1:E:231:GLN:HB3	1:E:234:ASP:OD2	2.17	0.44
1:G:193:ASP:OD1	1:G:198:MET:HB2	2.17	0.44
1:I:95:PHE:CG	1:I:96:PRO:HD2	2.53	0.44
1:G:155:THR:HG21	1:G:187:VAL:CB	2.47	0.44
1:A:72:CYS:O	1:A:73:THR:HG23	2.17	0.44
1:K:182:GLU:HG2	1:K:274:SER:HB3	1.98	0.44
2:J:410:LEU:HD12	2:J:435:ARG:NH1	2.25	0.44
2:J:410:LEU:HD13	2:J:435:ARG:NH1	2.31	0.44
1:C:197:GLN:CD	3:C:411:NAG:O7	2.56	0.44
1:E:197:GLN:HA	1:E:197:GLN:OE1	2.18	0.44
1:A:147:THR:O	1:A:148:ASN:OD1	2.36	0.44
1:C:165:THR:OG1	1:C:166:ALA:N	2.50	0.44
2:D:421:HIS:O	2:D:425:LEU:CD1	2.66	0.44
1:I:172:ILE:HG12	1:I:260:TYR:CE2	2.53	0.44
1:K:313:LYS:HB3	2:L:411:GLN:HA	1.99	0.44
1:G:163(C):ASN:O	1:G:165:THR:HG22	2.17	0.44
1:G:30:ILE:HG13	1:G:330:ASN:HB2	2.00	0.44
1:A:185:ILE:HB	1:A:271:TRP:HB2	2.00	0.44
1:I:135:TYR:CD1	1:I:159:ALA:HB1	2.53	0.44
1:C:152:PHE:CZ	1:C:265:LEU:HD21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:439:ILE:O	2:F:443:ILE:HG13	2.17	0.44
1:I:103:LYS:HB3	2:J:420:LEU:HD21	1.99	0.44
1:K:231:GLN:HG2	1:K:242:ARG:NH2	2.33	0.44
1:I:8:THR:HG23	2:J:364:MET:O	2.18	0.44
1:E:95:PHE:CG	1:E:96:PRO:HD2	2.53	0.44
1:I:107:LEU:HB3	1:I:108:PRO:HD3	1.99	0.44
1:G:165:THR:HA	1:G:203:GLY:HA3	1.99	0.44
1:C:30:ILE:HG13	1:C:330:ASN:HB2	2.00	0.44
1:K:85:HIS:ND1	1:K:86:GLU:HG3	2.32	0.44
2:J:421:HIS:O	2:J:425:LEU:CD1	2.66	0.44
1:A:131:PRO:HD2	1:A:172:ILE:CD1	2.47	0.44
1:E:284:LEU:CB	1:E:285:PRO:HA	2.36	0.44
1:A:53:LEU:HG	1:A:62:ASP:CG	2.38	0.44
1:K:94:CYS:O	1:K:235:GLY:N	2.46	0.44
1:E:53:LEU:O	1:E:76:ILE:HG23	2.18	0.44
1:A:165:THR:OG1	1:A:166:ALA:N	2.51	0.44
1:A:231:GLN:HB3	1:A:234:ASP:OD2	2.18	0.44
1:E:212:SER:HG	1:E:219:THR:HG1	1.66	0.44
1:G:104:ILE:HD13	1:G:245:VAL:HG12	2.00	0.44
1:A:150:ASN:OD1	1:A:150:ASN:N	2.50	0.44
1:C:131:PRO:O	1:C:170:LEU:HD13	2.17	0.44
2:J:470:LYS:NZ	2:L:479:GLU:CG	2.81	0.44
1:K:172:ILE:CG1	1:K:260:TYR:CE2	2.97	0.43
1:I:172:ILE:HG13	1:I:260:TYR:CE2	2.41	0.43
1:C:103:LYS:HB3	2:D:420:LEU:HD21	1.99	0.43
1:E:165:THR:OG1	1:E:166:ALA:N	2.51	0.43
1:E:215:ASN:ND2	1:E:215:ASN:C	2.64	0.43
1:I:281:LYS:HB2	1:I:295:GLU:HG2	2.00	0.43
1:A:95:PHE:CD1	1:A:96:PRO:HD2	2.53	0.43
1:E:187:VAL:O	1:E:267:PRO:HB3	2.18	0.43
1:K:30:ILE:HG13	1:K:330:ASN:HB2	1.99	0.43
2:J:496:LEU:HD12	2:J:499:ILE:HD12	2.00	0.43
1:G:184:GLN:OE1	1:G:270:VAL:HG11	2.18	0.43
1:A:197:GLN:HA	1:A:197:GLN:OE1	2.18	0.43
2:J:427:LEU:O	2:J:430:LYS:HB3	2.18	0.43
2:J:398:ASN:C	2:J:398:ASN:ND2	2.69	0.43
1:I:156:MET:HG3	1:I:265:LEU:HD23	2.00	0.43
2:D:395:ILE:HG12	2:D:454:ILE:HD13	2.00	0.43
2:J:408:LYS:H	2:J:435:ARG:NH2	2.16	0.43
1:G:131:PRO:CG	1:G:172:ILE:CD1	2.79	0.43
1:K:197:GLN:CD	3:K:411:NAG:O7	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:155:THR:HG23	1:I:187:VAL:HB	1.95	0.43
1:E:53:LEU:CD1	1:E:62:ASP:HB3	2.49	0.43
2:H:353:ILE:HG21	2:L:465:LEU:HD12	1.99	0.43
1:K:16:VAL:HG12	1:K:17:LYS:N	2.34	0.43
1:A:284:LEU:CB	1:A:285:PRO:HA	2.36	0.43
1:I:147:THR:HG22	1:I:148:ASN:N	2.33	0.43
2:H:387:SER:HB2	2:H:465:LEU:HD11	2.01	0.43
2:H:421:HIS:O	2:H:425:LEU:CD1	2.66	0.43
1:A:165:THR:HA	1:A:203:GLY:HA3	1.98	0.43
2:F:387:SER:HB2	2:F:465:LEU:HD11	2.01	0.43
1:G:135:TYR:HD2	1:G:161:PRO:HA	1.84	0.43
1:I:225:ILE:HA	1:I:225:ILE:HD13	1.78	0.43
1:C:57:CYS:O	1:C:60:CYS:HB2	2.18	0.43
1:C:104:ILE:HB	1:C:245:VAL:O	2.19	0.43
1:E:280:ILE:HD11	1:E:315:ILE:CG1	2.42	0.43
1:I:131:PRO:C	1:I:170:LEU:HD13	2.39	0.43
2:B:387:SER:HB2	2:B:465:LEU:HD11	2.01	0.43
1:I:231:GLN:HG2	1:I:242:ARG:NH2	2.33	0.43
1:C:172:ILE:CG1	1:C:260:TYR:CE2	2.97	0.43
1:K:95:PHE:CG	1:K:96:PRO:HD2	2.54	0.43
1:G:231:GLN:HG2	1:G:242:ARG:NH2	2.33	0.43
2:L:395:ILE:HG12	2:L:454:ILE:HD13	1.99	0.43
1:K:292:CYS:HB3	1:K:300:LEU:HD22	2.00	0.43
2:H:479:GLU:CG	2:L:470:LYS:NZ	2.80	0.43
1:C:20:THR:OG1	2:F:394:LYS:HD3	2.19	0.43
1:C:35:THR:OG1	1:C:308:THR:OG1	2.35	0.43
1:C:302:LYS:HD2	1:C:317:ASN:OD1	2.19	0.43
2:D:472:MET:H	2:D:472:MET:HG2	1.65	0.43
1:G:131:PRO:C	1:G:170:LEU:HD13	2.39	0.43
1:G:61:THR:HG23	1:G:92:SER:HB2	2.00	0.43
1:C:172:ILE:HG13	1:C:260:TYR:CE2	2.49	0.42
1:K:243:ILE:HD11	1:K:265:LEU:CD1	2.48	0.42
1:C:72:CYS:O	1:C:73:THR:HG23	2.19	0.42
1:E:85:HIS:ND1	1:E:86:GLU:HG3	2.33	0.42
1:G:85:HIS:ND1	1:G:86:GLU:HG3	2.34	0.42
1:I:57:CYS:O	1:I:60:CYS:HB2	2.19	0.42
1:G:172:ILE:CG1	1:G:260:TYR:CE2	2.97	0.42
1:I:131:PRO:HD2	1:I:172:ILE:CD1	2.49	0.42
1:I:172:ILE:HG12	1:I:260:TYR:HE2	1.78	0.42
1:I:21:GLN:HE22	2:J:348:GLY:HA2	1.84	0.42
2:F:472:MET:H	2:F:472:MET:HG2	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:102:THR:HG22	1:G:221:TYR:CE2	2.53	0.42
2:D:417:MET:HB2	2:D:421:HIS:CE1	2.54	0.42
2:H:420:LEU:HD12	2:H:421:HIS:HE1	1.84	0.42
1:C:176:TYR:OH	1:C:182:GLU:O	2.32	0.42
