



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:07 AM GMT

PDB ID : 2FK0
Title : Crystal Structure of a H5N1 influenza virus hemagglutinin.
Authors : Stevens, J.; Wilson, I.A.
Deposited on : 2006-01-03
Resolution : 2.95 Å(reported)

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

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

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

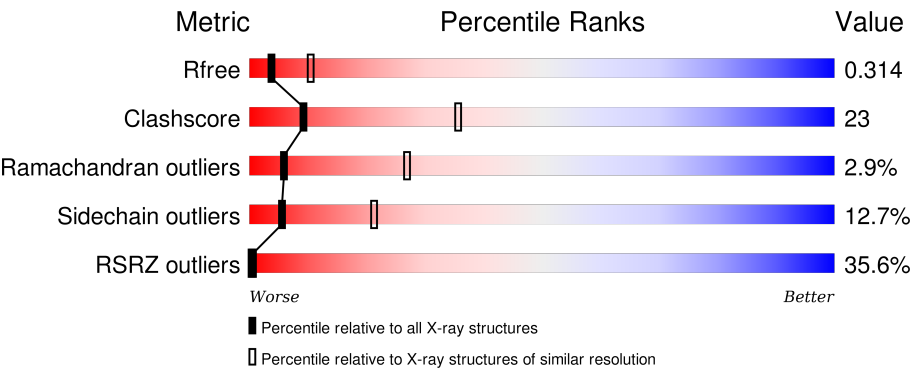
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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

Mol	Chain	Length	Quality of chain
1	A	334	<div><div>16%</div><div>61%</div><div>29%</div><div>6%</div><div>• •</div></div>
1	C	334	<div><div>15%</div><div>60%</div><div>31%</div><div>• • •</div></div>
1	E	334	<div><div>14%</div><div>56%</div><div>34%</div><div>6%</div><div>• •</div></div>
1	G	334	<div><div>12%</div><div>58%</div><div>32%</div><div>6%</div><div>• •</div></div>
1	I	334	<div><div>16%</div><div>57%</div><div>32%</div><div>7%</div><div>• •</div></div>

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Mol	Chain	Length	Quality of chain
1	K	334	
1	M	334	
1	O	334	
1	Q	334	
2	B	181	
2	D	181	
2	F	181	
2	H	181	
2	J	181	
2	L	181	
2	N	181	
2	P	181	
2	R	181	

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	3	X	-	-	-
3	NAG	I	3	X	-	-	-
3	NAG	K	3	X	-	-	X
3	NAG	M	3	X	-	-	X
3	NAG	O	3	X	-	-	X
4	NAG	A	3	X	-	-	-
4	NAG	E	3	X	-	-	-
4	BMA	E	5	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36202 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	C	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	E	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	G	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	I	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	K	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	M	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	O	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			
1	Q	322	Total	C	N	O	S	0	0	0
			2553	1613	441	484	15			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	ALA	-	CLONING ARTIFACT	GB 50296053
A	8	ASP	-	CLONING ARTIFACT	GB 50296053
A	9	PRO	-	CLONING ARTIFACT	GB 50296053
A	10	GLY	-	CLONING ARTIFACT	GB 50296053
C	7	ALA	-	CLONING ARTIFACT	GB 50296053
C	8	ASP	-	CLONING ARTIFACT	GB 50296053
C	9	PRO	-	CLONING ARTIFACT	GB 50296053
C	10	GLY	-	CLONING ARTIFACT	GB 50296053
E	7	ALA	-	CLONING ARTIFACT	GB 50296053
E	8	ASP	-	CLONING ARTIFACT	GB 50296053
E	9	PRO	-	CLONING ARTIFACT	GB 50296053

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Chain	Residue	Modelled	Actual	Comment	Reference
E	10	GLY	-	CLONING ARTIFACT	GB 50296053
G	7	ALA	-	CLONING ARTIFACT	GB 50296053
G	8	ASP	-	CLONING ARTIFACT	GB 50296053
G	9	PRO	-	CLONING ARTIFACT	GB 50296053
G	10	GLY	-	CLONING ARTIFACT	GB 50296053
I	7	ALA	-	CLONING ARTIFACT	GB 50296053
I	8	ASP	-	CLONING ARTIFACT	GB 50296053
I	9	PRO	-	CLONING ARTIFACT	GB 50296053
I	10	GLY	-	CLONING ARTIFACT	GB 50296053
K	7	ALA	-	CLONING ARTIFACT	GB 50296053
K	8	ASP	-	CLONING ARTIFACT	GB 50296053
K	9	PRO	-	CLONING ARTIFACT	GB 50296053
K	10	GLY	-	CLONING ARTIFACT	GB 50296053
M	7	ALA	-	CLONING ARTIFACT	GB 50296053
M	8	ASP	-	CLONING ARTIFACT	GB 50296053
M	9	PRO	-	CLONING ARTIFACT	GB 50296053
M	10	GLY	-	CLONING ARTIFACT	GB 50296053
O	7	ALA	-	CLONING ARTIFACT	GB 50296053
O	8	ASP	-	CLONING ARTIFACT	GB 50296053
O	9	PRO	-	CLONING ARTIFACT	GB 50296053
O	10	GLY	-	CLONING ARTIFACT	GB 50296053
Q	7	ALA	-	CLONING ARTIFACT	GB 50296053
Q	8	ASP	-	CLONING ARTIFACT	GB 50296053
Q	9	PRO	-	CLONING ARTIFACT	GB 50296053
Q	10	GLY	-	CLONING ARTIFACT	GB 50296053

- Molecule 2 is a protein called hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	D	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	F	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	H	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	J	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	L	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	N	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			
2	R	175	Total	C	N	O	S	0	0	0
			1416	880	246	282	8			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	CLONING ARTIFACT	GB 58618438
B	176	GLY	-	CLONING ARTIFACT	GB 58618438
B	177	ARG	-	CLONING ARTIFACT	GB 58618438
B	178	LEU	-	CLONING ARTIFACT	GB 58618438
B	179	VAL	-	CLONING ARTIFACT	GB 58618438
B	180	PRO	-	CLONING ARTIFACT	GB 58618438
B	181	ARG	-	CLONING ARTIFACT	GB 58618438
D	175	SER	-	CLONING ARTIFACT	GB 58618438
D	176	GLY	-	CLONING ARTIFACT	GB 58618438
D	177	ARG	-	CLONING ARTIFACT	GB 58618438
D	178	LEU	-	CLONING ARTIFACT	GB 58618438
D	179	VAL	-	CLONING ARTIFACT	GB 58618438
D	180	PRO	-	CLONING ARTIFACT	GB 58618438
D	181	ARG	-	CLONING ARTIFACT	GB 58618438
F	175	SER	-	CLONING ARTIFACT	GB 58618438
F	176	GLY	-	CLONING ARTIFACT	GB 58618438
F	177	ARG	-	CLONING ARTIFACT	GB 58618438
F	178	LEU	-	CLONING ARTIFACT	GB 58618438
F	179	VAL	-	CLONING ARTIFACT	GB 58618438
F	180	PRO	-	CLONING ARTIFACT	GB 58618438
F	181	ARG	-	CLONING ARTIFACT	GB 58618438
H	175	SER	-	CLONING ARTIFACT	GB 58618438
H	176	GLY	-	CLONING ARTIFACT	GB 58618438
H	177	ARG	-	CLONING ARTIFACT	GB 58618438
H	178	LEU	-	CLONING ARTIFACT	GB 58618438
H	179	VAL	-	CLONING ARTIFACT	GB 58618438
H	180	PRO	-	CLONING ARTIFACT	GB 58618438
H	181	ARG	-	CLONING ARTIFACT	GB 58618438
J	175	SER	-	CLONING ARTIFACT	GB 58618438
J	176	GLY	-	CLONING ARTIFACT	GB 58618438
J	177	ARG	-	CLONING ARTIFACT	GB 58618438
J	178	LEU	-	CLONING ARTIFACT	GB 58618438
J	179	VAL	-	CLONING ARTIFACT	GB 58618438
J	180	PRO	-	CLONING ARTIFACT	GB 58618438

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Chain	Residue	Modelled	Actual	Comment	Reference
J	181	ARG	-	CLONING ARTIFACT	GB 58618438
L	175	SER	-	CLONING ARTIFACT	GB 58618438
L	176	GLY	-	CLONING ARTIFACT	GB 58618438
L	177	ARG	-	CLONING ARTIFACT	GB 58618438
L	178	LEU	-	CLONING ARTIFACT	GB 58618438
L	179	VAL	-	CLONING ARTIFACT	GB 58618438
L	180	PRO	-	CLONING ARTIFACT	GB 58618438
L	181	ARG	-	CLONING ARTIFACT	GB 58618438
N	175	SER	-	CLONING ARTIFACT	GB 58618438
N	176	GLY	-	CLONING ARTIFACT	GB 58618438
N	177	ARG	-	CLONING ARTIFACT	GB 58618438
N	178	LEU	-	CLONING ARTIFACT	GB 58618438
N	179	VAL	-	CLONING ARTIFACT	GB 58618438
N	180	PRO	-	CLONING ARTIFACT	GB 58618438
N	181	ARG	-	CLONING ARTIFACT	GB 58618438
P	175	SER	-	CLONING ARTIFACT	GB 58618438
P	176	GLY	-	CLONING ARTIFACT	GB 58618438
P	177	ARG	-	CLONING ARTIFACT	GB 58618438
P	178	LEU	-	CLONING ARTIFACT	GB 58618438
P	179	VAL	-	CLONING ARTIFACT	GB 58618438
P	180	PRO	-	CLONING ARTIFACT	GB 58618438
P	181	ARG	-	CLONING ARTIFACT	GB 58618438
R	175	SER	-	CLONING ARTIFACT	GB 58618438
R	176	GLY	-	CLONING ARTIFACT	GB 58618438
R	177	ARG	-	CLONING ARTIFACT	GB 58618438
R	178	LEU	-	CLONING ARTIFACT	GB 58618438
R	179	VAL	-	CLONING ARTIFACT	GB 58618438
R	180	PRO	-	CLONING ARTIFACT	GB 58618438
R	181	ARG	-	CLONING ARTIFACT	GB 58618438

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

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

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

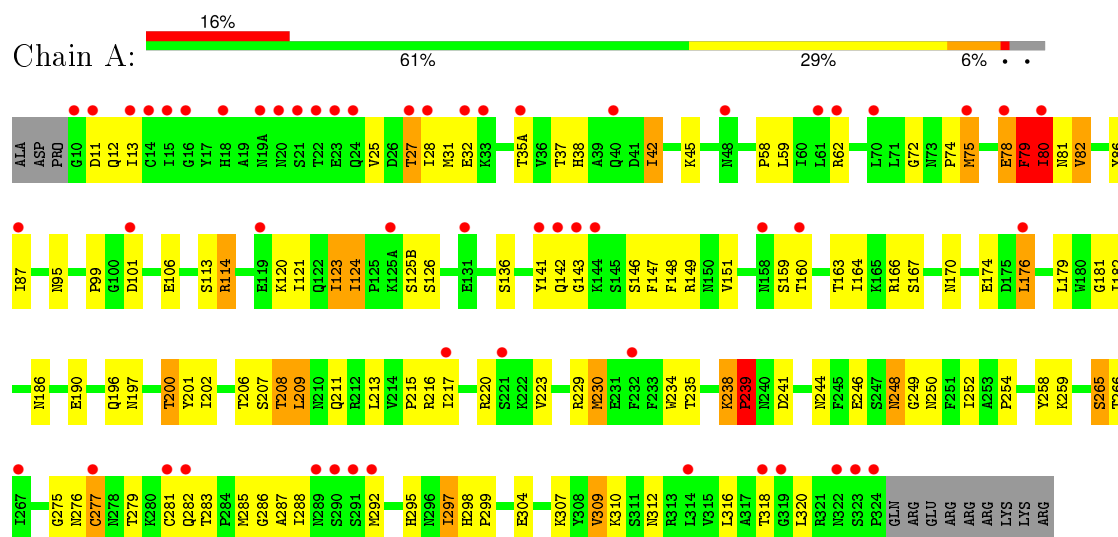
- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

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

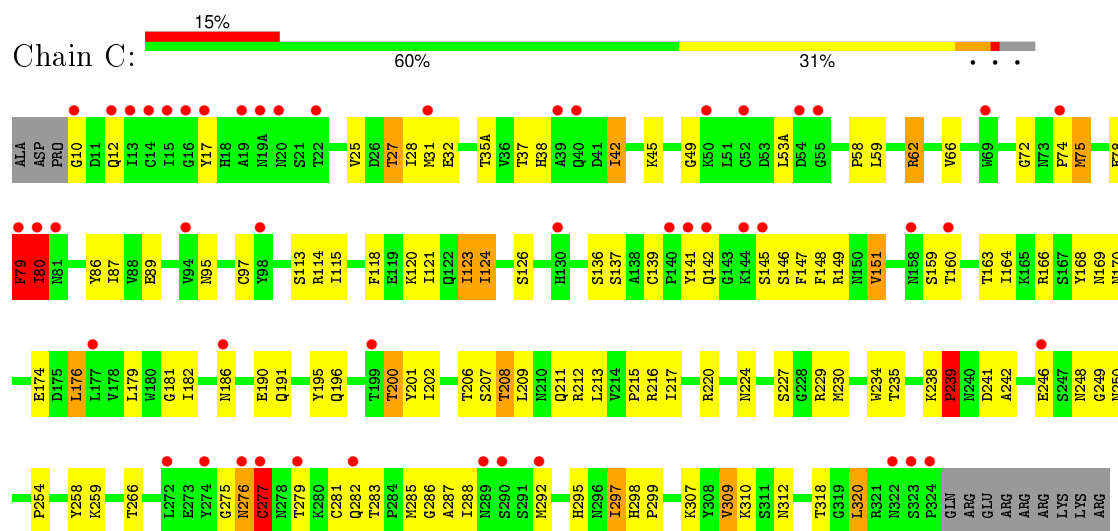
3 Residue-property plots [i](#)