1:C:152:PHE:CE2	1:C:265:LEU:HD21	2.54	0.42
1:G:170:LEU:HD12	1:G:260:TYR:CE1	2.54	0.42
1:A:20:THR:CG2	1:A:21:GLN:HG2	2.47	0.42
1:C:94:CYS:O	1:C:235:GLY:N	2.52	0.42
1:A:145:ASN:O	1:A:147:THR:N	2.52	0.42
1:K:104:ILE:HD13	1:K:245:VAL:HG12	2.00	0.42
1:G:165:THR:OG1	1:G:166:ALA:N	2.52	0.42
1:I:135:TYR:HD2	1:I:161:PRO:HA	1.84	0.42
2:F:496:LEU:HD12	2:F:499:ILE:HD12	2.01	0.42
1:I:111:LEU:HA	1:I:111:LEU:HD23	1.89	0.42
1:A:56:LYS:HZ2	1:A:75:LYS:HZ1	1.63	0.42
1:A:172:ILE:CG1	1:A:260:TYR:CE2	2.97	0.42
1:A:155:THR:CG2	1:A:187:VAL:CB	2.89	0.42
1:C:335:ARG:HB3	2:D:360:GLY:N	2.32	0.42
1:C:156:MET:HG3	1:C:265:LEU:HD23	2.01	0.42
1:A:90:VAL:HG12	1:A:91:THR:O	2.19	0.42
1:I:97:ILE:HG12	1:I:243:ILE:HG23	2.01	0.42
1:I:176:TYR:O	1:I:184:GLN:NE2	2.52	0.42
1:A:107:LEU:HB3	1:A:108:PRO:HD3	2.01	0.42
1:G:160:VAL:O	1:G:162:LYS:N	2.53	0.42
1:I:85:HIS:ND1	1:I:86:GLU:HG3	2.35	0.42
1:E:2:ARG:NH1	2:F:480:ILE:HD13	2.34	0.42
1:C:215:ASN:C	1:C:215:ASN:ND2	2.62	0.42
1:G:215:ASN:ND2	1:G:215:ASN:C	2.64	0.42
1:C:290:ALA:HB1	1:C:300:LEU:H	1.84	0.42
2:F:398:ASN:ND2	2:F:398:ASN:C	2.65	0.42
2:J:434:LEU:HD23	2:J:434:LEU:HA	1.86	0.42
1:C:53:LEU:CD1	1:C:62:ASP:HB3	2.50	0.42
2:F:395:ILE:HG12	2:F:454:ILE:HD13	2.02	0.42
1:E:135:TYR:CD1	1:E:159:ALA:HB1	2.54	0.42
2:L:410:LEU:HG	2:L:432:ASP:OD2	2.20	0.42
1:K:174:VAL:CG1	1:K:250:GLN:HE22	2.32	0.42
1:I:197:GLN:CD	3:I:411:NAG:O7	2.57	0.42
1:I:70:PRO:HG3	1:I:152:PHE:O	2.19	0.42
1:C:114:TYR:CG	1:C:273:ALA:HB1	2.55	0.42
1:C:39:SER:OG	1:C:40:HIS:N	2.52	0.42
1:C:48:GLU:HG2	1:C:48:GLU:H	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:280:ILE:HG22	1:K:281:LYS:N	2.35	0.42
1:A:292:CYS:CB	1:A:300:LEU:HD23	2.49	0.42
2:H:427:LEU:O	2:H:430:LYS:HB3	2.20	0.42
2:D:438:THR:HG23	2:F:439:ILE:HD11	2.01	0.42
1:K:9:SER:HB3	2:L:362:GLU:HB3	2.01	0.42
1:C:102:THR:HG22	1:C:221:TYR:CE2	2.55	0.42
1:G:95:PHE:CG	1:G:96:PRO:HD2	2.55	0.42
1:A:81:VAL:HG11	1:A:315:ILE:HD11	2.02	0.42
1:A:197:GLN:CD	3:A:412:NAG:O7	2.58	0.42
2:D:435:ARG:CD	2:D:439:ILE:HG13	2.49	0.42
1:C:135:TYR:CD1	1:C:159:ALA:HB1	2.54	0.42
1:C:82:SER:O	1:C:279:VAL:HA	2.19	0.42
2:D:455:ILE:HD13	2:D:455:ILE:HA	1.81	0.42
2:L:455:ILE:HD13	2:L:455:ILE:HA	1.87	0.42
1:A:237:LEU:HA	1:A:238:PRO:HD3	1.85	0.42
1:E:124:VAL:HG12	1:E:177:ILE:CG1	2.30	0.41
1:A:81:VAL:HG13	1:A:315:ILE:CD1	2.49	0.41
1:C:284:LEU:CB	1:C:285:PRO:HA	2.36	0.41
1:K:39:SER:OG	1:K:40:HIS:N	2.53	0.41
2:B:481:GLY:HA2	2:D:467:ARG:NH2	2.35	0.41
2:H:407:VAL:HG12	2:H:435:ARG:HH21	1.84	0.41
1:C:41:PHE:CE2	1:C:298:GLY:HA2	2.55	0.41
1:E:139:THR:HB	1:E:151:GLY:N	2.34	0.41
1:K:257:THR:HG22	1:K:258:ILE:N	2.35	0.41
1:A:57:CYS:O	1:A:60:CYS:HB2	2.20	0.41
2:B:496:LEU:HD12	2:B:499:ILE:HD12	2.01	0.41
1:I:131:PRO:CG	1:I:172:ILE:CD1	2.78	0.41
1:I:197:GLN:HA	1:I:197:GLN:OE1	2.21	0.41
2:B:435:ARG:CD	2:B:439:ILE:HG13	2.50	0.41
2:H:439:ILE:O	2:H:443:ILE:HG13	2.20	0.41
1:G:52:LYS:HD3	1:G:62:ASP:OD1	2.20	0.41
1:K:231:GLN:HB3	1:K:234:ASP:OD2	2.20	0.41
2:L:369:HIS:ND1	2:L:387:SER:OG	2.45	0.41
1:G:135:TYR:CD1	1:G:159:ALA:HB1	2.56	0.41
1:C:3:ILE:HA	2:D:372:THR:O	2.20	0.41
1:C:281:LYS:HD2	2:D:412:ARG:NH1	2.29	0.41
2:L:434:LEU:HD23	2:L:434:LEU:HA	1.90	0.41
1:A:176:TYR:OH	1:A:182:GLU:O	2.35	0.41
1:A:141:GLY:C	1:A:143:CYS:H	2.23	0.41
1:E:330:ASN:HA	2:F:395:ILE:HD13	2.03	0.41
1:C:72:CYS:O	1:C:73:THR:CG2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:182:GLU:HG2	1:G:274:SER:HB3	2.03	0.41
1:I:254:LYS:NZ	2:L:419:GLU:HG2	2.36	0.41
2:L:420:LEU:CD1	2:L:421:HIS:CE1	3.03	0.41
1:I:280:ILE:CG2	1:I:295:GLU:HG3	2.43	0.41
1:A:158:TRP:C	1:A:158:TRP:CD1	2.92	0.41
1:C:84:LEU:HD11	1:C:109:ASN:ND2	2.36	0.41
1:A:335:ARG:HD2	2:B:359:GLY:HA2	2.02	0.41
1:G:104:ILE:HB	1:G:245:VAL:O	2.21	0.41
1:K:160:VAL:O	1:K:162:LYS:N	2.53	0.41
2:J:463:LEU:HA	2:J:463:LEU:HD12	1.92	0.41
2:B:419:GLU:HG3	1:C:215:ASN:HB2	2.03	0.41
1:G:187:VAL:O	1:G:267:PRO:HB3	2.21	0.41
2:H:410:LEU:HD13	2:H:435:ARG:CZ	2.51	0.41
1:E:16:VAL:HG12	1:E:17:LYS:N	2.35	0.41
1:A:215:ASN:HB2	2:F:419:GLU:HG3	2.03	0.41
1:C:131:PRO:C	1:C:170:LEU:HD13	2.41	0.41
1:C:172:ILE:HG12	1:C:260:TYR:CE2	2.56	0.41
1:G:280:ILE:HD11	1:G:315:ILE:CG1	2.45	0.41
1:K:81:VAL:HG11	1:K:315:ILE:HD11	2.03	0.41
1:E:172:ILE:CG1	1:E:260:TYR:CE2	3.00	0.41
1:I:95:PHE:CD1	1:I:96:PRO:HD2	2.55	0.41
1:A:243:ILE:HD11	1:A:265:LEU:CD1	2.47	0.41
2:J:387:SER:HB2	2:J:465:LEU:HD11	2.03	0.41
1:K:135:TYR:HD2	1:K:161:PRO:HA	1.86	0.41
2:L:387:SER:HB2	2:L:465:LEU:HD11	2.02	0.41
2:B:440:SER:O	2:B:444:GLU:HG3	2.20	0.41
1:C:105:ARG:NH2	1:C:233:GLU:OE1	2.53	0.41
1:A:16:VAL:HG12	1:A:17:LYS:N	2.36	0.41
1:I:237:LEU:HA	1:I:238:PRO:HD3	1.81	0.41
2:L:496:LEU:HD12	2:L:499:ILE:HD12	2.02	0.41
1:G:281:LYS:HB2	1:G:295:GLU:HG2	2.03	0.41
1:C:124:VAL:HG12	1:C:177:ILE:CG1	2.37	0.41
1:A:53:LEU:O	1:A:76:ILE:HG23	2.21	0.41
2:H:427:LEU:HG	2:J:427:LEU:HD21	2.03	0.41
1:C:237:LEU:HA	1:C:238:PRO:HD3	1.85	0.41
2:B:449:LEU:HD11	2:D:449:LEU:HD13	2.03	0.41
1:E:171:THR:C	1:E:172:ILE:HG12	2.41	0.40
1:I:131:PRO:CD	1:I:172:ILE:CD1	2.99	0.40
2:H:479:GLU:HG2	2:L:470:LYS:HZ1	1.86	0.40
2:B:409:ASN:O	2:B:410:LEU:HB2	2.21	0.40
1:G:280:ILE:HG22	1:G:281:LYS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:PHE:CD1	1:C:96:PRO:HD2	2.56	0.40
1:K:16:VAL:CG1	1:K:17:LYS:N	2.85	0.40
1:C:135:TYR:HD2	1:C:161:PRO:HA	1.86	0.40
1:A:15:VAL:HG22	1:A:23:GLU:HG2	2.02	0.40
2:H:395:ILE:HG12	2:H:454:ILE:HD13	2.03	0.40
1:A:2:ARG:NH2	2:D:515:ASP:O	2.53	0.40
1:E:160:VAL:O	1:E:162:LYS:N	2.54	0.40
1:G:139:THR:HB	1:G:151:GLY:N	2.36	0.40
1:I:155:THR:HG21	1:I:187:VAL:CB	2.52	0.40
1:A:7:ILE:HD11	1:A:335:ARG:NE	2.36	0.40
1:G:189:GLY:HA3	1:G:244:VAL:O	2.21	0.40
1:C:160:VAL:O	1:C:162:LYS:N	2.54	0.40
1:K:225:ILE:HA	1:K:225:ILE:HD13	1.73	0.40
1:A:281:LYS:HB2	1:A:295:GLU:HG2	2.03	0.40
1:E:97:ILE:HG12	1:E:243:ILE:HG23	2.03	0.40
1:E:119:LEU:HD23	1:E:120:SER:O	2.21	0.40
2:D:387:SER:HB2	2:D:465:LEU:HD11	2.03	0.40
1:K:63:LEU:HA	1:K:108:PRO:HG3	2.03	0.40
1:E:114:TYR:CG	1:E:273:ALA:HB1	2.57	0.40
2:F:420:LEU:HD12	2:F:421:HIS:CE1	2.57	0.40
1:C:1:ASP:CG	2:D:490:LYS:HG2	2.42	0.40
1:I:176:TYR:HA	1:I:184:GLN:NE2	2.36	0.40
1:G:15:VAL:HG22	1:G:23:GLU:HG2	2.04	0.40
2:J:475:PRO:HD2	2:J:512:PRO:HB2	2.02	0.40
1:G:225:ILE:HD13	1:G:225:ILE:HA	1.78	0.40
2:J:361:TRP:NE1	2:J:372:THR:HG21	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	339/347 (98%)	311 (92%)	22 (6%)	6 (2%)	11	51
1	C	339/347 (98%)	314 (93%)	20 (6%)	5 (2%)	13	54
1	E	339/347 (98%)	314 (93%)	20 (6%)	5 (2%)	13	54
1	G	339/347 (98%)	314 (93%)	20 (6%)	5 (2%)	13	54
1	I	339/347 (98%)	314 (93%)	21 (6%)	4 (1%)	16	60
1	K	339/347 (98%)	316 (93%)	18 (5%)	5 (2%)	13	54
2	B	167/179 (93%)	162 (97%)	5 (3%)	0	100	100
2	D	167/179 (93%)	162 (97%)	5 (3%)	0	100	100
2	F	167/179 (93%)	162 (97%)	4 (2%)	1 (1%)	30	74
2	H	167/179 (93%)	162 (97%)	5 (3%)	0	100	100
2	J	167/179 (93%)	162 (97%)	5 (3%)	0	100	100
2	L	167/179 (93%)	162 (97%)	5 (3%)	0	100	100
All	All	3036/3156 (96%)	2855 (94%)	150 (5%)	31 (1%)	19	64

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	ILE
1	A	251	LYS
1	C	177	ILE
1	C	251	LYS
1	E	177	ILE
1	E	251	LYS
1	G	177	ILE
1	G	251	LYS
1	I	177	ILE
1	I	251	LYS
1	K	177	ILE
1	K	251	LYS
1	A	148	ASN
1	E	146	ILE
1	I	146	ILE
1	C	146	ILE
1	G	146	ILE
1	I	148	ASN
1	K	146	ILE
1	A	45	LYS
1	A	146	ILE
1	A	147	THR

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Mol	Chain	Res	Type
1	C	148	ASN
1	E	148	ASN
1	G	148	ASN
1	K	148	ASN
1	C	45	LYS
1	E	45	LYS
1	G	45	LYS
1	K	45	LYS
2	F	416	ALA

### 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	288/294 (98%)	283 (98%)	5 (2%)	68	89
1	C	288/294 (98%)	285 (99%)	3 (1%)	82	93
1	E	288/294 (98%)	285 (99%)	3 (1%)	82	93
1	G	288/294 (98%)	280 (97%)	8 (3%)	51	82
1	I	288/294 (98%)	284 (99%)	4 (1%)	74	90
1	K	288/294 (98%)	282 (98%)	6 (2%)	61	86
2	B	136/143 (95%)	134 (98%)	2 (2%)	72	90
2	D	136/143 (95%)	134 (98%)	2 (2%)	72	90
2	F	136/143 (95%)	133 (98%)	3 (2%)	60	86
2	H	136/143 (95%)	134 (98%)	2 (2%)	72	90
2	J	136/143 (95%)	135 (99%)	1 (1%)	88	95
2	L	136/143 (95%)	133 (98%)	3 (2%)	60	86
All	All	2544/2622 (97%)	2502 (98%)	42 (2%)	68	89

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	CYS

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Mol	Chain	Res	Type
1	A	105	ARG
1	A	118	ARG
1	A	202	TYR
1	A	215	ASN
2	B	421	HIS
2	B	435	ARG
1	C	54	CYS
1	C	118	ARG
1	C	215	ASN
2	D	398	ASN
2	D	435	ARG
1	E	54	CYS
1	E	118	ARG
1	E	215	ASN
2	F	398	ASN
2	F	421	HIS
2	F	435	ARG
1	G	54	CYS
1	G	105	ARG
1	G	118	ARG
1	G	184	GLN
1	G	202	TYR
1	G	212	SER
1	G	215	ASN
1	G	265	LEU
2	H	398	ASN
2	H	435	ARG
1	I	54	CYS
1	I	118	ARG
1	I	202	TYR
1	I	215	ASN
2	J	398	ASN
1	K	54	CYS
1	K	118	ARG
1	K	197	GLN
1	K	202	TYR
1	K	215	ASN
1	K	265	LEU
2	L	398	ASN
2	L	421	HIS
2	L	435	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	126	ASN
1	A	129	ASN
2	B	398	ASN
1	C	85	HIS
1	C	126	ASN
1	C	129	ASN
1	C	231	GLN
1	E	268	GLN
1	G	126	ASN
1	G	129	ASN
1	G	184	GLN
1	G	268	GLN
2	H	482	ASN
1	I	126	ASN
1	I	129	ASN
1	I	184	GLN
1	K	126	ASN
1	K	129	ASN
1	K	197	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 ⓘ

74 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	401	1,3	14,14,15	0.51	0	15,19,21	1.06	1 (6%)
3	NAG	A	402	3	14,14,15	0.47	0	15,19,21	0.85	1 (6%)
3	BMA	A	403	3	11,11,12	0.56	0	14,15,17	0.90	1 (7%)