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

• Molecule 1: hemagglutinin

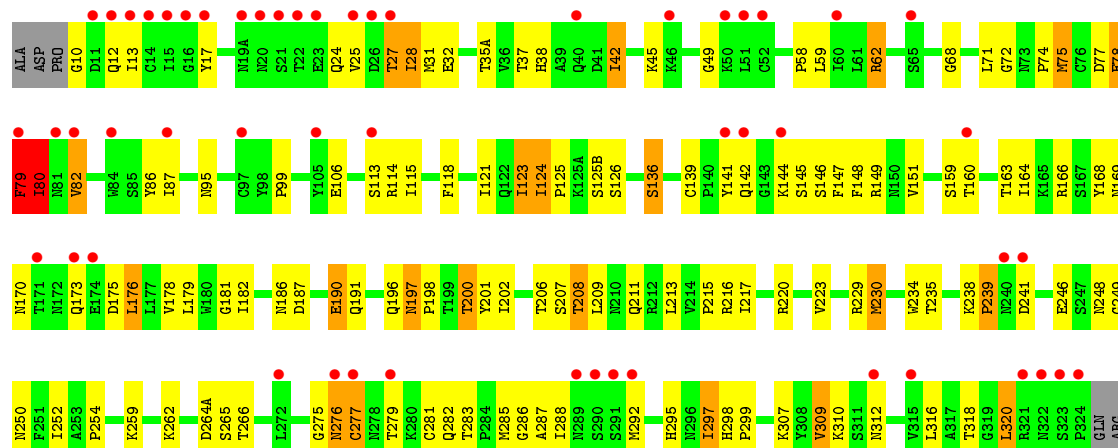


• Molecule 1: hemagglutinin



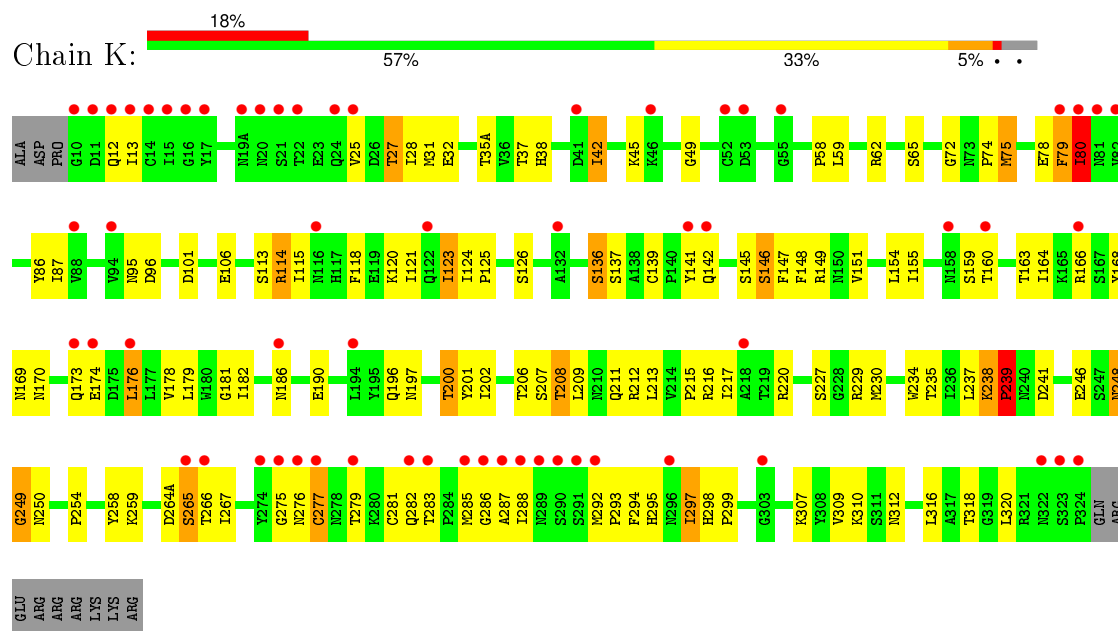
• Molecule 1: hemagglutinin



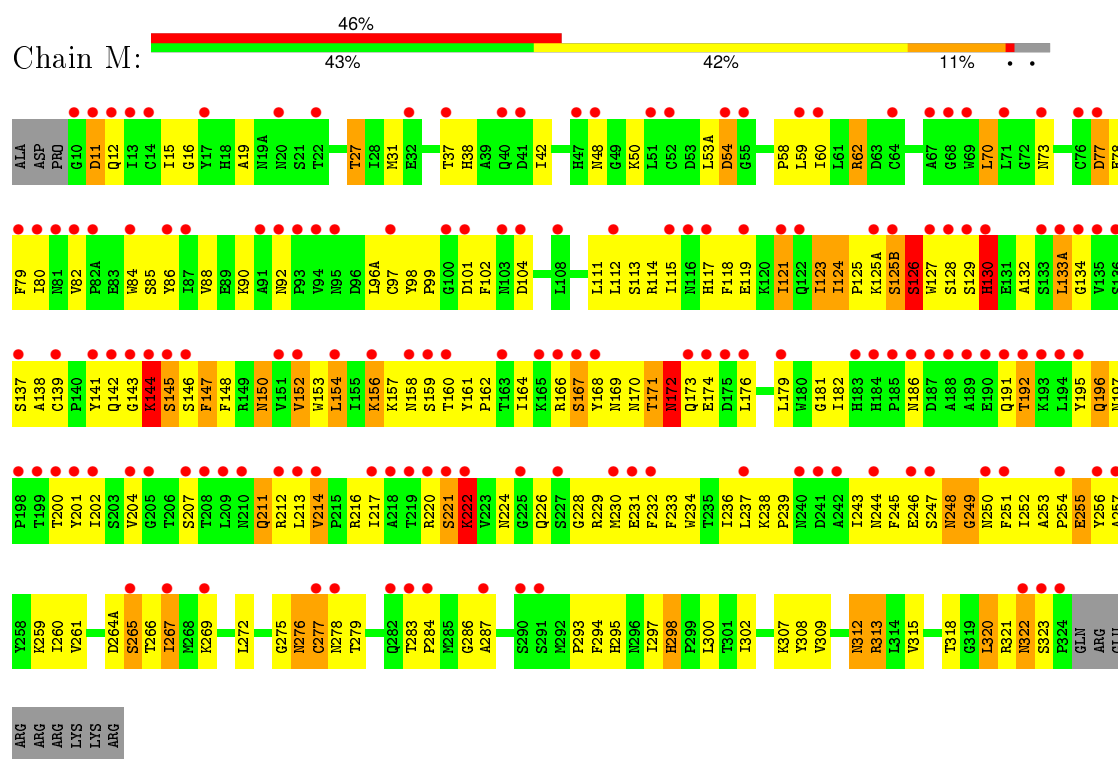


GLU
ARG
ARG
ARG
LYS
LYS
ARG

• Molecule 1: hemagglutinin

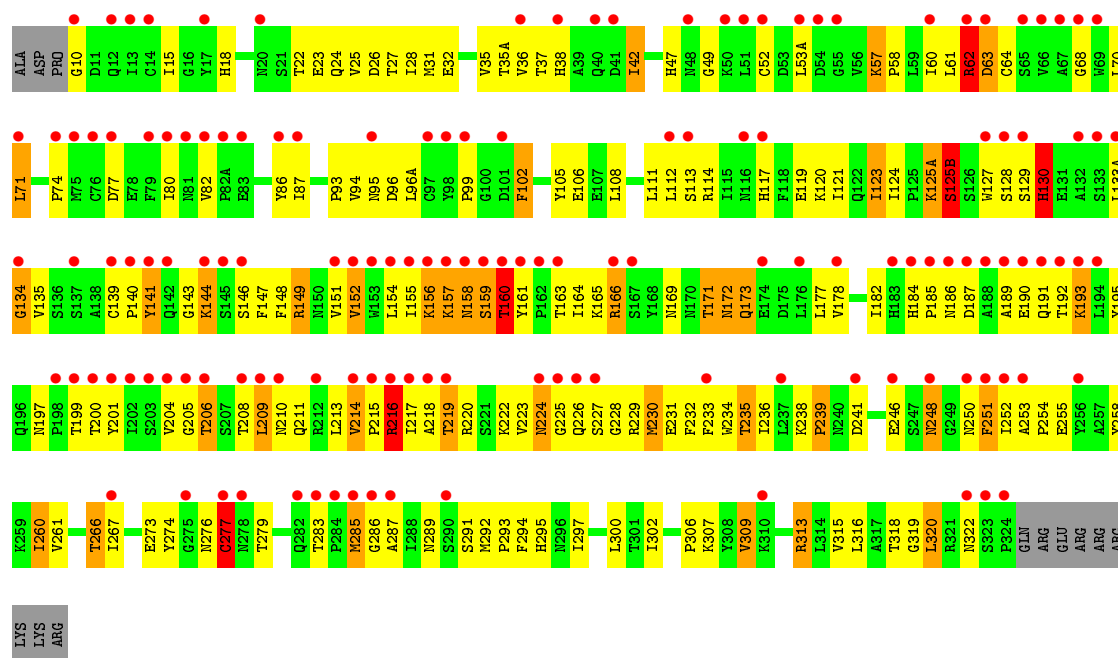


• Molecule 1: hemagglutinin

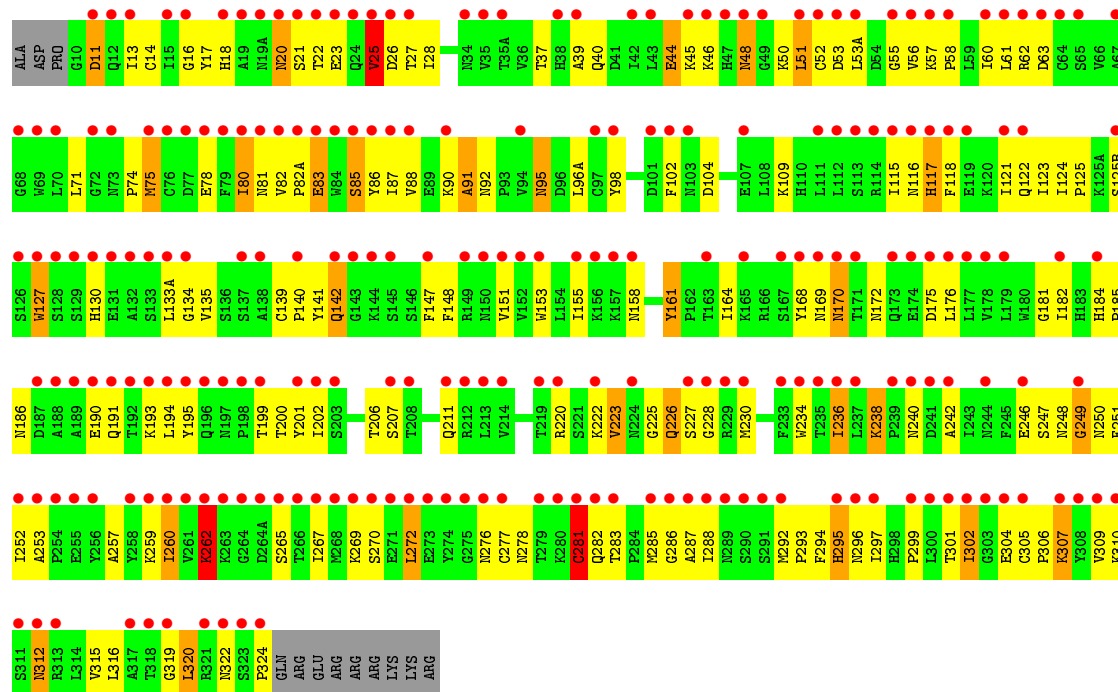


• Molecule 1: hemagglutinin

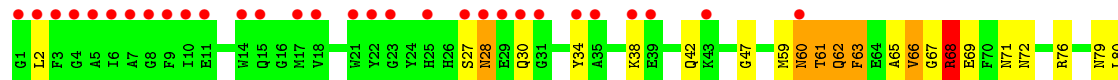
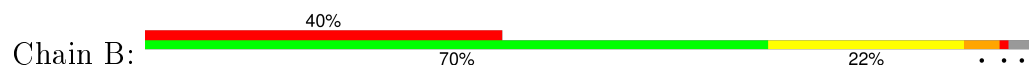


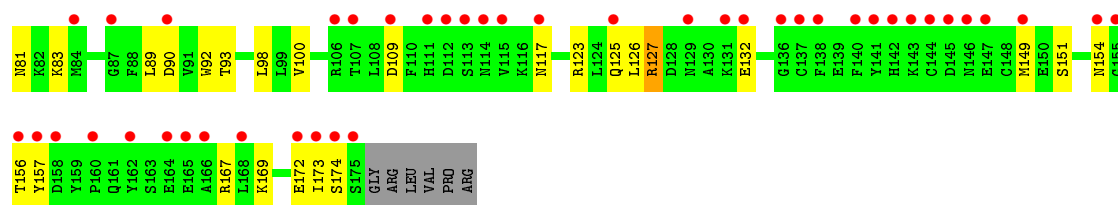


• Molecule 1: hemagglutinin



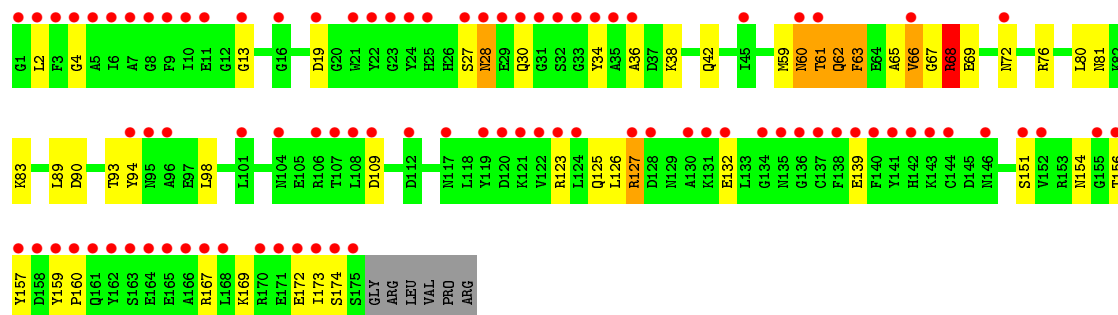
• Molecule 2: hemagglutinin





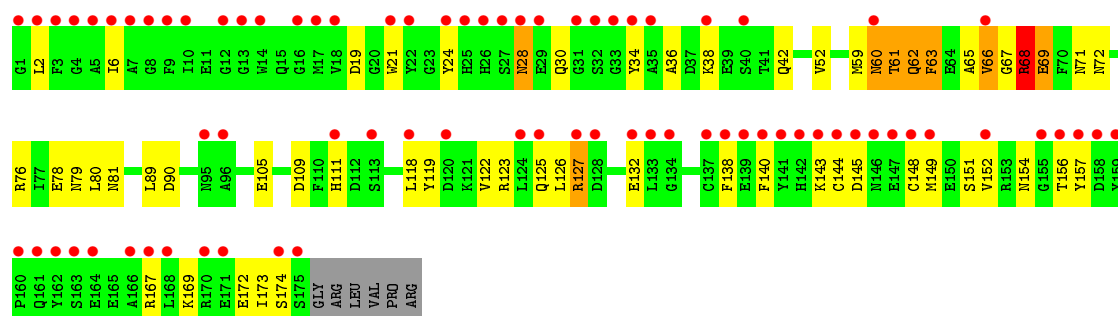
• Molecule 2: hemagglutinin

Chain D:



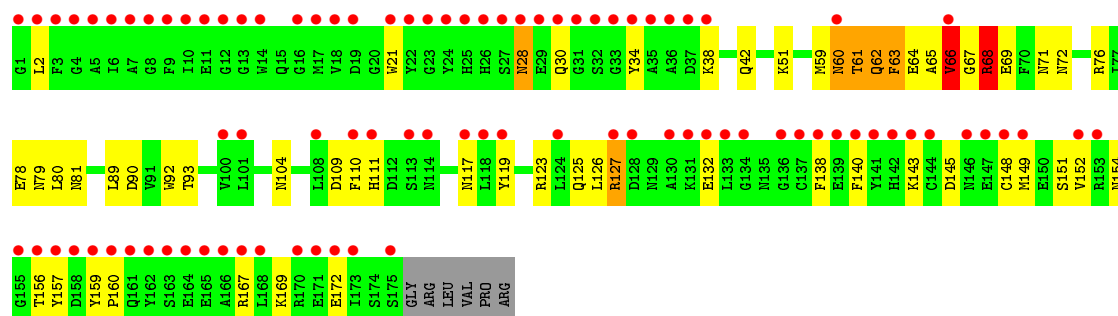
• Molecule 2: hemagglutinin

Chain F:

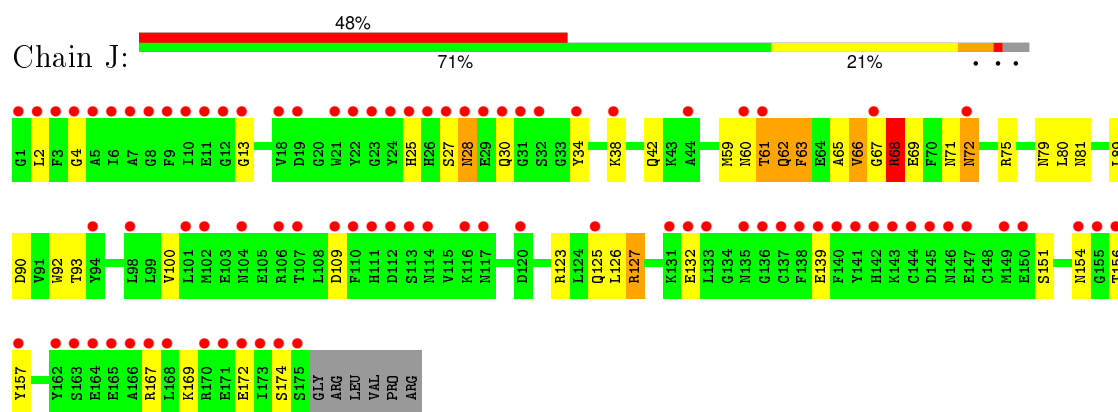


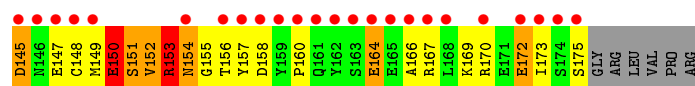
• Molecule 2: hemagglutinin

Chain H:

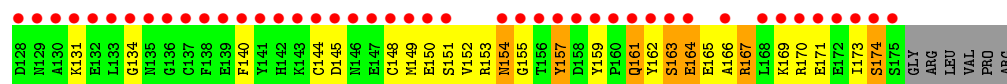
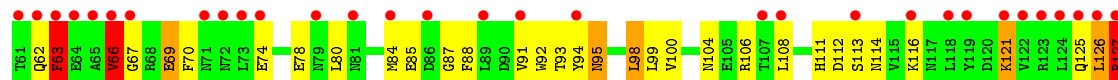
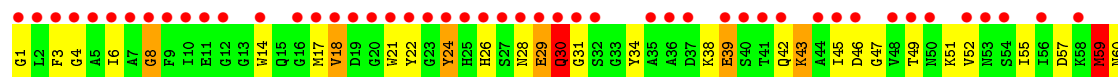


• Molecule 2: hemagglutinin





● Molecule 2: hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	197.94Å 197.94Å 134.69Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	171.50 – 2.95 49.49 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.9 (171.50-2.95) 98.9 (49.49-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.268 , 0.319 0.266 , 0.314	Depositor DCC
R_{free} test set	1233 reflections (1.02%)	DCC
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 98.8	EDS
Estimated twinning fraction	0.012 for -h,-k,l 0.008 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 122499 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	36202	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.76	0/2615	0.83	3/3551 (0.1%)
1	C	0.84	3/2615 (0.1%)	0.87	2/3551 (0.1%)
1	E	0.84	1/2615 (0.0%)	0.87	4/3551 (0.1%)
1	G	0.84	3/2615 (0.1%)	0.85	3/3551 (0.1%)
1	I	0.80	2/2615 (0.1%)	0.85	4/3551 (0.1%)
1	K	0.79	1/2615 (0.0%)	0.83	2/3551 (0.1%)
1	M	1.12	21/2615 (0.8%)	0.87	5/3551 (0.1%)
1	O	1.49	22/2615 (0.8%)	0.91	9/3551 (0.3%)
1	Q	0.65	2/2615 (0.1%)	0.70	0/3551
2	B	0.67	0/1443	0.70	3/1939 (0.2%)
2	D	0.68	0/1443	0.71	3/1939 (0.2%)
2	F	0.70	3/1443 (0.2%)	0.71	3/1939 (0.2%)
2	H	0.67	1/1443 (0.1%)	0.70	3/1939 (0.2%)
2	J	0.64	0/1443	0.68	2/1939 (0.1%)
2	L	0.67	1/1443 (0.1%)	0.67	2/1939 (0.1%)
2	N	1.29	7/1443 (0.5%)	0.86	5/1939 (0.3%)
2	P	1.38	13/1443 (0.9%)	0.88	5/1939 (0.3%)
2	R	0.74	5/1443 (0.3%)	0.69	0/1939
All	All	0.91	85/36522 (0.2%)	0.81	58/49410 (0.1%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	3
1	M	0	1
1	O	0	3
1	Q	0	1
2	B	0	3
2	D	0	3
2	F	0	3
2	H	0	3
2	J	0	2
2	L	0	3
2	N	0	2
2	P	0	2
3	C	1	0
3	I	1	0
3	K	1	0
3	M	1	0
3	O	1	0
4	A	1	0
4	E	1	0
All	All	7	38

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	125(B)	SER	CB-OG	34.55	1.87	1.42
2	N	38	LYS	CE-NZ	31.98	2.29	1.49
2	P	143	LYS	CE-NZ	27.78	2.18	1.49
1	O	157	LYS	CD-CE	22.51	2.07	1.51
1	O	130	HIS	CE1-NE2	20.34	1.79	1.32
1	O	125(A)	LYS	CE-NZ	18.91	1.96	1.49
1	M	130	HIS	CE1-NE2	18.73	1.75	1.32
2	P	38	LYS	CE-NZ	17.21	1.92	1.49
2	P	145	ASP	CG-OD1	16.80	1.64	1.25
1	O	157	LYS	CE-NZ	16.52	1.90	1.49
2	N	38	LYS	CD-CE	15.33	1.89	1.51
1	O	219	THR	CB-OG1	15.01	1.73	1.43
1	M	130	HIS	CG-ND1	14.75	1.71	1.38
1	M	247	SER	CB-OG	14.60	1.61	1.42
1	M	166	ARG	C-O	14.56	1.51	1.23
2	N	165	GLU	CD-OE2	14.41	1.41	1.25
1	O	160	THR	CB-OG1	14.28	1.71	1.43
1	O	159	SER	CB-OG	14.14	1.60	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	143	LYS	CD-CE	14.06	1.86	1.51
1	Q	130	HIS	CE1-NE2	13.35	1.63	1.32
1	O	125(A)	LYS	CD-CE	13.06	1.83	1.51
1	O	130	HIS	CG-ND1	12.82	1.67	1.38
1	M	159	SER	CB-OG	12.05	1.57	1.42
1	O	128	SER	CB-OG	11.90	1.57	1.42
2	R	150	GLU	CD-OE1	11.71	1.38	1.25
1	M	158	ASN	CG-OD1	11.48	1.49	1.24
2	N	38	LYS	CG-CD	11.47	1.91	1.52
1	M	158	ASN	CG-ND2	11.43	1.61	1.32
1	M	126	SER	CB-OG	11.06	1.56	1.42
2	P	145	ASP	CG-OD2	10.45	1.49	1.25
1	O	157	LYS	CG-CD	10.41	1.87	1.52
1	O	156	LYS	CE-NZ	10.31	1.74	1.49
2	P	175	SER	C-O	9.61	1.41	1.23
2	N	11	GLU	CG-CD	9.14	1.65	1.51
1	O	119	GLU	CD-OE2	8.90	1.35	1.25
2	P	125	GLN	CD-NE2	8.60	1.54	1.32
1	Q	130	HIS	CG-ND1	8.52	1.57	1.38
2	P	125	GLN	CG-CD	8.52	1.70	1.51
2	N	165	GLU	CD-OE1	8.35	1.34	1.25
1	M	137	SER	CB-OG	8.21	1.52	1.42
2	R	116	LYS	CD-CE	8.07	1.71	1.51
2	P	150	GLU	CD-OE1	7.94	1.34	1.25
2	R	39	GLU	CD-OE2	7.92	1.34	1.25
1	K	139	CYS	CB-SG	-7.75	1.69	1.82
1	M	166	ARG	CZ-NH1	7.71	1.43	1.33
1	O	165	LYS	CD-CE	7.71	1.70	1.51
2	R	39	GLU	CD-OE1	7.45	1.33	1.25
1	C	139	CYS	CB-SG	-7.40	1.69	1.82
1	M	154	LEU	CG-CD1	7.34	1.78	1.51
1	M	172	ASN	CG-OD1	7.33	1.40	1.24
1	E	277	CYS	CB-SG	-7.20	1.70	1.82
1	G	139	CYS	CB-SG	-7.14	1.70	1.82
1	M	172	ASN	CG-ND2	6.69	1.49	1.32
1	I	139	CYS	CB-SG	-6.67	1.71	1.82
1	M	222	LYS	CE-NZ	6.61	1.65	1.49
1	O	216	ARG	CZ-NH1	6.38	1.41	1.33
1	G	277	CYS	CB-SG	-6.33	1.71	1.82
2	L	78	GLU	CG-CD	6.29	1.61	1.51
2	P	125	GLN	CB-CG	6.21	1.69	1.52
2	P	150	GLU	CG-CD	6.20	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	64	CYS	CB-SG	-6.14	1.71	1.82
1	O	10	GLY	N-CA	6.13	1.55	1.46
2	N	11	GLU	CB-CG	6.10	1.63	1.52
2	P	125	GLN	CD-OE1	6.04	1.37	1.24
1	C	277	CYS	CB-SG	-6.03	1.72	1.82
2	R	150	GLU	CB-CG	5.99	1.63	1.52
1	M	73	ASN	CG-OD1	5.96	1.37	1.24
2	P	38	LYS	CD-CE	5.94	1.66	1.51
1	O	158	ASN	CG-OD1	5.93	1.37	1.24
2	H	78	GLU	CG-CD	5.78	1.60	1.51
1	M	152	VAL	C-O	5.76	1.34	1.23
1	M	166	ARG	CZ-NH2	5.68	1.40	1.33
1	M	128	SER	CB-OG	5.59	1.49	1.42
2	F	68	ARG	N-CA	5.58	1.57	1.46
1	M	166	ARG	C-N	5.54	1.46	1.34
1	O	160	THR	CB-CG2	5.41	1.70	1.52
1	M	186	ASN	CG-ND2	5.40	1.46	1.32
1	O	193	LYS	CE-NZ	5.38	1.62	1.49
1	O	210	ASN	C-O	5.32	1.33	1.23
1	C	151	VAL	CB-CG2	-5.30	1.41	1.52
2	F	69	GLU	CD-OE2	5.22	1.31	1.25
2	F	78	GLU	CG-CD	5.21	1.59	1.51
1	I	190	GLU	CG-CD	5.17	1.59	1.51
1	M	167	SER	CB-OG	5.16	1.49	1.42
1	O	219	THR	CB-CG2	5.08	1.69	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	38	LYS	CD-CE-NZ	-14.03	79.42	111.70
1	M	166	ARG	NE-CZ-NH2	-12.85	113.88	120.30
1	O	125(A)	LYS	CD-CE-NZ	-11.74	84.70	111.70
1	M	154	LEU	CB-CG-CD2	11.21	130.05	111.00
2	P	143	LYS	CD-CE-NZ	-10.31	87.98	111.70
2	P	145	ASP	CB-CG-OD1	-9.66	109.61	118.30
1	M	154	LEU	CB-CG-CD1	-8.27	96.94	111.00
1	O	157	LYS	CG-CD-CE	-8.05	87.74	111.90
1	A	176	LEU	CA-CB-CG	7.27	132.02	115.30
1	O	157	LYS	CD-CE-NZ	-7.16	95.24	111.70
2	F	76	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	K	176	LEU	CA-CB-CG	6.98	131.34	115.30
1	O	157	LYS	CB-CG-CD	-6.81	93.90	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	176	LEU	CA-CB-CG	6.79	130.92	115.30
2	N	38	LYS	CG-CD-CE	-6.72	91.74	111.90
2	D	68	ARG	N-CA-C	6.57	128.74	111.00
2	P	38	LYS	CD-CE-NZ	-6.48	96.80	111.70
1	G	176	LEU	CA-CB-CG	6.46	130.17	115.30
2	P	143	LYS	CG-CD-CE	-6.41	92.67	111.90
2	B	68	ARG	N-CA-C	6.38	128.24	111.00
2	H	68	ARG	N-CA-C	6.30	128.01	111.00
2	H	76	ARG	NE-CZ-NH2	-6.30	117.15	120.30
2	L	68	ARG	N-CA-C	6.15	127.61	111.00
1	K	80	ILE	N-CA-C	-6.13	94.44	111.00
1	E	176	LEU	CA-CB-CG	6.09	129.30	115.30
2	J	68	ARG	N-CA-C	6.00	127.21	111.00
1	C	176	LEU	CA-CB-CG	6.00	129.11	115.30
1	O	160	THR	CA-CB-CG2	-6.00	104.01	112.40
2	J	66	VAL	N-CA-C	5.99	127.17	111.00
1	E	63	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	O	125(B)	SER	CA-CB-OG	-5.93	95.20	111.20
2	F	68	ARG	N-CA-C	5.92	126.98	111.00
1	E	176	LEU	CB-CG-CD2	-5.89	100.98	111.00
2	D	66	VAL	N-CA-C	5.68	126.34	111.00
1	I	80	ILE	N-CA-C	-5.67	95.70	111.00
1	G	80	ILE	N-CA-C	-5.62	95.83	111.00
2	B	76	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	C	80	ILE	N-CA-C	-5.57	95.97	111.00
1	I	62	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	I	175	ASP	CB-CG-OD1	5.46	123.21	118.30
1	M	166	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	80	ILE	N-CA-C	-5.44	96.31	111.00
1	E	80	ILE	N-CA-C	-5.38	96.48	111.00
2	B	66	VAL	N-CA-C	5.37	125.50	111.00
2	F	66	VAL	N-CA-C	5.37	125.50	111.00
1	O	277	CYS	CA-CB-SG	5.32	123.58	114.00
2	H	66	VAL	N-CA-C	5.26	125.21	111.00
1	O	166	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	D	76	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	N	38	LYS	CB-CG-CD	-5.17	98.14	111.60
1	A	209	LEU	CB-CG-CD2	-5.17	102.22	111.00
1	O	216	ARG	NE-CZ-NH2	-5.15	117.72	120.30
2	P	59	MET	CA-CB-CG	-5.13	104.58	113.30
2	L	66	VAL	N-CA-C	5.13	124.85	111.00
2	N	165	GLU	OE1-CD-OE2	5.12	129.45	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	66	VAL	N-CA-C	5.10	124.77	111.00
1	M	154	LEU	CD1-CG-CD2	5.08	125.74	110.50
1	G	176	LEU	CB-CG-CD2	-5.06	102.41	111.00

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	3	NAG	C1
3	C	3	NAG	C1
4	E	3	NAG	C1
3	I	3	NAG	C1
3	K	3	NAG	C1
3	M	3	NAG	C1
3	O	3	NAG	C1

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	ASN	Peptide
1	A	276	ASN	Peptide
2	B	60	ASN	Peptide
2	B	61	THR	Peptide
2	B	68	ARG	Peptide
1	C	249	GLY	Peptide
1	C	276	ASN	Peptide
2	D	60	ASN	Peptide
2	D	61	THR	Peptide
2	D	68	ARG	Peptide
1	E	248	ASN	Peptide
1	E	276	ASN	Peptide
2	F	60	ASN	Peptide
2	F	61	THR	Peptide
2	F	68	ARG	Peptide
1	G	248	ASN	Peptide
1	G	276	ASN	Peptide
2	H	60	ASN	Peptide
2	H	61	THR	Peptide
2	H	68	ARG	Peptide
1	I	276	ASN	Peptide
2	J	61	THR	Peptide
2	J	68	ARG	Peptide
1	K	248	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	K	249	GLY	Peptide
1	K	276	ASN	Peptide
2	L	60	ASN	Peptide
2	L	61	THR	Peptide
2	L	68	ARG	Peptide
1	M	130	HIS	Sidechain
2	N	61	THR	Peptide
2	N	68	ARG	Peptide
1	O	225	GLY	Peptide
1	O	276	ASN	Peptide
1	O	313	ARG	Peptide
2	P	60	ASN	Peptide
2	P	61	THR	Peptide
1	Q	240	ASN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2553	0	2496	117	2
1	C	2553	0	2496	118	3
1	E	2553	0	2496	169	0
1	G	2553	0	2496	131	3
1	I	2553	0	2496	140	0
1	K	2553	0	2496	117	2
1	M	2553	0	2496	166	0
1	O	2553	0	2496	191	0
1	Q	2553	0	2498	132	0
2	B	1416	0	1320	47	0
2	D	1416	0	1320	46	0
2	F	1416	0	1320	72	0
2	H	1416	0	1320	60	0
2	J	1416	0	1320	42	0
2	L	1416	0	1320	39	0
2	N	1416	0	1320	75	0
2	P	1416	0	1320	82	0
2	R	1416	0	1320	77	0
3	A	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	56	0	50	1	0
3	E	28	0	25	0	0
3	G	28	0	25	2	0
3	I	56	0	50	1	0
3	K	56	0	50	0	0
3	M	56	0	50	4	0
3	O	56	0	50	2	0
4	A	39	0	34	3	0
4	E	39	0	34	3	0
4	G	39	0	34	0	0
All	All	36202	0	34773	1624	5

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 23.