4	NAG	A	404	1,4	14,14,15	0.38	0	15,19,21	1.86	2 (13%)
4	NAG	A	405	4	14,14,15	0.43	0	15,19,21	1.24	2 (13%)
4	NAG	A	406	1,4	14,14,15	0.37	0	15,19,21	2.01	1 (6%)
4	NAG	A	407	4	14,14,15	0.50	0	15,19,21	0.59	0
3	NAG	A	408	1,3	14,14,15	0.50	0	15,19,21	1.06	1 (6%)
3	NAG	A	409	3	14,14,15	0.46	0	15,19,21	0.84	1 (6%)
3	BMA	A	410	3	11,11,12	0.56	0	14,15,17	0.90	1 (7%)
3	NAG	A	412	1,3	14,14,15	0.50	0	15,19,21	1.53	3 (20%)
3	NAG	A	413	3	14,14,15	0.49	0	15,19,21	1.17	2 (13%)
3	BMA	A	414	3	11,11,12	0.62	0	14,15,17	1.45	3 (21%)
3	NAG	C	401	1,3	14,14,15	0.50	0	15,19,21	1.06	1 (6%)
3	NAG	C	402	3	14,14,15	0.47	0	15,19,21	0.84	1 (6%)
3	BMA	C	403	3	11,11,12	0.56	0	14,15,17	0.91	1 (7%)
4	NAG	C	405	1,4	14,14,15	0.36	0	15,19,21	2.02	1 (6%)
4	NAG	C	406	4	14,14,15	0.50	0	15,19,21	0.59	0
3	NAG	C	407	1,3	14,14,15	0.49	0	15,19,21	1.06	1 (6%)
3	NAG	C	408	3	14,14,15	0.47	0	15,19,21	0.84	1 (6%)
3	BMA	C	409	3	11,11,12	0.56	0	14,15,17	0.90	1 (7%)
3	NAG	C	411	1,3	14,14,15	0.49	0	15,19,21	1.53	4 (26%)
3	NAG	C	412	3	14,14,15	0.48	0	15,19,21	1.17	2 (13%)
3	BMA	C	413	3	11,11,12	0.61	0	14,15,17	1.45	3 (21%)
3	NAG	E	401	1,3	14,14,15	0.50	0	15,19,21	1.06	1 (6%)
3	NAG	E	402	3	14,14,15	0.45	0	15,19,21	0.84	1 (6%)
3	BMA	E	403	3	11,11,12	0.58	0	14,15,17	0.91	1 (7%)
4	NAG	E	404	1,4	14,14,15	0.38	0	15,19,21	1.85	2 (13%)
4	NAG	E	405	4	14,14,15	0.45	0	15,19,21	1.23	2 (13%)
4	NAG	E	406	1,4	14,14,15	0.37	0	15,19,21	2.02	1 (6%)
4	NAG	E	407	4	14,14,15	0.50	0	15,19,21	0.60	0
3	NAG	E	408	1,3	14,14,15	0.49	0	15,19,21	1.06	1 (6%)
3	NAG	E	409	3	14,14,15	0.45	0	15,19,21	0.84	1 (6%)
3	BMA	E	410	3	11,11,12	0.55	0	14,15,17	0.90	1 (7%)
3	NAG	E	412	1,3	14,14,15	0.51	0	15,19,21	1.53	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	E	413	3	14,14,15	0.48	0	15,19,21	1.17	2 (13%)
3	BMA	E	414	3	11,11,12	0.62	0	14,15,17	1.45	3 (21%)
3	NAG	G	401	1,3	14,14,15	0.50	0	15,19,21	1.06	1 (6%)
3	NAG	G	402	3	14,14,15	0.48	0	15,19,21	0.84	1 (6%)
3	BMA	G	403	3	11,11,12	0.55	0	14,15,17	0.90	1 (7%)
4	NAG	G	404	1,4	14,14,15	0.50	0	15,19,21	1.54	3 (20%)
4	NAG	G	405	4	14,14,15	0.49	0	15,19,21	1.18	2 (13%)
4	NAG	G	406	1,4	14,14,15	0.36	0	15,19,21	2.01	1 (6%)
4	NAG	G	407	4	14,14,15	0.50	0	15,19,21	0.59	0
3	NAG	G	408	1,3	14,14,15	0.49	0	15,19,21	1.07	1 (6%)
3	NAG	G	409	3	14,14,15	0.47	0	15,19,21	0.84	1 (6%)
3	BMA	G	410	3	11,11,12	0.57	0	14,15,17	0.90	1 (7%)
4	NAG	G	412	1,4	14,14,15	0.50	0	15,19,21	1.54	3 (20%)
4	NAG	G	413	4	14,14,15	0.49	0	15,19,21	1.17	2 (13%)
4	NAG	I	401	1,4	14,14,15	0.52	0	15,19,21	1.07	1 (6%)
4	NAG	I	402	4	14,14,15	0.47	0	15,19,21	0.85	1 (6%)
4	NAG	I	403	1,4	14,14,15	0.39	0	15,19,21	1.86	2 (13%)
4	NAG	I	404	4	14,14,15	0.44	0	15,19,21	1.23	2 (13%)
4	NAG	I	405	1,4	14,14,15	0.36	0	15,19,21	2.02	1 (6%)
4	NAG	I	406	4	14,14,15	0.50	0	15,19,21	0.59	0
3	NAG	I	407	1,3	14,14,15	0.49	0	15,19,21	1.06	1 (6%)
3	NAG	I	408	3	14,14,15	0.45	0	15,19,21	0.84	1 (6%)
3	BMA	I	409	3	11,11,12	0.56	0	14,15,17	0.90	1 (7%)
3	NAG	I	411	1,3	14,14,15	0.50	0	15,19,21	1.53	3 (20%)
3	NAG	I	412	3	14,14,15	0.49	0	15,19,21	1.18	2 (13%)
3	BMA	I	413	3	11,11,12	0.62	0	14,15,17	1.46	3 (21%)
3	NAG	K	401	1,3	14,14,15	0.50	0	15,19,21	1.06	1 (6%)
3	NAG	K	402	3	14,14,15	0.47	0	15,19,21	0.86	1 (6%)
3	BMA	K	403	3	11,11,12	0.56	0	14,15,17	0.90	1 (7%)
4	NAG	K	404	1,4	14,14,15	0.39	0	15,19,21	1.86	2 (13%)
4	NAG	K	405	4	14,14,15	0.45	0	15,19,21	1.24	2 (13%)
4	NAG	K	406	1,4	14,14,15	0.36	0	15,19,21	2.01	1 (6%)
4	NAG	K	407	4	14,14,15	0.51	0	15,19,21	0.59	0
3	NAG	K	408	1,3	14,14,15	0.51	0	15,19,21	1.06	1 (6%)
3	NAG	K	409	3	14,14,15	0.47	0	15,19,21	0.83	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BMA	K	410	3	11,11,12	0.56	0	14,15,17	0.90	1 (7%)
3	NAG	K	411	1,3	14,14,15	0.50	0	15,19,21	1.53	3 (20%)
3	NAG	K	412	3	14,14,15	0.48	0	15,19,21	1.17	2 (13%)
3	BMA	K	413	3	11,11,12	0.62	0	14,15,17	1.45	3 (21%)

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	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	402	3	-	0/6/23/26	0/1/1/1
3	BMA	A	403	3	-	0/2/19/22	0/1/1/1
4	NAG	A	404	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	405	4	-	0/6/23/26	0/1/1/1
4	NAG	A	406	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	407	4	-	0/6/23/26	0/1/1/1
3	NAG	A	408	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	409	3	-	0/6/23/26	0/1/1/1
3	BMA	A	410	3	-	0/2/19/22	0/1/1/1
3	NAG	A	412	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	413	3	-	0/6/23/26	0/1/1/1
3	BMA	A	414	3	-	0/2/19/22	0/1/1/1
3	NAG	C	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	402	3	-	0/6/23/26	0/1/1/1
3	BMA	C	403	3	-	0/2/19/22	0/1/1/1