All (1624) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:154:LEU:CD1	1:M:154:LEU:CG	1.79	1.60
1:M:130:HIS:CG	1:M:130:HIS:ND1	1.71	1.54
1:M:130:HIS:NE2	1:M:130:HIS:CE1	1.75	1.53
1:O:125(A):LYS:CE	1:O:125(A):LYS:CD	1.83	1.52
2:P:143:LYS:CE	2:P:143:LYS:CD	1.86	1.51
2:N:38:LYS:CD	2:N:38:LYS:CE	1.89	1.49
2:N:38:LYS:CD	2:N:38:LYS:CG	1.91	1.48
1:O:157:LYS:CG	1:O:157:LYS:CD	1.87	1.48
1:O:156:LYS:NZ	1:O:156:LYS:CE	1.74	1.45
1:O:160:THR:CB	1:O:160:THR:OG1	1.71	1.37
1:O:157:LYS:NZ	1:O:157:LYS:CE	1.90	1.34
1:O:219:THR:OG1	1:O:219:THR:CB	1.73	1.34
2:P:145:ASP:CG	2:P:145:ASP:OD1	1.64	1.34
1:G:141:TYR:HE2	1:G:142:GLN:NE2	1.28	1.31
2:P:38:LYS:CE	2:P:38:LYS:NZ	1.92	1.31
1:O:157:LYS:CD	1:O:157:LYS:CE	2.07	1.31
1:I:141:TYR:HE2	1:I:142:GLN:NE2	1.29	1.31
1:E:141:TYR:HE2	1:E:142:GLN:NE2	1.26	1.30
1:O:130:HIS:NE2	1:O:130:HIS:CE1	1.79	1.30
1:O:125(A):LYS:CE	1:O:125(A):LYS:NZ	1.96	1.29
1:C:141:TYR:HE2	1:C:142:GLN:NE2	1.27	1.27
1:A:141:TYR:HE2	1:A:142:GLN:NE2	1.31	1.26
1:E:78:GLU:OE2	1:I:142:GLN:OE1	1.56	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:125(B):SER:OG	1:O:125(B):SER:CB	1.87	1.22
1:K:141:TYR:HE2	1:K:142:GLN:NE2	1.41	1.16
1:Q:206:THR:HG22	1:Q:207:SER:H	1.04	1.14
1:G:75:MET:HB2	1:G:95:ASN:ND2	1.66	1.10
1:E:200:THR:HG21	1:E:250:ASN:OD1	1.51	1.10
1:K:200:THR:HG21	1:K:250:ASN:OD1	1.52	1.10
1:E:75:MET:HB2	1:E:95:ASN:ND2	1.67	1.09
1:G:200:THR:HG21	1:G:250:ASN:OD1	1.49	1.09
1:E:182:ILE:HD12	1:E:202:ILE:HD13	1.34	1.08
1:I:200:THR:HG21	1:I:250:ASN:OD1	1.51	1.07
1:A:75:MET:HB2	1:A:95:ASN:ND2	1.69	1.07
2:P:143:LYS:CE	2:P:143:LYS:NZ	2.18	1.07
1:A:75:MET:HB2	1:A:95:ASN:HD22	1.21	1.04
1:M:130:HIS:CG	1:M:130:HIS:CE1	2.40	1.04
1:K:182:ILE:HD12	1:K:202:ILE:HD13	1.38	1.04
1:A:200:THR:HG21	1:A:250:ASN:OD1	1.55	1.04
1:I:75:MET:HB2	1:I:95:ASN:ND2	1.73	1.04
1:C:75:MET:HB2	1:C:95:ASN:ND2	1.73	1.04
1:G:182:ILE:HD11	1:G:213:LEU:HD12	1.40	1.03
1:G:75:MET:HB2	1:G:95:ASN:HD22	1.24	1.02
1:E:75:MET:HB2	1:E:95:ASN:HD22	1.23	1.01
1:G:79:PHE:C	1:G:79:PHE:HD1	1.65	1.00
1:C:200:THR:HG21	1:C:250:ASN:OD1	1.61	0.99
2:B:59:MET:O	2:B:61:THR:N	1.94	0.99
1:E:13:ILE:CD1	2:F:152:VAL:HG11	1.93	0.98
2:R:165:GLU:O	2:R:169:LYS:HB3	1.64	0.98
2:P:59:MET:O	2:P:61:THR:N	1.95	0.98
1:K:75:MET:HB2	1:K:95:ASN:ND2	1.79	0.98
1:Q:282:GLN:O	1:Q:301:THR:HB	1.64	0.98
1:C:283:THR:HB	1:C:286:GLY:O	1.64	0.97
1:A:79:PHE:HD1	1:A:79:PHE:C	1.68	0.97
2:F:59:MET:O	2:F:61:THR:N	1.97	0.97
1:I:283:THR:HB	1:I:286:GLY:O	1.64	0.97
1:C:75:MET:HB2	1:C:95:ASN:HD22	1.29	0.97
1:E:283:THR:HB	1:E:286:GLY:O	1.65	0.97
2:N:150:GLU:O	2:N:154:ASN:HB2	1.64	0.96
1:O:283:THR:HG22	1:O:285:MET:H	1.30	0.96
1:G:182:ILE:HD12	1:G:202:ILE:HD13	1.46	0.96
1:E:182:ILE:HD11	1:E:213:LEU:HD12	1.47	0.96
2:N:38:LYS:NZ	2:N:38:LYS:CE	2.29	0.95
1:I:182:ILE:HD11	1:I:213:LEU:HD12	1.46	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:79:PHE:C	1:I:79:PHE:HD1	1.70	0.95
1:A:182:ILE:HD12	1:A:202:ILE:HD13	1.49	0.95
1:E:11:ASP:OD2	2:F:143:LYS:HA	1.66	0.95
1:E:79:PHE:HD1	1:E:79:PHE:C	1.68	0.94
1:O:28:ILE:HD11	2:P:102:MET:HG3	1.47	0.94
1:I:182:ILE:HD12	1:I:202:ILE:HD13	1.47	0.94
1:C:182:ILE:HD12	1:C:202:ILE:HD13	1.44	0.94
1:I:75:MET:HB2	1:I:95:ASN:HD22	1.32	0.94
1:O:141:TYR:HB2	1:O:146:SER:HB3	1.46	0.94
1:O:251:PHE:CE1	1:O:253:ALA:HA	2.03	0.93
1:E:272:LEU:HD21	1:M:171:THR:HG21	1.51	0.93
1:G:283:THR:HB	1:G:286:GLY:O	1.69	0.93
1:M:27:THR:HG22	1:M:31:MET:H	1.31	0.93
1:K:275:GLY:O	1:K:277:CYS:HB3	1.69	0.92
1:G:275:GLY:O	1:G:277:CYS:HB3	1.69	0.92
2:J:59:MET:O	2:J:61:THR:N	2.02	0.92
1:Q:206:THR:CG2	1:Q:207:SER:H	1.83	0.92
1:C:182:ILE:HD11	1:C:213:LEU:HD12	1.52	0.92
2:R:30:GLN:HA	2:R:30:GLN:HE21	1.35	0.92
1:E:275:GLY:O	1:E:277:CYS:HB3	1.70	0.91
2:R:127:ARG:HB2	2:R:127:ARG:HH11	1.36	0.91
1:A:283:THR:HB	1:A:286:GLY:O	1.70	0.91
1:G:283:THR:HG22	1:G:285:MET:H	1.35	0.90
1:M:50:LYS:HD3	1:M:275:GLY:HA3	1.50	0.90
2:L:59:MET:O	2:L:61:THR:N	2.04	0.90
1:K:79:PHE:HD1	1:K:79:PHE:C	1.74	0.90
1:K:182:ILE:HD11	1:K:213:LEU:HD12	1.53	0.90
2:H:59:MET:O	2:H:61:THR:N	2.05	0.90
1:A:182:ILE:HD11	1:A:213:LEU:HD12	1.53	0.90
2:P:145:ASP:OD1	2:P:148:CYS:HB2	1.71	0.90
2:N:145:ASP:O	2:N:148:CYS:HB3	1.72	0.90
1:Q:206:THR:HG22	1:Q:207:SER:N	1.85	0.90
1:M:275:GLY:O	1:M:277:CYS:HB3	1.71	0.89
1:I:79:PHE:O	1:I:80:ILE:HD13	1.72	0.89
2:P:151:SER:HB2	2:P:157:TYR:HA	1.55	0.89
1:C:275:GLY:O	1:C:277:CYS:HB3	1.71	0.89
1:E:13:ILE:HD12	2:F:152:VAL:HG11	1.53	0.89
1:C:79:PHE:C	1:C:79:PHE:HD1	1.76	0.89
1:A:275:GLY:O	1:A:277:CYS:HB3	1.73	0.89
1:M:201:TYR:H	1:M:248:ASN:HB2	1.38	0.88
1:Q:16:GLY:HA3	2:R:14:TRP:HD1	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:157:LYS:CB	1:O:157:LYS:CD	2.53	0.87
1:K:79:PHE:CD1	1:K:79:PHE:C	2.46	0.87
1:E:79:PHE:C	1:E:79:PHE:CD1	2.42	0.86
1:A:159:SER:O	1:A:196:GLN:HG3	1.74	0.86
1:I:283:THR:HG22	1:I:285:MET:H	1.40	0.86
2:H:63:PHE:N	2:H:63:PHE:HD1	1.73	0.86
2:D:59:MET:O	2:D:61:THR:N	2.09	0.85
1:M:200:THR:HA	1:M:248:ASN:HB3	1.57	0.85
1:K:283:THR:HB	1:K:286:GLY:O	1.75	0.84
1:O:135:VAL:HG22	1:O:146:SER:HA	1.58	0.84
1:A:79:PHE:C	1:A:79:PHE:CD1	2.42	0.84
1:C:124:ILE:HD11	1:C:254:PRO:O	1.77	0.84
1:I:275:GLY:O	1:I:277:CYS:HB3	1.76	0.84
1:E:283:THR:HG22	1:E:285:MET:H	1.43	0.84
1:C:79:PHE:CD1	1:C:79:PHE:C	2.49	0.84
1:I:79:PHE:C	1:I:79:PHE:CD1	2.44	0.84
1:M:114:ARG:HB2	1:M:265:SER:HB3	1.59	0.84
1:I:288:ILE:HD11	1:I:297:ILE:HG13	1.59	0.83
2:L:63:PHE:HD1	2:L:63:PHE:N	1.73	0.83
2:P:143:LYS:CE	2:P:143:LYS:CG	2.55	0.83
2:P:63:PHE:HD1	2:P:63:PHE:N	1.77	0.83
1:M:130:HIS:CE1	1:M:130:HIS:CD2	2.66	0.83
1:A:283:THR:HG22	1:A:285:MET:H	1.44	0.83
1:G:79:PHE:C	1:G:79:PHE:CD1	2.39	0.83
1:M:38:HIS:HB2	1:M:318:THR:HB	1.61	0.83
1:M:154:LEU:CB	1:M:154:LEU:CD1	2.56	0.82
1:K:75:MET:HB2	1:K:95:ASN:HD22	1.42	0.82
1:K:283:THR:HG22	1:K:285:MET:H	1.44	0.82
1:E:27:THR:HG22	1:E:31:MET:H	1.43	0.82
1:E:272:LEU:CD2	1:M:171:THR:HG21	2.10	0.82
1:G:288:ILE:HD11	1:G:297:ILE:HG13	1.60	0.82
2:N:144:CYS:SG	2:N:149:MET:HG3	2.20	0.81
1:E:79:PHE:CG	1:I:144:LYS:HE3	2.16	0.81
1:E:126:SER:HB2	1:E:166:ARG:HH22	1.45	0.81
1:Q:44:GLU:HB2	1:Q:294:PHE:O	1.81	0.81
2:H:63:PHE:CD1	2:H:63:PHE:N	2.45	0.80
1:C:79:PHE:O	1:C:80:ILE:HD13	1.82	0.80
2:J:63:PHE:N	2:J:63:PHE:HD1	1.78	0.80
2:H:61:THR:OG1	1:I:310:LYS:HD3	1.82	0.80
1:O:53(A):LEU:HD11	1:O:302:ILE:HG22	1.62	0.80
1:K:79:PHE:O	1:K:80:ILE:HD13	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:27:THR:HG22	1:I:31:MET:H	1.47	0.80
1:M:267:ILE:HD12	1:M:267:ILE:H	1.45	0.80
2:L:63:PHE:N	2:L:63:PHE:CD1	2.44	0.80
2:D:63:PHE:N	2:D:63:PHE:HD1	1.78	0.80
2:N:143:LYS:H	2:N:143:LYS:HD3	1.44	0.79
1:K:288:ILE:HD11	1:K:297:ILE:HG13	1.64	0.79
1:C:27:THR:HG22	1:C:31:MET:H	1.46	0.79
1:Q:225:GLY:O	1:Q:226:GLN:HB2	1.83	0.79
1:K:27:THR:HG22	1:K:31:MET:H	1.44	0.79
1:K:126:SER:HB2	1:K:166:ARG:HH22	1.48	0.79
2:F:63:PHE:HD1	2:F:63:PHE:N	1.80	0.79
1:E:87:ILE:HD12	1:E:113:SER:HA	1.64	0.79
1:M:266:THR:HG21	2:N:67:GLY:H	1.47	0.78
1:E:279:THR:HG21	1:E:287:ALA:HB1	1.64	0.78
2:R:95:ASN:O	2:R:99:LEU:HB2	1.84	0.78
1:A:288:ILE:HD11	1:A:297:ILE:HG13	1.66	0.78
1:Q:260:ILE:HG23	1:Q:262:LYS:HB3	1.64	0.78
1:C:283:THR:HG22	1:C:285:MET:H	1.49	0.78
1:M:265:SER:OG	1:M:266:THR:N	2.15	0.78
1:E:288:ILE:HD11	1:E:297:ILE:HG13	1.65	0.78
1:G:179:LEU:HD23	1:G:234:TRP:HB3	1.66	0.77
2:B:167:ARG:HD3	2:D:174:SER:HA	1.66	0.77
1:K:179:LEU:HD23	1:K:234:TRP:HB3	1.65	0.77
1:E:18:HIS:HB2	2:F:21:TRP:HA	1.65	0.77
2:P:63:PHE:N	2:P:63:PHE:CD1	2.48	0.77
1:K:141:TYR:CE2	1:K:142:GLN:NE2	2.29	0.77
1:A:121:ILE:HG22	1:A:123:ILE:HD13	1.64	0.77
1:O:238:LYS:HG3	1:O:239:PRO:HD2	1.65	0.77
1:G:27:THR:HG22	1:G:31:MET:H	1.48	0.77
1:C:288:ILE:HD11	1:C:297:ILE:HG13	1.66	0.77
1:G:79:PHE:O	1:G:79:PHE:CD1	2.39	0.76
1:I:79:PHE:CD1	1:I:79:PHE:O	2.39	0.76
2:D:63:PHE:N	2:D:63:PHE:CD1	2.50	0.76
1:E:11:ASP:HB2	2:F:140:PHE:HD1	1.51	0.76
1:I:59:LEU:HD11	1:I:80:ILE:HG23	1.67	0.76
2:N:132:GLU:O	2:N:134:GLY:N	2.18	0.76
1:O:307:LYS:HD2	2:P:92:TRP:CE2	2.21	0.76
2:D:167:ARG:HD3	2:F:174:SER:HA	1.67	0.76
1:C:179:LEU:HD23	1:C:234:TRP:HB3	1.67	0.75
1:E:282:GLN:HE21	1:E:283:THR:H	1.34	0.75
1:A:282:GLN:HE21	1:A:283:THR:H	1.32	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:300:LEU:HD21	2:P:68:ARG:HH21	1.51	0.75
1:M:283:THR:HG22	1:M:284:PRO:HD2	1.67	0.75
2:F:63:PHE:CD1	2:F:63:PHE:N	2.52	0.75
1:E:11:ASP:O	2:F:140:PHE:N	2.16	0.75
2:R:4:GLY:HA2	2:R:8:GLY:HA3	1.68	0.75