4	NAG	C	405	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	406	4	-	0/6/23/26	0/1/1/1
3	NAG	C	407	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	408	3	-	0/6/23/26	0/1/1/1
3	BMA	C	409	3	-	0/2/19/22	0/1/1/1
3	NAG	C	411	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	412	3	-	0/6/23/26	0/1/1/1
3	BMA	C	413	3	-	0/2/19/22	0/1/1/1
3	NAG	E	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	402	3	-	0/6/23/26	0/1/1/1
3	BMA	E	403	3	-	0/2/19/22	0/1/1/1
4	NAG	E	404	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	405	4	-	0/6/23/26	0/1/1/1
4	NAG	E	406	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	407	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	408	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	409	3	-	0/6/23/26	0/1/1/1
3	BMA	E	410	3	-	0/2/19/22	0/1/1/1
3	NAG	E	412	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	413	3	-	0/6/23/26	0/1/1/1
3	BMA	E	414	3	-	0/2/19/22	0/1/1/1
3	NAG	G	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	402	3	-	0/6/23/26	0/1/1/1
3	BMA	G	403	3	-	0/2/19/22	0/1/1/1
4	NAG	G	404	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	405	4	-	0/6/23/26	0/1/1/1
4	NAG	G	406	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	407	4	-	0/6/23/26	0/1/1/1
3	NAG	G	408	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	409	3	-	0/6/23/26	0/1/1/1
3	BMA	G	410	3	-	0/2/19/22	0/1/1/1
4	NAG	G	412	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	413	4	-	0/6/23/26	0/1/1/1
4	NAG	I	401	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	402	4	-	0/6/23/26	0/1/1/1
4	NAG	I	403	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	404	4	-	0/6/23/26	0/1/1/1
4	NAG	I	405	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	406	4	-	0/6/23/26	0/1/1/1
3	NAG	I	407	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	408	3	-	0/6/23/26	0/1/1/1
3	BMA	I	409	3	-	0/2/19/22	0/1/1/1
3	NAG	I	411	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	412	3	-	0/6/23/26	0/1/1/1
3	BMA	I	413	3	-	0/2/19/22	0/1/1/1
3	NAG	K	401	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	402	3	-	0/6/23/26	0/1/1/1
3	BMA	K	403	3	-	0/2/19/22	0/1/1/1
4	NAG	K	404	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	405	4	-	0/6/23/26	0/1/1/1
4	NAG	K	406	1,4	-	0/6/23/26	0/1/1/1
4	NAG	K	407	4	-	0/6/23/26	0/1/1/1
3	NAG	K	408	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	409	3	-	0/6/23/26	0/1/1/1
3	BMA	K	410	3	-	0/2/19/22	0/1/1/1
3	NAG	K	411	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	412	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	K	413	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	404	NAG	O7-C7-C8	-2.88	116.78	122.06
4	K	405	NAG	C2-N2-C7	-2.85	119.37	123.04
3	E	412	NAG	O7-C7-C8	-2.85	116.83	122.06
4	A	405	NAG	C2-N2-C7	-2.85	119.38	123.04
4	G	412	NAG	O7-C7-C8	-2.83	116.86	122.06
3	I	411	NAG	O7-C7-C8	-2.83	116.87	122.06
3	A	412	NAG	O7-C7-C8	-2.82	116.88	122.06
4	E	405	NAG	C2-N2-C7	-2.82	119.41	123.04
3	K	411	NAG	O7-C7-C8	-2.82	116.89	122.06
4	I	404	NAG	C2-N2-C7	-2.82	119.42	123.04
3	C	411	NAG	O7-C7-C8	-2.81	116.91	122.06
3	C	411	NAG	C4-C3-C2	-2.67	107.08	111.23
3	K	412	NAG	O5-C5-C6	-2.66	101.59	107.35
3	C	412	NAG	O5-C5-C6	-2.65	101.61	107.35
3	I	411	NAG	C4-C3-C2	-2.65	107.11	111.23
3	A	413	NAG	O5-C5-C6	-2.65	101.62	107.35
4	G	405	NAG	O5-C5-C6	-2.65	101.62	107.35
4	G	412	NAG	C4-C3-C2	-2.65	107.11	111.23
4	G	413	NAG	O5-C5-C6	-2.65	101.62	107.35
3	K	411	NAG	C4-C3-C2	-2.65	107.12	111.23
3	E	413	NAG	O5-C5-C6	-2.64	101.62	107.35
3	A	412	NAG	C4-C3-C2	-2.64	107.12	111.23
3	I	412	NAG	O5-C5-C6	-2.64	101.63	107.35
3	E	412	NAG	C4-C3-C2	-2.63	107.14	111.23
4	G	404	NAG	C4-C3-C2	-2.59	107.21	111.23
3	A	409	NAG	C2-N2-C7	-2.51	119.81	123.04
3	G	409	NAG	C2-N2-C7	-2.51	119.81	123.04
3	E	409	NAG	C2-N2-C7	-2.51	119.81	123.04
3	E	402	NAG	C2-N2-C7	-2.51	119.81	123.04
3	C	408	NAG	C2-N2-C7	-2.50	119.83	123.04
3	I	408	NAG	C2-N2-C7	-2.50	119.83	123.04
3	K	409	NAG	C2-N2-C7	-2.49	119.84	123.04
3	K	402	NAG	C2-N2-C7	-2.48	119.85	123.04
3	A	402	NAG	C2-N2-C7	-2.47	119.86	123.04
3	I	413	BMA	O4-C4-C5	-2.46	102.72	109.24
3	E	414	BMA	O4-C4-C5	-2.46	102.73	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	NAG	C2-N2-C7	-2.45	119.89	123.04
3	A	414	BMA	O4-C4-C5	-2.45	102.75	109.24
4	I	402	NAG	C2-N2-C7	-2.45	119.89	123.04
3	C	413	BMA	O4-C4-C5	-2.44	102.76	109.24
3	K	413	BMA	O4-C4-C5	-2.44	102.77	109.24
3	G	402	NAG	C2-N2-C7	-2.44	119.91	123.04
3	K	413	BMA	C6-C5-C4	-2.31	107.31	113.02
3	E	414	BMA	C6-C5-C4	-2.31	107.33	113.02
3	A	414	BMA	C6-C5-C4	-2.30	107.35	113.02
3	I	413	BMA	C6-C5-C4	-2.30	107.35	113.02