1:E:47:HIS:HE1	1:M:171:THR:O	1.69	0.75
1:O:293:PRO:HG2	1:O:294:PHE:CD1	2.22	0.75
1:K:13:ILE:HD11	2:L:149:MET:HG2	1.68	0.74
1:C:59:LEU:HD11	1:C:80:ILE:HG23	1.69	0.74
1:Q:16:GLY:HA3	2:R:14:TRP:CD1	2.20	0.74
1:M:201:TYR:H	1:M:248:ASN:CB	2.00	0.74
1:C:124:ILE:CG1	1:C:254:PRO:O	2.35	0.74
1:G:206:THR:HG22	1:G:207:SER:N	2.02	0.74
1:K:80:ILE:O	1:K:80:ILE:HG22	1.88	0.74
1:I:146:SER:OG	1:I:147:PHE:N	2.19	0.74
1:G:124:ILE:HD11	1:G:254:PRO:O	1.88	0.74
1:E:179:LEU:HD23	1:E:234:TRP:HB3	1.67	0.74
1:A:206:THR:HB	1:A:209:LEU:H	1.52	0.74
2:J:63:PHE:CD1	2:J:63:PHE:N	2.50	0.74
1:I:279:THR:HG21	1:I:287:ALA:HB1	1.68	0.74
1:M:204:VAL:HA	1:M:244:ASN:O	1.88	0.73
1:A:79:PHE:CD1	1:A:79:PHE:O	2.42	0.73
1:O:206:THR:HB	1:O:208:THR:H	1.53	0.73
1:G:206:THR:HG22	1:G:208:THR:H	1.54	0.73
1:I:266:THR:HG21	2:J:67:GLY:H	1.53	0.73
2:B:63:PHE:N	2:B:63:PHE:HD1	1.87	0.73
2:P:37:ASP:O	2:P:41:THR:OG1	2.07	0.73
2:P:164:GLU:HA	2:P:167:ARG:HB2	1.69	0.73
1:I:179:LEU:HD23	1:I:234:TRP:HB3	1.70	0.73
1:C:182:ILE:HD13	1:C:182:ILE:N	2.02	0.73
4:A:4:NAG:H5	4:A:4:NAG:HN2	1.54	0.73
1:A:126:SER:HB2	1:A:166:ARG:HH22	1.54	0.73
3:A:1:NAG:H62	3:A:2:NAG:H2	1.70	0.73
1:E:11:ASP:CB	2:F:140:PHE:HD1	2.02	0.72
1:C:124:ILE:CD1	1:C:254:PRO:O	2.37	0.72
1:O:219:THR:HG22	1:O:220:ARG:H	1.54	0.72
1:E:79:PHE:O	1:E:79:PHE:CD1	2.42	0.72
1:I:124:ILE:HD11	1:I:254:PRO:O	1.89	0.72
2:P:25:HIS:HA	2:P:34:TYR:HB3	1.71	0.72
1:E:272:LEU:HD21	1:M:171:THR:CG2	2.20	0.72
2:R:30:GLN:HA	2:R:30:GLN:NE2	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:211:GLN:NE2	1:M:213:LEU:HD21	2.05	0.72
1:Q:104:ASP:HB2	1:Q:234:TRP:HE1	1.55	0.72
1:G:279:THR:HG21	1:G:287:ALA:HB1	1.72	0.72
1:G:79:PHE:O	1:G:80:ILE:HD13	1.90	0.72
1:M:37:THR:HB	1:M:320:LEU:H	1.54	0.72
1:C:279:THR:HG21	1:C:287:ALA:HB1	1.72	0.72
1:E:59:LEU:HD11	1:E:80:ILE:HG23	1.70	0.71
1:E:121:ILE:HG22	1:E:123:ILE:HD13	1.72	0.71
1:O:134:GLY:HA2	1:O:155:ILE:HD13	1.72	0.71
1:A:179:LEU:HD23	1:A:234:TRP:HB3	1.72	0.71
1:A:27:THR:HG22	1:A:31:MET:H	1.55	0.71
1:C:307:LYS:NZ	2:D:62:GLN:HB3	2.06	0.71
1:C:141:TYR:CE2	1:C:142:GLN:NE2	2.18	0.71
1:O:27:THR:HG22	1:O:31:MET:H	1.55	0.71
1:O:200:THR:HG21	1:O:250:ASN:HB2	1.73	0.71
1:Q:56:VAL:O	1:Q:85:SER:OG	2.09	0.71
1:C:159:SER:O	1:C:196:GLN:HG3	1.91	0.71
1:O:27:THR:HB	1:O:32:GLU:HB2	1.73	0.71
1:G:159:SER:O	1:G:196:GLN:HG3	1.91	0.71
1:E:75:MET:CB	1:E:95:ASN:ND2	2.52	0.70
1:I:159:SER:O	1:I:196:GLN:HG3	1.90	0.70
1:M:123:ILE:HG23	1:M:124:ILE:HG12	1.72	0.70
1:K:124:ILE:HD11	1:K:254:PRO:O	1.90	0.70
1:C:80:ILE:O	1:C:80:ILE:HG22	1.90	0.70
1:O:62:ARG:HD2	1:O:63:ASP:HB2	1.74	0.70
1:O:125(A):LYS:CE	1:O:125(A):LYS:CG	2.70	0.70
1:G:59:LEU:HD11	1:G:80:ILE:HG23	1.71	0.70
1:E:11:ASP:HB2	2:F:140:PHE:CD1	2.26	0.70
1:Q:87:ILE:HD11	1:Q:267:ILE:HA	1.73	0.70
1:M:200:THR:HA	1:M:248:ASN:CB	2.21	0.70
1:K:307:LYS:NZ	2:L:62:GLN:HB3	2.06	0.70
1:I:182:ILE:HD13	1:I:182:ILE:N	2.07	0.70
1:C:181:GLY:C	1:C:182:ILE:HD13	2.11	0.70
1:A:206:THR:HG22	1:A:208:THR:H	1.56	0.70
1:A:72:GLY:O	1:A:148:PHE:HA	1.92	0.70
1:C:126:SER:HB2	1:C:166:ARG:HH22	1.56	0.70
1:G:11:ASP:OD2	2:H:143:LYS:HA	1.92	0.70
1:E:206:THR:HG22	1:E:207:SER:N	2.07	0.70
1:C:206:THR:HG22	1:C:207:SER:N	2.06	0.70
1:O:223:VAL:O	1:O:224:ASN:HB2	1.91	0.70
1:E:206:THR:HB	1:E:209:LEU:H	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:159:SER:O	1:K:196:GLN:HG3	1.92	0.70
1:A:59:LEU:HD11	1:A:80:ILE:HG23	1.72	0.69
1:Q:181:GLY:O	1:Q:182:ILE:HD13	1.92	0.69
2:N:37:ASP:O	2:N:39:GLU:N	2.24	0.69
2:N:38:LYS:CD	2:N:38:LYS:CB	2.69	0.69
2:P:59:MET:C	2:P:61:THR:H	1.95	0.69
1:G:121:ILE:HG22	1:G:123:ILE:HD13	1.72	0.69
2:H:65:ALA:C	2:H:66:VAL:HG13	2.11	0.69
2:B:63:PHE:CD1	2:B:63:PHE:N	2.59	0.69
1:O:125(A):LYS:CD	1:O:125(A):LYS:NZ	2.56	0.69
1:Q:16:GLY:CA	2:R:14:TRP:HD1	2.04	0.69
1:M:202:ILE:HB	1:M:213:LEU:HD12	1.74	0.69
1:G:206:THR:CG2	1:G:207:SER:N	2.55	0.69
1:C:141:TYR:CD2	1:C:142:GLN:HG3	2.28	0.69
1:M:243:ILE:HG12	1:M:245:PHE:CE1	2.27	0.69
2:F:65:ALA:C	2:F:66:VAL:HG13	2.13	0.69
1:E:146:SER:OG	1:E:147:PHE:N	2.26	0.69
1:E:124:ILE:HD11	1:E:254:PRO:O	1.92	0.69
1:I:124:ILE:CG1	1:I:254:PRO:O	2.40	0.69
1:M:279:THR:HG21	1:M:287:ALA:HB1	1.73	0.69
1:C:87:ILE:HD12	1:C:113:SER:HA	1.75	0.69
1:I:282:GLN:HE21	1:I:283:THR:H	1.40	0.69
2:N:117:ASN:O	2:N:121:LYS:HG2	1.93	0.69
1:M:114:ARG:HH11	1:M:265:SER:HB2	1.59	0.68
1:A:206:THR:HG22	1:A:207:SER:N	2.08	0.68
1:A:206:THR:HG22	1:A:208:THR:N	2.09	0.68
1:I:206:THR:HG22	1:I:207:SER:N	2.08	0.68
1:C:206:THR:CG2	1:C:207:SER:N	2.56	0.68
1:I:38:HIS:HB2	1:I:318:THR:HB	1.75	0.68
1:G:206:THR:HB	1:G:209:LEU:H	1.57	0.68
1:O:295:HIS:HD2	1:O:297:ILE:H	1.39	0.68
1:I:121:ILE:HG22	1:I:123:ILE:HD13	1.75	0.68
1:A:279:THR:HG21	1:A:287:ALA:HB1	1.73	0.68
1:E:18:HIS:N	2:F:21:TRP:O	2.25	0.68
1:I:126:SER:HB2	1:I:166:ARG:HH22	1.59	0.68
1:Q:172:ASN:ND2	1:Q:259:LYS:HE2	2.09	0.68
2:P:59:MET:HE1	2:P:62:GLN:HG3	1.75	0.67
1:G:72:GLY:O	1:G:148:PHE:HA	1.94	0.67
1:I:72:GLY:O	1:I:148:PHE:HA	1.94	0.67
1:A:75:MET:CB	1:A:95:ASN:ND2	2.54	0.67
1:A:124:ILE:HD13	1:A:254:PRO:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLY:C	1:A:182:ILE:HD13	2.14	0.67
1:A:229:ARG:HH21	1:E:207:SER:HA	1.59	0.67
1:G:13:ILE:CD1	2:H:152:VAL:HG11	2.24	0.67
1:E:307:LYS:NZ	2:F:62:GLN:HB3	2.08	0.67
1:M:202:ILE:HA	1:M:246:GLU:O	1.94	0.67
1:E:124:ILE:HD13	1:E:254:PRO:HG2	1.75	0.67
1:C:79:PHE:O	1:C:79:PHE:CD1	2.48	0.67
1:O:182:ILE:HG23	1:O:215:PRO:HB3	1.77	0.67
1:K:124:ILE:HD13	1:K:254:PRO:HG2	1.76	0.67
1:K:59:LEU:HD11	1:K:80:ILE:HG23	1.76	0.67
1:A:124:ILE:CG1	1:A:254:PRO:O	2.42	0.67
1:A:124:ILE:HD11	1:A:254:PRO:O	1.95	0.67
1:C:206:THR:HG22	1:C:208:THR:H	1.59	0.67
1:G:126:SER:HB2	1:G:166:ARG:HH22	1.60	0.67
1:O:211:GLN:NE2	1:O:213:LEU:HD11	2.09	0.67
1:E:126:SER:CB	1:E:166:ARG:HH22	2.06	0.66
1:I:27:THR:HG22	1:I:32:GLU:H	1.60	0.66
2:N:120:ASP:OD1	2:N:123:ARG:NH1	2.28	0.66
1:K:206:THR:HG22	1:K:207:SER:N	2.11	0.66
1:K:121:ILE:HG22	1:K:123:ILE:HD13	1.75	0.66
1:Q:14:CYS:O	2:R:24:TYR:HB3	1.95	0.66
1:I:181:GLY:C	1:I:182:ILE:HD13	2.15	0.66
1:K:282:GLN:HE21	1:K:283:THR:H	1.41	0.66
1:M:172:ASN:H	1:M:172:ASN:HD22	1.43	0.66
1:E:72:GLY:O	1:E:148:PHE:HA	1.95	0.66
1:I:206:THR:CG2	1:I:207:SER:N	2.58	0.66
2:N:38:LYS:CE	2:N:38:LYS:CG	2.73	0.66
1:E:206:THR:CG2	1:E:207:SER:N	2.59	0.66
1:G:266:THR:HG21	2:H:67:GLY:H	1.60	0.66
1:K:206:THR:CG2	1:K:207:SER:N	2.58	0.66
2:P:27:SER:HA	2:P:32:SER:HB2	1.76	0.66
2:N:59:MET:O	2:N:61:THR:N	2.29	0.66
1:C:282:GLN:HE21	1:C:283:THR:H	1.42	0.66
2:P:63:PHE:HD1	2:P:63:PHE:H	1.43	0.66
1:I:206:THR:HB	1:I:209:LEU:H	1.61	0.66
1:C:72:GLY:O	1:C:148:PHE:HA	1.96	0.66
1:K:279:THR:HG21	1:K:287:ALA:HB1	1.78	0.66
1:K:146:SER:OG	1:K:147:PHE:N	2.27	0.66
1:G:282:GLN:HE21	1:G:283:THR:H	1.42	0.65
2:B:90:ASP:OD1	2:F:63:PHE:HE1	1.79	0.65
1:K:206:THR:HG22	1:K:208:THR:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:166:ALA:HA	2:N:169:LYS:HB3	1.78	0.65
1:O:157:LYS:CG	1:O:157:LYS:CE	2.74	0.65
2:P:80:LEU:HD12	2:P:83:LYS:HE3	1.78	0.65
1:A:141:TYR:CE2	1:A:142:GLN:NE2	2.22	0.65
1:O:58:PRO:HB3	1:O:86:TYR:CE2	2.30	0.65
1:I:206:THR:HG22	1:I:208:THR:H	1.61	0.65
1:O:27:THR:HG23	2:P:105:GLU:HB2	1.79	0.65
4:A:4:NAG:H5	4:A:4:NAG:N2	2.08	0.65
1:C:38:HIS:HB2	1:C:318:THR:HB	1.77	0.65
1:G:75:MET:CB	1:G:95:ASN:ND2	2.55	0.65
1:G:206:THR:HG22	1:G:208:THR:N	2.10	0.65
2:R:166:ALA:HB1	2:R:170:ARG:HD3	1.78	0.65
1:E:79:PHE:O	1:E:80:ILE:HD13	1.96	0.65
1:O:123:ILE:N	1:O:255:GLU:O	2.27	0.65
1:K:186:ASN:HB3	1:K:190:GLU:OE2	1.97	0.65
1:M:277:CYS:SG	1:M:278:ASN:N	2.69	0.65
1:C:27:THR:HG22	1:C:32:GLU:H	1.62	0.65
1:A:27:THR:HG22	1:A:32:GLU:H	1.61	0.65
1:I:206:THR:HG22	1:I:208:THR:N	2.12	0.65
2:N:133:LEU:HB2	2:N:137:CYS:O	1.97	0.65
2:P:128:ASP:HB3	2:P:170:ARG:HH12	1.62	0.65
1:E:126:SER:HB3	1:I:79:PHE:CZ	2.32	0.65
1:O:38:HIS:HD2	1:O:319:GLY:HA3	1.62	0.65
1:C:141:TYR:CE2	1:C:142:GLN:HG3	2.32	0.64
1:Q:200:THR:HG23	1:Q:249:GLY:H	1.62	0.64
1:K:79:PHE:CD1	1:K:79:PHE:O	2.50	0.64
1:A:275:GLY:O	1:A:277:CYS:CB	2.45	0.64
2:B:174:SER:HA	2:F:167:ARG:HD3	1.77	0.64
1:E:50:LYS:HZ2	1:M:121:ILE:HG23	1.60	0.64
1:O:177:LEU:HD23	1:O:258:TYR:HD1	1.62	0.64
1:A:79:PHE:O	1:A:80:ILE:HD13	1.97	0.64
2:N:57:ASP:O	2:N:60:ASN:HB2	1.98	0.64
1:I:80:ILE:HG22	1:I:80:ILE:O	1.96	0.64
2:H:66:VAL:HG21	2:J:79:ASN:HD21	1.63	0.64
1:M:221:SER:O	1:M:229:ARG:NH2	2.29	0.64
2:P:133:LEU:HD21	2:P:139:GLU:HB2	1.78	0.64