3	C	413	BMA	C6-C5-C4	-2.29	107.37	113.02
4	G	405	NAG	C4-C3-C2	-2.25	107.73	111.23
3	I	412	NAG	C4-C3-C2	-2.24	107.75	111.23
3	E	413	NAG	C4-C3-C2	-2.22	107.78	111.23
3	A	413	NAG	C4-C3-C2	-2.22	107.78	111.23
4	G	413	NAG	C4-C3-C2	-2.21	107.79	111.23
3	K	412	NAG	C4-C3-C2	-2.20	107.81	111.23
3	C	412	NAG	C4-C3-C2	-2.19	107.82	111.23
4	K	405	NAG	C4-C3-C2	-2.08	108.00	111.23
4	A	405	NAG	C4-C3-C2	-2.07	108.01	111.23
3	I	409	BMA	O5-C1-C2	-2.07	107.50	110.86
3	G	410	BMA	O5-C1-C2	-2.06	107.51	110.86
3	E	410	BMA	O5-C1-C2	-2.06	107.51	110.86
3	E	403	BMA	O5-C1-C2	-2.06	107.52	110.86
3	A	410	BMA	O5-C1-C2	-2.05	107.52	110.86
3	C	403	BMA	O5-C1-C2	-2.05	107.53	110.86
4	E	405	NAG	C4-C3-C2	-2.05	108.05	111.23
3	K	403	BMA	O5-C1-C2	-2.05	107.54	110.86
4	I	404	NAG	C4-C3-C2	-2.04	108.05	111.23
3	K	410	BMA	O5-C1-C2	-2.04	107.54	110.86
3	C	409	BMA	O5-C1-C2	-2.04	107.55	110.86
3	A	403	BMA	O5-C1-C2	-2.04	107.55	110.86
3	G	403	BMA	O5-C1-C2	-2.01	107.60	110.86
3	C	411	NAG	C3-C4-C5	2.00	113.69	110.20
4	I	403	NAG	C3-C4-C5	2.26	114.14	110.20
4	K	404	NAG	C3-C4-C5	2.28	114.18	110.20
4	E	404	NAG	C3-C4-C5	2.31	114.22	110.20
4	A	404	NAG	C3-C4-C5	2.34	114.28	110.20
3	C	411	NAG	C3-C2-N2	2.44	116.39	110.56
3	I	411	NAG	C3-C2-N2	2.44	116.40	110.56
3	A	412	NAG	C3-C2-N2	2.44	116.40	110.56
3	K	411	NAG	C3-C2-N2	2.44	116.41	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	412	NAG	C3-C2-N2	2.44	116.41	110.56
4	G	412	NAG	C3-C2-N2	2.45	116.43	110.56
4	G	404	NAG	C3-C2-N2	2.47	116.47	110.56
3	I	413	BMA	O2-C2-C3	2.90	115.95	110.12
3	C	413	BMA	O2-C2-C3	2.91	115.98	110.12
3	E	414	BMA	O2-C2-C3	2.93	116.00	110.12
3	K	413	BMA	O2-C2-C3	2.93	116.00	110.12
3	A	414	BMA	O2-C2-C3	2.93	116.00	110.12
3	K	401	NAG	C1-O5-C5	3.33	116.47	112.25
3	C	401	NAG	C1-O5-C5	3.33	116.47	112.25
3	E	401	NAG	C1-O5-C5	3.33	116.47	112.25
3	A	401	NAG	C1-O5-C5	3.33	116.48	112.25
3	G	401	NAG	C1-O5-C5	3.34	116.48	112.25
4	I	401	NAG	C1-O5-C5	3.34	116.49	112.25
3	E	408	NAG	C1-O5-C5	3.34	116.49	112.25
3	C	407	NAG	C1-O5-C5	3.34	116.49	112.25
3	A	408	NAG	C1-O5-C5	3.34	116.49	112.25
3	K	408	NAG	C1-O5-C5	3.35	116.50	112.25
3	I	407	NAG	C1-O5-C5	3.35	116.50	112.25
3	G	408	NAG	C1-O5-C5	3.37	116.52	112.25
4	E	404	NAG	C1-O5-C5	6.30	120.24	112.25
4	A	404	NAG	C1-O5-C5	6.32	120.27	112.25
4	I	403	NAG	C1-O5-C5	6.35	120.30	112.25
4	K	404	NAG	C1-O5-C5	6.35	120.31	112.25
4	G	406	NAG	C1-O5-C5	7.17	121.35	112.25
4	K	406	NAG	C1-O5-C5	7.20	121.39	112.25
4	A	406	NAG	C1-O5-C5	7.21	121.40	112.25
4	E	406	NAG	C1-O5-C5	7.22	121.41	112.25
4	I	405	NAG	C1-O5-C5	7.22	121.42	112.25
4	C	405	NAG	C1-O5-C5	7.23	121.42	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAG	1	0
3	A	412	NAG	6	0
3	C	411	NAG	7	0
3	E	401	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	412	NAG	7	0
4	G	404	NAG	1	0
4	G	405	NAG	7	0
4	G	412	NAG	5	0
3	I	411	NAG	6	0
3	K	403	BMA	3	0
3	K	411	NAG	3	0

## 5.6 Ligand geometry [i](#)

17 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	A	411	1	14,14,15	0.51	0	15,19,21	0.74	0
5	NAG	A	415	1	14,14,15	0.46	0	15,19,21	1.02	1 (6%)
5	NAG	B	600	2	14,14,15	0.48	0	15,19,21	0.71	0
5	NAG	C	404	1	14,14,15	0.38	0	15,19,21	1.85	2 (13%)
5	NAG	C	410	1	14,14,15	0.49	0	15,19,21	1.53	3 (20%)
5	NAG	C	414	1	14,14,15	0.47	0	15,19,21	1.02	1 (6%)
5	NAG	D	600	2	14,14,15	0.48	0	15,19,21	0.71	0
5	NAG	E	411	1	14,14,15	0.52	0	15,19,21	0.74	0
5	NAG	E	415	1	14,14,15	0.46	0	15,19,21	1.02	1 (6%)
5	NAG	F	600	2	14,14,15	0.47	0	15,19,21	0.71	0
5	NAG	G	411	1	14,14,15	0.51	0	15,19,21	0.74	0
5	NAG	G	414	1	14,14,15	0.45	0	15,19,21	1.02	1 (6%)
5	NAG	H	600	2	14,14,15	0.49	0	15,19,21	0.71	0
5	NAG	I	410	1	14,14,15	0.52	0	15,19,21	0.74	0
5	NAG	I	414	1	14,14,15	0.46	0	15,19,21	1.01	1 (6%)
5	NAG	J	600	2	14,14,15	0.47	0	15,19,21	0.71	0
5	NAG	K	414	1	14,14,15	0.47	0	15,19,21	1.02	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	411	1	-	0/6/23/26	0/1/1/1
5	NAG	A	415	1	-	0/6/23/26	0/1/1/1
5	NAG	B	600	2	-	0/6/23/26	0/1/1/1
5	NAG	C	404	1	-	0/6/23/26	0/1/1/1
5	NAG	C	410	1	-	0/6/23/26	0/1/1/1
5	NAG	C	414	1	-	0/6/23/26	0/1/1/1
5	NAG	D	600	2	-	0/6/23/26	0/1/1/1
5	NAG	E	411	1	-	0/6/23/26	0/1/1/1
5	NAG	E	415	1	-	0/6/23/26	0/1/1/1
5	NAG	F	600	2	-	0/6/23/26	0/1/1/1
5	NAG	G	411	1	-	0/6/23/26	0/1/1/1
5	NAG	G	414	1	-	0/6/23/26	0/1/1/1
5	NAG	H	600	2	-	0/6/23/26	0/1/1/1
5	NAG	I	410	1	-	0/6/23/26	0/1/1/1
5	NAG	I	414	1	-	0/6/23/26	0/1/1/1
5	NAG	J	600	2	-	0/6/23/26	0/1/1/1
5	NAG	K	414	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	410	NAG	O7-C7-C8	-2.83	116.87	122.06
5	C	410	NAG	C4-C3-C2	-2.61	107.17	111.23
5	C	404	NAG	C3-C4-C5	2.30	114.22	110.20
5	C	410	NAG	C3-C2-N2	2.46	116.45	110.56