1:A:12:GLN:HB2	2:B:27:SER:OG	1.98	0.64
2:N:63:PHE:CD1	2:N:63:PHE:N	2.62	0.64
1:A:206:THR:CG2	1:A:207:SER:N	2.61	0.64
2:N:151:SER:HB2	2:N:156:THR:O	1.98	0.64
1:Q:320:LEU:HD12	2:R:6:ILE:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:53(A):LEU:O	1:Q:278:ASN:HA	1.98	0.64
1:A:266:THR:HG21	2:B:67:GLY:H	1.62	0.64
2:H:68:ARG:HG3	2:H:68:ARG:O	1.96	0.64
1:O:57:LYS:H	1:O:57:LYS:CD	2.11	0.64
1:Q:22:THR:CG2	1:Q:324:PRO:HD3	2.27	0.64
2:P:59:MET:CE	2:P:62:GLN:HG3	2.28	0.64
1:K:38:HIS:HB2	1:K:318:THR:HB	1.80	0.64
1:O:172:ASN:N	1:O:172:ASN:ND2	2.47	0.63
1:G:38:HIS:HB2	1:G:318:THR:HB	1.80	0.63
1:K:181:GLY:C	1:K:182:ILE:HD13	2.17	0.63
1:I:79:PHE:O	1:I:80:ILE:CD1	2.46	0.63
1:C:206:THR:HB	1:C:209:LEU:H	1.63	0.63
1:Q:104:ASP:CB	1:Q:234:TRP:HE1	2.11	0.63
1:K:182:ILE:N	1:K:182:ILE:HD13	2.12	0.63
1:E:171:THR:HB	1:I:121:ILE:HD13	1.81	0.63
1:E:47:HIS:CE1	1:M:171:THR:O	2.51	0.63
1:M:172:ASN:N	1:M:172:ASN:HD22	1.97	0.63
1:G:206:THR:HG23	1:G:241:ASP:OD2	1.99	0.63
1:E:266:THR:HG21	2:F:67:GLY:H	1.64	0.63
1:K:141:TYR:CD2	1:K:142:GLN:HG3	2.32	0.63
1:O:38:HIS:HB2	1:O:318:THR:HB	1.81	0.63
1:C:206:THR:HG22	1:C:208:THR:N	2.14	0.62
1:M:228:GLY:O	1:M:229:ARG:NH1	2.32	0.62
1:E:38:HIS:HB2	1:E:318:THR:HB	1.81	0.62
1:O:214:VAL:O	1:O:216:ARG:HD3	2.00	0.62
1:O:102:PHE:HB3	1:O:105:TYR:HB2	1.81	0.62
1:Q:11:ASP:HB2	2:R:140:PHE:HD1	1.65	0.62
1:I:182:ILE:HD11	1:I:213:LEU:CD1	2.28	0.62
1:O:146:SER:OG	1:O:147:PHE:N	2.32	0.62
1:M:114:ARG:NH1	1:M:265:SER:HB2	2.14	0.62
1:K:126:SER:CB	1:K:166:ARG:HH22	2.11	0.62
1:K:201:TYR:CE2	1:K:248:ASN:HB2	2.34	0.62
1:M:170:ASN:ND2	1:M:239:PRO:HA	2.14	0.62
2:H:63:PHE:HE1	2:J:90:ASP:OD1	1.81	0.62
1:I:27:THR:CG2	1:I:31:MET:H	2.12	0.62
2:B:62:GLN:N	2:B:62:GLN:CD	2.51	0.62
1:O:313:ARG:HB3	1:O:315:VAL:HG23	1.81	0.62
1:Q:90:LYS:HD3	1:Q:270:SER:O	2.00	0.62
1:Q:63:ASP:HB3	1:Q:95:ASN:HD21	1.65	0.62
1:I:141:TYR:CD2	1:I:142:GLN:HG3	2.35	0.61
1:K:27:THR:HG22	1:K:32:GLU:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:63:PHE:HD1	2:N:63:PHE:H	1.48	0.61
1:Q:316:LEU:HD13	2:R:100:VAL:HG22	1.82	0.61
1:K:141:TYR:CE2	1:K:142:GLN:HG3	2.35	0.61
1:C:124:ILE:HG12	1:C:254:PRO:O	2.00	0.61
1:E:206:THR:HG22	1:E:208:THR:N	2.14	0.61
1:C:27:THR:CG2	1:C:31:MET:H	2.11	0.61
2:R:95:ASN:O	2:R:99:LEU:N	2.31	0.61
1:M:313:ARG:HD2	1:M:315:VAL:HG21	1.82	0.61
1:M:182:ILE:CD1	1:M:202:ILE:HD13	2.30	0.61
1:A:182:ILE:HD13	1:A:182:ILE:N	2.16	0.61
1:M:167:SER:HB2	1:M:243:ILE:O	2.00	0.61
1:G:87:ILE:HD12	1:G:113:SER:HA	1.83	0.61
2:N:63:PHE:HD1	2:N:63:PHE:N	1.99	0.61
1:G:170:ASN:O	1:G:239:PRO:O	2.18	0.61
1:K:206:THR:HG22	1:K:208:THR:H	1.66	0.61
1:A:38:HIS:HB2	1:A:318:THR:HB	1.83	0.61
1:G:283:THR:HG22	1:G:285:MET:N	2.14	0.61
1:E:15:ILE:HD13	2:F:119:TYR:HA	1.82	0.61
1:G:80:ILE:HG22	1:G:80:ILE:O	2.01	0.61
1:A:282:GLN:NE2	1:A:283:THR:H	1.97	0.61
1:E:179:LEU:CD2	1:E:234:TRP:HB3	2.30	0.61
1:C:206:THR:CG2	1:C:207:SER:H	2.14	0.61
1:E:117:HIS:CD2	1:I:125(B):SER:HB3	2.35	0.61
1:Q:127:TRP:CE3	1:Q:127:TRP:HA	2.35	0.61
1:M:171:THR:H	1:M:172:ASN:HD22	1.49	0.61
1:G:11:ASP:HB2	2:H:140:PHE:HD1	1.66	0.61
1:O:172:ASN:HD22	1:O:172:ASN:H	1.49	0.61
2:R:145:ASP:O	2:R:148:CYS:HB3	2.00	0.61
1:E:27:THR:CG2	1:E:31:MET:H	2.12	0.60
1:O:127:TRP:CZ3	1:O:154:LEU:HD11	2.36	0.60
2:N:164:GLU:HA	2:N:167:ARG:HB2	1.83	0.60
1:G:179:LEU:CD2	1:G:234:TRP:HB3	2.31	0.60
1:E:320:LEU:HB3	2:F:111:HIS:CD2	2.34	0.60
2:J:167:ARG:HD3	2:L:174:SER:HA	1.83	0.60
1:C:79:PHE:O	1:C:80:ILE:CD1	2.49	0.60
1:M:123:ILE:HD13	1:M:257:ALA:HB3	1.83	0.60
1:Q:53:ASP:HB2	1:Q:276:ASN:ND2	2.16	0.60
1:E:141:TYR:CE2	1:E:142:GLN:NE2	2.18	0.60
1:M:283:THR:HG22	1:M:284:PRO:CD	2.31	0.60
1:G:124:ILE:CG1	1:G:254:PRO:O	2.49	0.60
1:M:134:GLY:HA3	1:M:153:TRP:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:72:GLY:O	1:K:148:PHE:HA	2.02	0.60
1:E:282:GLN:NE2	1:E:283:THR:H	1.98	0.60
1:K:182:ILE:HD11	1:K:213:LEU:CD1	2.30	0.60
1:G:79:PHE:O	1:G:79:PHE:HD1	1.79	0.60
2:P:65:ALA:C	2:P:66:VAL:HG13	2.22	0.60
1:G:181:GLY:C	1:G:182:ILE:HD13	2.22	0.60
1:I:124:ILE:CD1	1:I:254:PRO:O	2.49	0.60
2:N:37:ASP:C	2:N:39:GLU:H	2.04	0.60
1:O:177:LEU:HD23	1:O:258:TYR:CD1	2.36	0.60
1:O:172:ASN:N	1:O:172:ASN:HD22	1.99	0.60
1:A:230:MET:SD	1:A:252:ILE:HD11	2.42	0.60
1:G:141:TYR:CD2	1:G:142:GLN:HG3	2.36	0.60
1:A:310:LYS:HD3	2:F:61:THR:OG1	2.01	0.60
1:O:283:THR:HB	1:O:286:GLY:O	2.02	0.60
1:C:275:GLY:O	1:C:277:CYS:CB	2.48	0.60
1:G:124:ILE:CD1	1:G:254:PRO:O	2.50	0.60
1:G:121:ILE:HG13	1:G:259:LYS:HE3	1.84	0.60
2:P:59:MET:C	2:P:61:THR:N	2.55	0.60
1:Q:262:LYS:HG3	1:Q:262:LYS:O	2.02	0.60
1:E:206:THR:HG22	1:E:208:THR:H	1.67	0.60
1:G:59:LEU:HD11	1:G:80:ILE:CG2	2.32	0.60
1:M:152:VAL:HG23	1:M:255:GLU:HG3	1.82	0.60
2:R:164:GLU:HA	2:R:167:ARG:HD2	1.83	0.59
2:D:81:ASN:HD22	2:F:80:LEU:HD13	1.66	0.59
1:E:141:TYR:CD2	1:E:142:GLN:HG3	2.37	0.59
1:M:172:ASN:N	1:M:172:ASN:ND2	2.49	0.59
1:E:179:LEU:HD23	1:E:234:TRP:CB	2.32	0.59
1:G:307:LYS:NZ	2:H:62:GLN:HB3	2.17	0.59
1:M:15:ILE:HD12	1:M:15:ILE:H	1.68	0.59
1:O:218:ALA:HB3	1:O:220:ARG:HH21	1.66	0.59
1:G:27:THR:HG22	1:G:32:GLU:H	1.66	0.59
1:G:13:ILE:HD12	2:H:152:VAL:HG11	1.84	0.59
1:E:159:SER:O	1:E:196:GLN:HG3	2.02	0.59
1:Q:80:ILE:C	1:Q:82:VAL:H	2.06	0.59
1:Q:260:ILE:HG22	1:Q:260:ILE:O	2.02	0.59
1:A:124:ILE:CD1	1:A:254:PRO:HG2	2.31	0.59
1:O:222:LYS:HD2	1:O:222:LYS:N	2.18	0.59
1:E:182:ILE:HD11	1:E:213:LEU:CD1	2.26	0.59
1:M:123:ILE:HG22	1:M:255:GLU:C	2.23	0.59
1:O:184:HIS:HB2	1:O:220:ARG:HH12	1.67	0.59
1:O:222:LYS:HA	1:O:226:GLN:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:THR:OG1	1:E:310:LYS:HD3	2.02	0.59
1:O:295:HIS:HD2	1:O:297:ILE:N	2.00	0.59
1:K:206:THR:HB	1:K:209:LEU:H	1.66	0.59
1:M:313:ARG:HD2	1:M:315:VAL:CG2	2.33	0.59
2:P:120:ASP:OD1	2:P:123:ARG:NH1	2.36	0.59
2:N:159:TYR:N	2:N:160:PRO:HD2	2.18	0.59
1:M:101:ASP:HB3	1:M:231:GLU:HG3	1.84	0.59
2:R:93:THR:HG22	2:R:93:THR:O	2.03	0.59
1:I:124:ILE:HD13	1:I:254:PRO:HG2	1.84	0.59
1:Q:320:LEU:HA	2:R:108:LEU:HD23	1.85	0.59
2:D:62:GLN:N	2:D:62:GLN:CD	2.53	0.58
1:O:124:ILE:HD11	1:O:254:PRO:HG2	1.84	0.58
2:P:9:PHE:HD1	2:P:10:ILE:HG13	1.67	0.58
2:B:61:THR:OG1	1:C:310:LYS:HD3	2.04	0.58
1:Q:53:ASP:HB2	1:Q:276:ASN:HD22	1.68	0.58
1:M:161:TYR:CZ	1:M:249:GLY:HA2	2.39	0.58
1:Q:282:GLN:H	1:Q:302:ILE:HG22	1.67	0.58
1:M:27:THR:HG22	1:M:31:MET:N	2.10	0.58
1:G:310:LYS:HD3	2:L:61:THR:OG1	2.02	0.58
2:D:63:PHE:HE1	2:F:90:ASP:OD1	1.87	0.58
1:O:15:ILE:HD11	2:P:122:VAL:HG21	1.84	0.58
1:G:275:GLY:O	1:G:277:CYS:CB	2.49	0.58
1:E:18:HIS:CB	2:F:21:TRP:HA	2.33	0.58
1:I:179:LEU:CD2	1:I:234:TRP:HB3	2.32	0.58
1:C:266:THR:HG21	2:D:67:GLY:H	1.68	0.58
1:M:27:THR:CG2	1:M:31:MET:H	2.11	0.58
1:K:206:THR:HG23	1:K:241:ASP:OD2	2.04	0.58
2:B:2:LEU:HB2	2:B:109:ASP:OD2	2.04	0.58
2:D:59:MET:O	2:D:61:THR:O	2.22	0.58
1:A:126:SER:CB	1:A:166:ARG:HH22	2.16	0.58
2:P:24:TYR:CE1	2:P:153:ARG:HB3	2.39	0.58
1:Q:296:ASN:HB3	1:Q:309:VAL:O	2.03	0.58
1:A:87:ILE:HD12	1:A:113:SER:HA	1.85	0.58
1:K:74:PRO:HB3	1:K:141:TYR:HD1	1.69	0.58
1:M:169:ASN:HB3	1:M:171:THR:HG23	1.86	0.58
2:P:150:GLU:HA	2:P:153:ARG:CZ	2.33	0.58
1:O:293:PRO:HG2	1:O:294:PHE:HD1	1.65	0.58
2:F:62:GLN:N	2:F:62:GLN:CD	2.58	0.58
1:Q:200:THR:HG21	1:Q:250:ASN:HB2	1.85	0.58
1:E:13:ILE:HD13	2:F:152:VAL:HG11	1.80	0.57
1:K:124:ILE:CG1	1:K:254:PRO:O	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:ASN:HB2	1:I:144:LYS:NZ	2.19	0.57
1:C:124:ILE:HD13	1:C:254:PRO:HG2	1.86	0.57
2:L:2:LEU:HB2	2:L:109:ASP:OD2	2.04	0.57
1:M:114:ARG:HH11	1:M:265:SER:CB	2.17	0.57
1:G:11:ASP:O	2:H:140:PHE:N	2.30	0.57
1:M:293:PRO:HG2	1:M:294:PHE:CD1	2.39	0.57
1:A:141:TYR:CD2	1:A:142:GLN:HG3	2.39	0.57
1:G:75:MET:HB2	1:G:95:ASN:HD21	1.64	0.57
2:P:128:ASP:CB	2:P:170:ARG:HH12	2.16	0.57
1:Q:74:PRO:HG3	1:Q:139:CYS:HB3	1.86	0.57
1:O:178:VAL:O	1:O:234:TRP:HA	2.04	0.57
2:R:87:GLY:O	2:R:91:VAL:HG23	2.04	0.57
1:E:74:PRO:HB3	1:E:141:TYR:HD1	1.68	0.57
1:M:125:PRO:HB2	1:M:126:SER:OG	2.05	0.57
1:E:206:THR:CG2	1:E:207:SER:H	2.18	0.57
1:Q:11:ASP:H	2:R:140:PHE:HB2	1.69	0.57
1:K:266:THR:HG21	2:L:67:GLY:H	1.69	0.57
1:E:141:TYR:CE2	1:E:142:GLN:HG3	2.40	0.57
1:C:201:TYR:HE1	1:C:246:GLU:HG2	1.69	0.57
1:O:141:TYR:HB2	1:O:146:SER:CB	2.27	0.57
1:A:27:THR:CG2	1:A:31:MET:H	2.16	0.57
1:C:146:SER:OG	1:C:147:PHE:N	2.34	0.57
1:K:316:LEU:HD23	2:L:52:VAL:HG22	1.86	0.57
1:G:206:THR:CG2	1:G:207:SER:H	2.17	0.57
1:O:124:ILE:HG21	1:O:166:ARG:HE	1.70	0.57
1:G:42:ILE:O	1:G:292:MET:HB3	2.05	0.57
1:K:27:THR:CG2	1:K:31:MET:H	2.13	0.57
1:G:179:LEU:HD23	1:G:234:TRP:CB	2.33	0.57
2:P:38:LYS:CD	2:P:38:LYS:NZ	2.68	0.57
1:E:59:LEU:HD11	1:E:80:ILE:CG2	2.35	0.57
1:M:320:LEU:H	1:M:320:LEU:HD23	1.69	0.57
1:C:206:THR:HG23	1:C:241:ASP:OD2	2.05	0.57
1:Q:134:GLY:HA3	1:Q:153:TRP:HB3	1.87	0.57
1:C:126:SER:CB	1:C:166:ARG:HH22	2.18	0.56
1:O:87:ILE:HD11	1:O:112:LEU:O	2.04	0.56
1:M:90:LYS:O	1:M:269:LYS:HD3	2.04	0.56
2:D:2:LEU:HB2	2:D:109:ASP:OD2	2.05	0.56
2:L:59:MET:O	2:L:61:THR:O	2.22	0.56
2:P:79:ASN:ND2	2:P:83:LYS:HE2	2.20	0.56
1:M:144:LYS:HD2	1:M:145:SER:OG	2.05	0.56
2:J:2:LEU:HB2	2:J:109:ASP:OD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:109:ASP:HA	2:N:112:ASP:HB2	1.87	0.56
2:B:68:ARG:HG3	2:B:68:ARG:O	2.05	0.56
1:Q:230:MET:SD	1:Q:252:ILE:HD11	2.45	0.56
1:M:59:LEU:HD11	1:M:80:ILE:HG21	1.86	0.56
1:O:24:GLN:HE22	3:O:1:NAG:H61	1.71	0.56
2:L:151:SER:HA	2:L:154:ASN:HB2	1.88	0.56
2:N:38:LYS:CD	2:N:38:LYS:NZ	2.69	0.56
2:F:59:MET:C	2:F:61:THR:N	2.59	0.56
1:O:266:THR:HG21	2:P:67:GLY:H	1.70	0.56
1:O:87:ILE:HD12	1:O:113:SER:HA	1.86	0.56
2:H:151:SER:HA	2:H:154:ASN:HB2	1.88	0.56
1:A:186:ASN:HB3	1:A:190:GLU:OE2	2.06	0.56
2:R:63:PHE:N	2:R:63:PHE:CD1	2.73	0.56
1:Q:13:ILE:HD13	2:R:152:VAL:HG11	1.87	0.56
1:O:151:VAL:HG23	1:O:254:PRO:HA	1.88	0.56
1:C:186:ASN:HB3	1:C:190:GLU:OE2	2.06	0.56
1:G:182:ILE:HD11	1:G:213:LEU:CD1	2.27	0.56
1:I:282:GLN:NE2	1:I:283:THR:H	2.02	0.56
1:M:266:THR:CG2	1:M:302:ILE:HD11	2.36	0.56
1:O:291:SER:HB2	1:O:292:MET:CE	2.35	0.56
1:E:121:ILE:HG13	1:E:259:LYS:HE3	1.86	0.56
1:Q:251:PHE:CE2	1:Q:253:ALA:HB2	2.40	0.56
1:K:282:GLN:NE2	1:K:283:THR:H	2.04	0.56
1:E:27:THR:HG22	1:E:32:GLU:H	1.71	0.56
1:A:124:ILE:CD1	1:A:254:PRO:O	2.54	0.56
1:I:121:ILE:HG13	1:I:259:LYS:HE3	1.87	0.56
1:G:141:TYR:CE2	1:G:142:GLN:HG3	2.41	0.56
1:I:141:TYR:CE2	1:I:142:GLN:NE2	2.21	0.56
1:I:75:MET:HB2	1:I:95:ASN:HD21	1.68	0.56
1:K:75:MET:HB2	1:K:95:ASN:HD21	1.68	0.56
1:I:126:SER:CB	1:I:166:ARG:HH22	2.18	0.56
1:O:307:LYS:HD2	2:P:92:TRP:CZ2	2.41	0.56
1:K:307:LYS:HG3	2:L:59:MET:SD	2.46	0.56
2:B:79:ASN:HD21	2:F:66:VAL:HG21	1.70	0.56
1:Q:155:ILE:HG12	1:Q:194:LEU:HD22	1.88	0.56
1:M:212:ARG:O	1:M:213:LEU:HD23	2.06	0.55
1:K:275:GLY:O	1:K:277:CYS:CB	2.50	0.55
2:H:59:MET:O	2:H:61:THR:O	2.23	0.55
1:G:207:SER:HA	1:I:229:ARG:HH21	1.72	0.55
1:O:204:VAL:HG12	1:O:205:GLY:N	2.21	0.55
1:C:170:ASN:O	1:C:239:PRO:O	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:CYS:O	2:F:24:TYR:HA	2.06	0.55
1:E:79:PHE:HD1	1:E:79:PHE:O	1.81	0.55
1:E:80:ILE:HG22	1:E:80:ILE:O	2.06	0.55
1:I:141:TYR:CE2	1:I:142:GLN:HG3	2.41	0.55
1:E:124:ILE:CD1	1:E:254:PRO:HG2	2.36	0.55
1:G:282:GLN:NE2	1:G:283:THR:H	2.04	0.55
1:C:295:HIS:HD2	1:C:297:ILE:H	1.52	0.55
1:I:206:THR:HG23	1:I:241:ASP:OD2	2.07	0.55
2:D:65:ALA:C	2:D:66:VAL:HG13	2.26	0.55
2:L:59:MET:O	2:L:61:THR:C	2.45	0.55
1:Q:98:TYR:CD2	1:Q:230:MET:HB2	2.41	0.55
1:A:80:ILE:C	1:A:82:VAL:H	2.10	0.55
1:E:272:LEU:HD21	1:M:171:THR:CB	2.37	0.55
1:G:27:THR:CG2	1:G:31:MET:H	2.16	0.55
1:C:121:ILE:HG22	1:C:123:ILE:HD13	1.86	0.55
1:M:19:ALA:HB1	1:M:322:ASN:ND2	2.21	0.55
2:J:66:VAL:HG21	2:L:79:ASN:HD21	1.71	0.55
1:K:124:ILE:CD1	1:K:254:PRO:HG2	2.36	0.55
1:I:206:THR:CG2	1:I:207:SER:H	2.18	0.55
1:G:120:LYS:HG3	1:G:258:TYR:CE2	2.42	0.55
3:M:3:NAG:O6	3:M:4:NAG:N2	2.40	0.55
1:Q:293:PRO:HB2	1:Q:294:PHE:CD1	2.42	0.55
1:G:126:SER:CB	1:G:166:ARG:HH22	2.19	0.55
1:C:121:ILE:HG13	1:C:259:LYS:HE3	1.88	0.55
2:H:80:LEU:HD13	2:L:81:ASN:HD22	1.71	0.55
1:G:106:GLU:OE2	2:H:71:ASN:HB3	2.07	0.55
2:B:59:MET:C	2:B:61:THR:H	2.10	0.55
1:O:141:TYR:CB	1:O:146:SER:HB3	2.31	0.55
2:R:127:ARG:NH1	2:R:159:TYR:OH	2.40	0.55
1:K:295:HIS:HD2	1:K:297:ILE:H	1.53	0.55
1:Q:127:TRP:HA	1:Q:127:TRP:HE3	1.72	0.55
2:P:23:GLY:HA2	2:P:36:ALA:HA	1.89	0.55
1:M:283:THR:CG2	1:M:298:HIS:HB3	2.37	0.55
2:B:80:LEU:HD13	2:F:81:ASN:HD22	1.71	0.55
1:G:79:PHE:O	1:G:80:ILE:CD1	2.55	0.55
1:E:124:ILE:CG1	1:E:254:PRO:O	2.55	0.55
1:A:11:ASP:OD1	2:B:28:ASN:HA	2.07	0.55
2:F:68:ARG:O	2:F:68:ARG:HG3	2.06	0.55
1:I:74:PRO:HB3	1:I:141:TYR:HD1	1.71	0.54
1:A:141:TYR:CE2	1:A:142:GLN:HG3	2.42	0.54
1:O:125(B):SER:OG	1:O:125(B):SER:CA	2.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:14:TRP:HB3	2:R:34:TYR:HE2	1.72	0.54
1:E:15:ILE:HG23	2:F:118:LEU:HD23	1.90	0.54
2:R:94:TYR:O	2:R:98:LEU:HB2	2.07	0.54
1:G:141:TYR:CE2	1:G:142:GLN:NE2	2.20	0.54
1:G:123:ILE:HD11	1:G:168:TYR:CZ	2.42	0.54
1:O:71:LEU:H	1:O:71:LEU:HD23	1.72	0.54
1:G:320:LEU:HB3	2:H:111:HIS:CD2	2.43	0.54
1:I:79:PHE:HD1	1:I:79:PHE:O	1.84	0.54
2:J:59:MET:O	2:J:61:THR:O	2.25	0.54
1:I:27:THR:HG22	1:I:32:GLU:N	2.22	0.54
2:N:159:TYR:OH	2:N:167:ARG:NH2	2.40	0.54
1:I:106:GLU:OE2	2:J:71:ASN:HB3	2.08	0.54
1:I:216:ARG:O	1:I:220:ARG:NH2	2.41	0.54
4:E:5:BMA:H62	1:Q:55:GLY:HA2	1.88	0.54
1:K:179:LEU:CD2	1:K:234:TRP:HB3	2.35	0.54
1:O:206:THR:HG22	1:O:241:ASP:OD2	2.07	0.54
1:C:27:THR:HG22	1:C:32:GLU:N	2.23	0.54
1:O:211:GLN:HE22	1:O:213:LEU:HD11	1.72	0.54
2:P:9:PHE:CD1	2:P:10:ILE:HG13	2.42	0.54
2:R:52:VAL:HA	2:R:55:ILE:HD12	1.89	0.54
1:O:135:VAL:CG2	1:O:146:SER:HA	2.32	0.54
1:Q:25:VAL:HG13	1:Q:26:ASP:N	2.23	0.54
2:R:165:GLU:O	2:R:169:LYS:CB	2.49	0.54
1:A:206:THR:HG23	1:A:241:ASP:OD2	2.07	0.54
1:K:124:ILE:CD1	1:K:254:PRO:O	2.55	0.54
1:Q:109:LYS:HE3	1:Q:267:ILE:HG12	1.90	0.54
1:E:307:LYS:HZ3	2:F:62:GLN:HB3	1.70	0.54
1:A:124:ILE:HG12	1:A:254:PRO:O	2.07	0.54
2:N:141:TYR:HB3	2:N:169:LYS:HG2	1.88	0.54
1:O:125(B):SER:OG	1:O:125(B):SER:N	2.40	0.54
1:G:80:ILE:C	1:G:82:VAL:H	2.12	0.54
1:M:320:LEU:HD23	1:M:320:LEU:N	2.22	0.54
1:O:238:LYS:HG3	1:O:239:PRO:CD	2.36	0.54
1:O:209:LEU:HD12	1:O:211:GLN:HB3	1.90	0.54
2:P:29:GLU:CD	2:P:29:GLU:H	2.11	0.54
1:M:267:ILE:HD12	1:M:267:ILE:N	2.20	0.54
1:G:124:ILE:HD13	1:G:254:PRO:HG2	1.89	0.54
1:Q:121:ILE:HD11	1:Q:259:LYS:HE3	1.90	0.54
1:E:42:ILE:O	1:E:292:MET:HB3	2.07	0.54
2:B:151:SER:HA	2:B:154:ASN:HB2	1.90	0.54
2:B:59:MET:O	2:B:61:THR:C	2.46	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:124:ILE:CD1	1:E:254:PRO:O	2.56	0.53
1:I:78:GLU:O	1:I:80:ILE:N	2.40	0.53
1:C:307:LYS:HZ1	2:D:62:GLN:HB3	1.71	0.53
1:M:37:THR:HB	1:M:320:LEU:N	2.21	0.53
1:M:295:HIS:CE1	1:M:308:TYR:HB2	2.43	0.53
2:J:62:GLN:CD	2:J:62:GLN:N	2.61	0.53
2:F:151:SER:HA	2:F:154:ASN:HB2	1.89	0.53
2:J:61:THR:OG1	1:K:310:LYS:HD3	2.07	0.53
1:E:206:THR:HB	1:E:209:LEU:HB3	1.90	0.53
1:Q:320:LEU:HD12	2:R:6:ILE:CG2	2.38	0.53
2:P:52:VAL:O	2:P:55:ILE:HG22	2.08	0.53
1:C:59:LEU:HD11	1:C:80:ILE:CG2	2.36	0.53
1:O:53(A):LEU:HD11	1:O:302:ILE:CG2	2.35	0.53
1:Q:90:LYS:O	1:Q:92:ASN:N	2.42	0.53
2:R:100:VAL:O	2:R:104:ASN:HB2	2.09	0.53
1:M:141:TYR:HB3	1:M:146:SER:HB2	1.90	0.53
2:F:2:LEU:HB2	2:F:109:ASP:OD2	2.07	0.53
1:M:220:ARG:O	1:M:222:LYS:NZ	2.32	0.53
1:G:182:ILE:N	1:G:182:ILE:HD13	2.23	0.53
1:C:282:GLN:NE2	1:C:283:THR:H	2.06	0.53
1:I:59:LEU:HD11	1:I:80:ILE:CG2	2.36	0.53
1:A:106:GLU:OE2	2:B:71:ASN:HB3	2.08	0.53
1:E:79:PHE:O	1:E:80:ILE:CD1	2.56	0.53
1:G:181:GLY:O	1:G:182:ILE:HD13	2.08	0.53
2:P:153:ARG:O	2:P:155:GLY:N	2.41	0.53
1:A:146:SER:OG	1:A:147:PHE:N	2.41	0.53
1:I:309:VAL:HG22	2:J:93:THR:HA	1.91	0.53
1:A:42:ILE:O	1:A:292:MET:HB3	2.08	0.53
2:D:151:SER:HA	2:D:154:ASN:HB2	1.90	0.53
1:E:164:ILE:O	1:E:246:GLU:HA	2.07	0.53
1:C:75:MET:CB	1:C:95:ASN:ND2	2.61	0.53
1:A:121:ILE:HG13	1:A:259:LYS:HE3	1.89	0.53
1:O:18:HIS:HB2	2:P:21:TRP:HA	1.90	0.53
1:G:279:THR:HB	1:G:281:CYS:H	1.74	0.53
1:M:152:VAL:CG2	1:M:255:GLU:HG3	2.39	0.53
2:H:117:ASN:HD21	2:J:4:GLY:N	2.05	0.53
1:Q:190:GLU:HA	1:Q:193:LYS:HB2	1.90	0.53
1:G:18:HIS:HB2	2:H:21:TRP:HA	1.91	0.53
1:M:191:GLN:HE21	1:M:195:TYR:HB2	1.74	0.53
1:Q:260:ILE:CG2	1:Q:260:ILE:O	2.57	0.53
1:G:124:ILE:O	1:G:124:ILE:CG1	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:312:ASN:ND2	1:M:312:ASN:N	2.57	0.53
1:Q:78:GLU:O	1:Q:78:GLU:HG2	2.09	0.53
1:K:206:THR:CG2	1:K:207:SER:H	2.21	0.53
1:G:146:SER:OG	1:G:147:PHE:N	2.41	0.53
2:B:59:MET:C	2:B:61:THR:N	2.60	0.53
1:A:59:LEU:HD11	1:A:80:ILE:CG2	2.37	0.53
1:K:283:THR:HG22	1:K:285:MET:N	2.18	0.53
2:H:65:ALA:C	2:H:66:VAL:CG1	2.76	0.53
1:Q:22:THR:HG21	1:Q:324:PRO:HD3	1.89	0.53
1:M:182:ILE:HD11	1:M:202:ILE:HD13	1.90	0.53
1:C:74:PRO:HB3	1:C:141:TYR:HD1	1.73	0.53
1:C:201:TYR:CE2	1:C:248:ASN:HB2	2.44	0.53
1:O:200:THR:HG21	1:O:250:ASN:CB	2.39	0.53
1:A:279:THR:HB	1:A:281:CYS:H	1.73	0.53
1:M:156:LYS:HD2	1:M:156:LYS:O	2.09	0.53
1:O:309:VAL:HG22	2:P:93:THR:HA	1.91	0.53
2:H:79:ASN:HD21	2:L:66:VAL:HG21	1.74	0.53
2:J:151:SER:HA	2:J:154:ASN:HB2	1.91	0.53
2:J:59:MET:C	2:J:61:THR:N	2.63	0.52
1:O:57:LYS:HD2	1:O:57:LYS:H	1.73	0.52
2:R:63:PHE:N	2:R:63:PHE:HD1	2.07	0.52
2:R:144:CYS:SG	2:R:149:MET:HG3	2.49	0.52
1:I:24:GLN:OE1	3:I:1:NAG:H61	2.08	0.52
1:O:157:LYS:CD	1:O:157:LYS:HB3	2.37	0.52
1:Q:16:GLY:CA	2:R:14:TRP:CD1	2.88	0.52
1:A:206:THR:CG2	1:A:207:SER:H	2.22	0.52
1:M:156:LYS:HB3	1:M:161:TYR:HB2	1.90	0.52
1:E:216:ARG:O	1:E:220:ARG:NH2	2.42	0.52
2:B:47:GLY:O	1:C:31:MET:HG2	2.09	0.52
2:L:68:ARG:HG3	2:L:68:ARG:O	2.08	0.52
2:F:59:MET:O	2:F:61:THR:C	2.48	0.52
1:I:279:THR:HB	1:I:281:CYS:H	1.73	0.52
1:O:151:VAL:HG22	1:O:252:ILE:HG22	1.90	0.52
1:E:13:ILE:HD11	2:F:149:MET:HG2	1.91	0.52
1:O:74:PRO:HG2	1:O:139:CYS:HB3	1.92	0.52
2:D:59:MET:O	2:D:61:THR:C	2.48	0.52
1:Q:44:GLU:OE1	1:Q:292:MET:HB2	2.09	0.52
2:N:68:ARG:O	2:N:68:ARG:HG3	2.09	0.52
1:I:42:ILE:O	1:I:292:MET:HB3	2.10	0.52
2:B:59:MET:O	2:B:61:THR:O	2.26	0.52
1:E:11:ASP:OD2	2:F:143:LYS:CA	2.48	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:59:MET:C	2:J:61:THR:H	2.13	0.52
1:K:58:PRO:HB3	1:K:86:TYR:CZ	2.44	0.52
2:H:51:LYS:HA	1:I:28:ILE:O	2.09	0.52
2:B:65:ALA:C	2:B:66:VAL:HG13	2.30	0.52
1:I:298:HIS:ND1	1:I:299:PRO:HD2	2.25	0.52
1:C:80:ILE:CG2	1:C:80:ILE:O	2.58	0.52
1:G:13:ILE:HD11	2:H:149:MET:HG2	1.91	0.52
2:J:81:ASN:HD22	2:L:80:LEU:HD13	1.75	0.52
1:M:297:ILE:O	1:M:298:HIS:HB2	2.10	0.52
1:K:201:TYR:HE1	1:K:246:GLU:HG2	1.75	0.52
2:D:66:VAL:HG21	2:F:79:ASN:HD21	1.74	0.52
1:C:10:GLY:HA3	2:D:139:GLU:OE2	2.09	0.52
1:O:228:GLY:O	1:O:229:ARG:NH1	2.42	0.52
1:O:220:ARG:HG2	1:O:229:ARG:NH2	2.25	0.52
1:G:74:PRO:HB3	1:G:141:TYR:HD1	1.75	0.52
1:E:122:GLN:OE1	1:I:77:ASP:HB2	2.09	0.52
1:A:170:ASN:O	1:A:239:PRO:O	2.28	0.52
1:M:176:LEU:HD23	1:M:237:LEU:HD23	1.91	0.51
1:I:170:ASN:O	1:I:239:PRO:O	2.28	0.51
1:K:115:ILE:HG21	1:K:118:PHE:HB2	1.92	0.51
2:P:149:MET:HA	2:P:152:VAL:CG2	2.40	0.51
2:H:2:LEU:HB2	2:H:109:ASP:OD2	2.10	0.51
1:I:283:THR:HG22	1:I:285:MET:N	2.18	0.51
1:E:279:THR:CG2	1:E:287:ALA:HB1	2.38	0.51
2:B:63:PHE:HE1	2:D:90:ASP:OD1	1.93	0.51
1:O:123:ILE:HG23	1:O:124:ILE:HG12	1.91	0.51
1:Q:22:THR:HG22	1:Q:324:PRO:HD3	1.90	0.51
1:K:42:ILE:O	1:K:292:MET:HB3	2.10	0.51
2:N:24:TYR:CE1	2:N:153:ARG:HG2	2.45	0.51
2:R:42:GLN:HA	2:R:45:ILE:HD12	1.92	0.51
1:M:295:HIS:HD2	1:M:297:ILE:HG12	1.75	0.51
1:C:42:ILE:O	1:C:292:MET:HB3	2.10	0.51
1:M:321:ARG:HH11	1:M:321:ARG:HB3	1.75	0.51
1:A:200:THR:HG22	1:A:215:PRO:CD	2.40	0.51
1:K:179:LEU:HD23	1:K:234:TRP:CB	2.36	0.51
1:I:72:GLY:HA3	1:I:149:ARG:HB2	1.91	0.51
2:P:82:LYS:O	2:P:83:LYS:C	2.49	0.51
1:I:164:ILE:O	1:I:246:GLU:HA	2.10	0.51
1:Q:123:ILE:HG12	1:Q:257:ALA:HB3	1.92	0.51
1:M:200:THR:HG21	1:M:250:ASN:HB2	1.93	0.51
1:C:279:THR:HB	1:C:281:CYS:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:HG22	1:A:32:GLU:N	2.24	0.51
1:O:200:THR:HG21	1:O:250:ASN:OD1	2.10	0.51
1:A:164:ILE:O	1:A:246:GLU:HA	2.11	0.51
1:Q:91:ALA:HA	1:Q:269:LYS:HD2	1.93	0.51
1:E:80:ILE:C	1:E:82:VAL:H	2.13	0.51
1:E:122:GLN:HE22	1:I:77:ASP:CB	2.24	0.51
2:L:59:MET:C	2:L:61:THR:N	2.64	0.51
1:E:279:THR:HB	1:E:281:CYS:H	1.75	0.51
1:M:192:THR:HG23	1:M:196:GLN:HA	1.92	0.51
1:M:70:LEU:HD13	1:M:179:LEU:HD11	1.92	0.51
1:I:10:GLY:HA3	2:J:139:GLU:OE2	2.10	0.51
1:Q:225:GLY:O	1:Q:226:GLN:CB	2.57	0.51
1:Q:182:ILE:HD11	1:Q:202:ILE:HG21	1.93	0.51
1:G:72:GLY:HA3	1:G:149:ARG:HB2	1.92	0.51
2:H:68:ARG:HH11	2:H:68:ARG:HB2	1.76	0.51
1:M:156:LYS:HG2	1:M:196:GLN:HG2	1.93	0.51
2:N:27:SER:HA	2:N:32:SER:HB3	1.92	0.51
2:F:59:MET:C	2:F:61:THR:H	2.14	0.51
1:K:80:ILE:O	1:K:80:ILE:CG2	2.58	0.51
1:O:52:CYS:HA	1:O:277:CYS:HB3	1.93	0.51
2:J:68:ARG:HG3	2:J:68:ARG:O	2.10	0.51
1:E:81:ASN:H	1:I:144:LYS:HZ2	1.57	0.51
1:I:124:ILE:HG12	1:I:254:PRO:O	2.09	0.51
1:Q:182:ILE:HD11	1:Q:202:ILE:HG12	1.92	0.51
2:F:65:ALA:C	2:F:66:VAL:CG1	2.78	0.51
2:H:59:MET:C	2:H:61:THR:N	2.64	0.51
1:M:16:GLY:HA3	2:N:14:TRP:NE1	2.26	0.51
1:M:182:ILE:HD12	1:M:202:ILE:HD13	1.93	0.50
1:I:49:GLY:HA2	1:I:285:MET:O	2.11	0.50
1:E:124:ILE:O	1:E:124:ILE:CG1	2.58	0.50
1:G:295:HIS:HD2	1:G:297:ILE:H	1.58	0.50
1:M:283:THR:CG2	1:M:284:PRO:HD2	2.40	0.50
1:C:238:LYS:HG3	1:C:239:PRO:HD2	1.93	0.50
1:K:87:ILE:HD12	1:K:113:SER:HA	1.92	0.50
1:A:238:LYS:HG3	1:A:239:PRO:HD2	1.92	0.50
3:C:1:NAG:O3	3:C:1:NAG:C7	2.60	0.50
1:O:156:LYS:NZ	1:O:156:LYS:CD	2.69	0.50
1:A:79:PHE:O	1:A:80:ILE:CD1	2.59	0.50
2:F:59:MET:O	2:F:61:THR:O	2.29	0.50
2:P:150:GLU:HA	2:P:153:ARG:NH1	2.26	0.50
1:O:291:SER:HB2	1:O:292:MET:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:65:ALA:C	2:L:66:VAL:HG13	2.32	0.50
1:E:238:LYS:HG3	1:E:239:PRO:HD2	1.93	0.50
1:C:216:ARG:O	1:C:220:ARG:NH2	2.44	0.50
2:N:158:ASP:OD1	2:N:161:GLN:HG3	2.11	0.50
2:R:47:GLY:O	2:R:51:LYS:HB3	2.11	0.50
1:K:238:LYS:HG3	1:K:239:PRO:HD2	1.93	0.50
1:E:283:THR:HG22	1:E:285:MET:N	2.19	0.50
1:C:276:ASN:O	1:C:277:CYS:HB2	2.11	0.50
1:G:124:ILE:HG12	1:G:254:PRO:O	2.11	0.50
1:C:123:ILE:HD11	1:C:168:TYR:CZ	2.46	0.50
1:E:58:PRO:HB3	1:E:86:TYR:CZ	2.46	0.50
1:E:11:ASP:H	2:F:140:PHE:HB2	1.76	0.50
1:O:74:PRO:HB3	1:O:141:TYR:HA	1.94	0.50
1:O:291:SER:CB	1:O:292:MET:HE2	2.42	0.50
1:I:179:LEU:HD23	1:I:234:TRP:CB	2.38	0.50
1:Q:92:ASN:O	1:Q:92:ASN:ND2	2.45	0.50
1:E:298:HIS:ND1	1:E:299:PRO:HD2	2.26	0.50
1:G:45:LYS:HE2	1:G:312:ASN:O	2.12	0.50
2:F:125:GLN:HG2	2:F:157:TYR:HB3	1.94	0.50
1:O:226:GLN:HE22	1:O:228:GLY:H	1.59	0.50
1:I:282:GLN:HG3	1:I:283:THR:N	2.25	0.50
2:J:59:MET:O	2:J:61:THR:C	2.50	0.50
2:H:59:MET:O	2:H:61:THR:C	2.49	0.50
1:O:292:MET:HB3	1:O:293:PRO:CD	2.41	0.50
2:P:34:TYR:N	2:P:34:TYR:CD1	2.79	0.50
1:G:216:ARG:HG2	1:K:212:ARG:HB2	1.92	0.50
1:A:283:THR:HG22	1:A:285:MET:N	2.19	0.50
1:E:27:THR:HG22	1:E:31:MET:N	2.19	0.50
1:C:58:PRO:HB3	1:C:86:TYR:CZ	2.47	0.50
2:J:65:ALA:C	2:J:66:VAL:HG13	2.32	0.50
1:O:320:LEU:HD23	1:O:320:LEU:N	2.27	0.50
1:O:232:PHE:N	1:O:232:PHE:CD1	2.78	0.50
2:J:63:PHE:HE1	2:L:90:ASP:OD1	1.94	0.50
2:N:166:ALA:C	2:N:168:LEU:H	2.13	0.50
3:M:4:NAG:H83	3:M:4:NAG:H3	1.92	0.50
1:O:23:GLU:O	1:O:35(A):THR:HA	2.12	0.50
2:D:68:ARG:HG3	2:D:68:ARG:O	2.11	0.50
1:A:179:LEU:CD2	1:A:234:TRP:HB3	2.40	0.50
2:J:38:LYS:O	2:J:42:GLN:HB2	2.12	0.50
1:E:114:ARG:HH11	1:E:265:SER:HB3	1.77	0.50
1:K:216:ARG:O	1:K:220:ARG:NH2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:189:ALA:O	1:O:193:LYS:N	2.36	0.50
1:C:283:THR:HG22	1:C:285:MET:N	2.22	0.50
1:I:279:THR:CG2	1:I:287:ALA:HB1	2.38	0.50
1:O:195:TYR:CZ	1:O:250:ASN:HA	2.47	0.50
1:O:295:HIS:CD2	1:O:297:ILE:H	2.26	0.50
1:O:68:GLY:O	1:O:71:LEU:O	2.29	0.50
2:N:68:ARG:HA	2:N:69:GLU:OE1	2.11	0.50
1:I:201:TYR:HE1	1:I:246:GLU:HG2	1.76	0.50
1:M:179:LEU:O	1:M:254:PRO:HB3	2.12	0.50
1:O:52:CYS:SG	1:O:287:ALA:HB2	2.52	0.50
2:R:171:GLU:HA	2:R:174:SER:HB3	1.93	0.50
1:E:182:ILE:CD1	1:E:202:ILE:HD13	2.24	0.49
2:R:30:GLN:HE21	2:R:30:GLN:CA	2.17	0.49
1:K:79:PHE:O	1:K:80:ILE:CD1	2.54	0.49
1:K:164:ILE:O	1:K:246:GLU:HA	2.12	0.49
1:A:58:PRO:HB3	1:A:86:TYR:CZ	2.48	0.49
2:J:125:GLN:HG2	2:J:157:TYR:HB3	1.94	0.49
2:P:65:ALA:C	2:P:66:VAL:CG1	2.80	0.49
1:O:37:THR:OG1	1:O:320:LEU:N	2.45	0.49
1:E:72:GLY:HA3	1:E:149:ARG:HB2	1.94	0.49
1:M:295:HIS:CD2	1:M:297:ILE:H	2.29	0.49
1:E:206:THR:HG23	1:E:241:ASP:OD2	2.13	0.49
1:A:201:TYR:HE1	1:A:246:GLU:HG2	1.77	0.49
1:G:164:ILE:O	1:G:246:GLU:HA	2.13	0.49
1:Q:267:ILE:H	1:Q:267:ILE:HD12	1.78	0.49
1:A:307:LYS:HD2	2:B:92:TRP:CE2	2.47	0.49
3:G:1:NAG:H62	3:G:2:NAG:HN2	1.78	0.49
1:M:212:ARG:C	1:M:213:LEU:HD23	2.32	0.49
1:O:157:LYS:O	1:O:159:SER:N	2.46	0.49
1:C:75:MET:HB2	1:C:95:ASN:HD21	1.71	0.49
2:P:150:GLU:O	2:P:154:ASN:HB2	2.12	0.49
1:Q:234:TRP:HZ3	1:Q:236:ILE:HG13	1.78	0.49
1:O:120:LYS:HE3	1:O:258:TYR:HE2	1.77	0.49
1:E:45:LYS:HE2	1:E:312:ASN:O	2.12	0.49
1:E:321:ARG:HD2	2:F:6:ILE:HD12	1.94	0.49
1:Q:98:TYR:HD2	1:Q:230:MET:HB2	1.77	0.49
1:I:307:LYS:NZ	2:J:62:GLN:HB3	2.28	0.49
2:R:38:LYS:O	2:R:42:GLN:HG2	2.12	0.49
1:Q:37:THR:HB	1:Q:319:GLY:HA3	1.95	0.49
1:C:307:LYS:HZ3	2:D:62:GLN:HB3	1.76	0.49
2:D:59:MET:C	2:D:61:THR:N	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:27:THR:HG22	1:I:31:MET:N	2.22	0.49
2:H:68:ARG:NH1	2:H:68:ARG:HB2	2.28	0.49
1:M:139:CYS:O	1:M:146:SER:O	2.31	0.49
1:E:170:ASN:O	1:E:239:PRO:O	2.31	0.49
1:O:94:VAL:HG12	1:O:95:ASN:OD1	2.12	0.49
1:E:200:THR:HG22	1:E:215:PRO:CD	2.42	0.49
1:E:295:HIS:HD2	1:E:297:