5	I	414	NAG	C1-O5-C5	2.55	115.48	112.25
5	G	414	NAG	C1-O5-C5	2.56	115.50	112.25
5	K	414	NAG	C1-O5-C5	2.57	115.50	112.25
5	A	415	NAG	C1-O5-C5	2.57	115.50	112.25
5	E	415	NAG	C1-O5-C5	2.57	115.51	112.25
5	C	414	NAG	C1-O5-C5	2.58	115.53	112.25
5	C	404	NAG	C1-O5-C5	6.32	120.27	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	341/347 (98%)	0.26	16 (4%) 35 30	33, 64, 133, 208	0
1	C	341/347 (98%)	0.14	10 (2%) 55 48	30, 61, 135, 195	0
1	E	341/347 (98%)	0.17	11 (3%) 51 45	26, 63, 141, 237	0
1	G	341/347 (98%)	0.23	10 (2%) 55 48	35, 73, 151, 210	0
1	I	341/347 (98%)	0.17	9 (2%) 59 52	39, 71, 141, 193	0
1	K	341/347 (98%)	0.41	19 (5%) 28 25	45, 77, 157, 209	0
2	B	169/179 (94%)	0.49	13 (7%) 16 15	30, 142, 219, 275	0
2	D	169/179 (94%)	0.55	20 (11%) 6 7	30, 132, 212, 252	0
2	F	169/179 (94%)	0.40	15 (8%) 12 12	34, 130, 207, 274	0
2	H	169/179 (94%)	0.64	23 (13%) 4 5	42, 143, 202, 255	0
2	J	169/179 (94%)	0.52	16 (9%) 10 11	40, 138, 225, 266	0
2	L	169/179 (94%)	0.72	23 (13%) 4 5	43, 149, 223, 260	0
All	All	3060/3156 (96%)	0.34	185 (6%) 25 22	26, 77, 195, 275	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	383	ALA	8.3
2	B	516	SER	7.8
2	L	382	ALA	5.7
2	D	372	THR	5.4
2	H	382	ALA	5.3
2	L	361	TRP	4.9
2	F	381	VAL	4.9
2	D	361	TRP	4.8
2	H	383	ALA	4.5
2	F	516	SER	4.5
2	H	503	THR	4.4

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Mol	Chain	Res	Type	RSRZ
2	J	381	VAL	4.3
2	L	488	LYS	4.2
2	D	381	VAL	4.2
2	H	516	SER	4.2
1	K	180	GLU	4.2
2	D	382	ALA	4.2
2	F	514	PHE	4.1
1	C	2	ARG	4.1
2	L	374	HIS	4.1
2	H	366	ALA	4.0
2	L	383	ALA	3.9
2	F	479	GLU	3.9
2	J	516	SER	3.9
1	C	28	GLY	3.9
2	J	371	TYR	3.8
2	D	373	SER	3.8
2	F	507	GLY	3.8
2	H	504	PHE	3.6
2	H	371	TYR	3.6
2	D	374	HIS	3.6
2	H	374	HIS	3.6
2	L	371	TYR	3.6
2	F	363	GLY	3.5
2	L	511	LEU	3.5
1	K	218	THR	3.5
2	J	512	PRO	3.5
1	I	11	ASN	3.5
2	B	503	THR	3.5
2	D	379	VAL	3.4
2	B	367	GLY	3.4
2	D	368	TRP	3.4
1	K	252	SER	3.4
2	B	382	ALA	3.3
2	B	508	GLU	3.3
2	D	371	TYR	3.3
2	L	473	LEU	3.2
1	A	180	GLU	3.2
1	K	3	ILE	3.2
1	A	338	ALA	3.2
2	H	365	ILE	3.1
2	D	516	SER	3.1
2	H	494	THR	3.1

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Mol	Chain	Res	Type	RSRZ
2	L	494	THR	3.1
2	L	372	THR	3.1
2	L	384	ASP	3.1
2	B	369	HIS	3.1
1	G	319	PRO	3.0
2	F	375	GLY	3.0
1	K	11	ASN	3.0
1	K	283	SER	2.9
2	L	368	TRP	2.9
2	J	366	ALA	2.9
1	C	289	GLU	2.9
2	F	382	ALA	2.9
2	J	379	VAL	2.9
1	K	201	LEU	2.9
2	B	371	TYR	2.8
1	K	193	ASP	2.8
2	D	515	ASP	2.8
2	J	348	GLY	2.8
1	G	307	TYR	2.7
2	L	476	SER	2.7
1	I	204	ASP	2.7
2	L	376	ALA	2.7
2	H	488	LYS	2.7
1	C	29	VAL	2.7
2	L	381	VAL	2.7
1	G	163	ASN	2.7
1	E	29	VAL	2.7
1	A	201	LEU	2.7
1	E	42	ALA	2.7
2	H	512	PRO	2.7
1	A	10	SER	2.6
2	L	375	GLY	2.6
1	G	283	SER	2.6
2	D	490	LYS	2.6
2	H	361	TRP	2.6
2	H	511	LEU	2.6
2	L	380	ALA	2.6
1	A	289	GLU	2.6
1	C	287	ILE	2.6
2	J	480	ILE	2.6
1	A	218	THR	2.6
2	L	472	MET	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	F	505	ASP	2.5
1	K	163(C)	ASN	2.5
2	H	498	ARG	2.5
2	J	374	HIS	2.5
2	F	366	ALA	2.5
1	I	197	GLN	2.4
2	B	370	GLY	2.4
1	A	293	LEU	2.4
2	H	457	SER	2.4
1	E	12	SER	2.4
2	B	491	CYS	2.4
2	H	509	PHE	2.4
1	E	193	ASP	2.4
1	K	1	ASP	2.4
1	E	252	SER	2.4
2	B	366	ALA	2.4
1	K	319	PRO	2.3
1	K	163	ASN	2.3
2	L	373	SER	2.3
2	D	367	GLY	2.3
1	C	40	HIS	2.3
2	H	505	ASP	2.3
1	E	14	HIS	2.3
1	A	193	ASP	2.3
2	B	383	ALA	2.3
2	H	381	VAL	2.3
1	G	218	THR	2.3
2	D	369	HIS	2.3
2	H	363	GLY	2.3
1	E	163(C)	ASN	2.3
2	H	460	GLU	2.3
1	G	252	SER	2.3
2	B	515	ASP	2.2
2	J	505	ASP	2.2
1	C	251	LYS	2.2
1	G	315	ILE	2.2
2	F	362	GLU	2.2
1	E	15	VAL	2.2
1	K	81	VAL	2.2
2	D	485	PHE	2.2
2	L	474	GLY	2.2
2	L	369	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	284	LEU	2.2
1	A	127	ALA	2.2
1	I	15	VAL	2.2
1	E	300	LEU	2.2
2	F	361	TRP	2.2
2	J	367	GLY	2.2
1	A	298	GLY	2.2
1	C	331	GLY	2.2
1	I	201	LEU	2.2
1	C	15	VAL	2.2
1	A	252	SER	2.2
2	F	513	THR	2.2
1	K	286	LEU	2.2
1	E	329	ALA	2.2
1	A	5	THR	2.2
1	I	218	THR	2.1
2	D	479	GLU	2.1
1	K	314	ALA	2.1
2	D	380	ALA	2.1
2	J	435	ARG	2.1
1	A	6	GLY	2.1
1	K	334	TYR	2.1
2	F	498	ARG	2.1
1	A	290	ALA	2.1
2	F	515	ASP	2.1
1	G	282	GLY	2.1
2	H	495	CYS	2.1
2	D	505	ASP	2.1
2	B	361	TRP	2.1
1	C	42	ALA	2.1
1	K	2	ARG	2.1
2	L	348	GLY	2.1
2	J	361	TRP	2.1
1	A	41	PHE	2.1
1	K	127	ALA	2.1
2	H	489	HIS	2.1
1	A	42	ALA	2.1
1	I	193	ASP	2.1
1	E	127	ALA	2.1
1	G	219	THR	2.0
1	I	14	HIS	2.0
2	J	504	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
2	J	488	LYS	2.0
2	D	365	ILE	2.0
2	L	499	ILE	2.0
1	I	48	GLU	2.0
1	K	212	SER	2.0
2	J	418	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	E	401	14/15	0.79	0.25	1.32	84,93,101,102	0
4	NAG	I	401	14/15	0.72	0.28	0.66	94,99,102,105	0
4	NAG	G	406	14/15	0.81	0.20	-0.01	126,139,148,148	0
3	NAG	A	401	14/15	0.86	0.20	-0.19	79,85,89,90	0
4	NAG	K	406	14/15	0.79	0.24	-0.76	125,137,147,147	0
4	NAG	I	405	14/15	0.74	0.27	-0.81	102,115,124,125	0
4	NAG	C	405	14/15	0.83	0.17	-1.03	96,109,118,118	0
3	NAG	K	401	14/15	0.89	0.18	-1.07	95,101,105,106	0
4	NAG	E	406	14/15	0.82	0.23	-1.13	108,122,133,133	0
4	NAG	A	406	14/15	0.93	0.11	-1.33	123,135,144,144	0
3	NAG	G	408	14/15	0.82	0.29	-	116,128,139,139	0
4	NAG	G	407	14/15	0.82	0.16	-	133,143,154,156	0
4	NAG	A	407	14/15	0.87	0.14	-	131,141,153,155	0
3	NAG	C	408	14/15	0.74	0.36	-	131,144,152,153	0
3	BMA	I	409	11/12	0.70	0.26	-	157,161,173,174	0
4	NAG	K	405	14/15	0.71	0.38	-	134,138,145,150	0
3	NAG	K	408	14/15	0.88	0.26	-	116,128,138,138	0
4	NAG	I	402	14/15	0.71	0.43	-	96,101,106,107	0
3	BMA	A	414	11/12	0.47	0.35	-	161,166,172,174	0
3	NAG	K	402	14/15	0.80	0.26	-	95,100,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BMA	E	403	11/12	0.61	0.28	-	107,111,121,124	0
3	BMA	C	403	11/12	0.69	0.23	-	100,104,110,110	0
3	BMA	C	409	11/12	0.50	0.24	-	157,160,173,174	0
3	NAG	I	408	14/15	0.79	0.24	-	149,162,170,171	0
3	NAG	C	412	14/15	0.73	0.41	-	134,138,141,142	0
3	BMA	C	413	11/12	0.55	0.43	-	156,159,163,164	0
3	NAG	C	411	14/15	0.80	0.28	-	92,101,107,107	0
4	NAG	K	404	14/15	0.91	0.26	-	100,110,121,123	0
3	NAG	G	402	14/15	0.76	0.46	-	83,88,97,98	0
3	NAG	A	408	14/15	0.88	0.23	-	133,145,154,154	0
4	NAG	G	413	14/15	0.64	0.54	-	152,155,158,159	0
3	NAG	A	409	14/15	0.84	0.19	-	138,151,159,160	0
3	NAG	E	413	14/15	0.70	0.47	-	153,158,161,163	0
3	BMA	E	414	11/12	0.47	0.40	-	179,186,190,193	0
4	NAG	E	404	14/15	0.90	0.27	-	80,91,102,105	0
3	BMA	K	410	11/12	0.51	0.24	-	184,188,200,201	0
3	BMA	A	403	11/12	0.61	0.29	-	100,104,110,111	0
3	BMA	G	410	11/12	0.57	0.20	-	171,174,187,188	0
3	NAG	G	401	14/15	0.88	0.24	-	85,91,95,95	0
3	NAG	I	411	14/15	0.66	0.26	-	98,105,109,110	0
3	NAG	E	409	14/15	0.82	0.37	-	135,150,159,160	0
3	NAG	K	411	14/15	0.66	0.30	-	127,132,137,139	0
3	NAG	C	401	14/15	0.85	0.23	-	78,83,86,88	0
3	NAG	A	402	14/15	0.82	0.33	-	79,85,92,93	0
3	BMA	G	403	11/12	0.64	0.36	-	101,105,111,113	0
3	NAG	I	412	14/15	0.66	0.30	-	139,142,144,145	0
3	NAG	K	409	14/15	0.82	0.22	-	145,159,167,167	0
4	NAG	I	403	14/15	0.87	0.22	-	76,87,99,101	0
3	NAG	E	408	14/15	0.78	0.34	-	112,127,138,139	0
4	NAG	A	405	14/15	0.79	0.36	-	106,110,116,120	0
4	NAG	E	407	14/15	0.85	0.27	-	117,129,142,144	0
4	NAG	A	404	14/15	0.90	0.43	-	92,101,112,113	0
3	NAG	C	407	14/15	0.79	0.32	-	107,119,128,128	0
3	NAG	A	413	14/15	0.64	0.45	-	136,141,145,146	0
3	NAG	K	412	14/15	0.66	0.41	-	156,159,163,165	0
4	NAG	I	406	14/15	0.72	0.22	-	115,125,137,138	0
3	NAG	A	412	14/15	0.79	0.31	-	96,104,110,111	0
3	BMA	K	413	11/12	0.68	0.32	-	136,141,144,147	0
3	BMA	E	410	11/12	0.64	0.23	-	167,171,185,186	0
3	NAG	I	407	14/15	0.86	0.25	-	106,118,127,127	0
4	NAG	G	405	14/15	0.62	0.34	-	134,141,145,146	0
3	NAG	E	402	14/15	0.76	0.26	-	85,94,106,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	C	406	14/15	0.72	0.25	-	135,144,156,157	0
3	NAG	E	412	14/15	0.67	0.32	-	99,110,115,116	0
3	NAG	C	402	14/15	0.89	0.19	-	80,84,89,90	0
4	NAG	I	404	14/15	0.73	0.32	-	127,132,138,141	0
4	NAG	K	407	14/15	0.74	0.22	-	131,142,155,157	0
4	NAG	G	412	14/15	0.79	0.23	-	104,111,114,115	0
3	NAG	G	409	14/15	0.82	0.23	-	147,160,168,169	0
4	NAG	G	404	14/15	0.79	0.30	-	100,105,109,109	0
4	NAG	E	405	14/15	0.70	0.28	-	98,104,113,119	0
3	BMA	K	403	11/12	0.48	0.28	-	114,118,124,126	0
3	BMA	I	413	11/12	0.47	0.40	-	166,170,173,175	0
3	BMA	A	410	11/12	0.64	0.20	-	182,186,198,199	0

## 6.4 Ligands ⓘ

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( $\text{\AA}^2$ )	Q<0.9
5	NAG	C	404	14/15	0.74	0.29	-0.17	85,96,107,109	0
5	NAG	J	600	14/15	0.58	0.38	-	197,206,213,214	0
5	NAG	E	411	14/15	0.57	0.56	-	126,134,139,142	0
5	NAG	A	415	14/15	0.90	0.16	-	117,130,138,139	0
5	NAG	B	600	14/15	0.74	0.26	-	194,202,209,210	0
5	NAG	G	411	14/15	0.84	0.36	-	130,138,142,145	0
5	NAG	D	600	14/15	0.41	0.44	-	200,206,211,213	0
5	NAG	A	411	14/15	0.81	0.35	-	80,87,91,93	0
5	NAG	I	410	14/15	0.64	0.42	-	119,125,127,129	0
5	NAG	G	414	14/15	0.55	0.37	-	106,119,127,128	0
5	NAG	C	410	14/15	0.76	0.27	-	103,107,111,111	0
5	NAG	F	600	14/15	0.58	0.26	-	186,193,200,200	0
5	NAG	K	414	14/15	0.74	0.23	-	106,117,125,126	0
5	NAG	I	414	14/15	0.46	0.54	-	150,161,168,169	0
5	NAG	C	414	14/15	0.56	0.51	-	111,122,129,129	0
5	NAG	E	415	14/15	0.80	0.22	-	109,119,127,129	0
5	NAG	H	600	14/15	0.64	0.27	-	203,207,210,211	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.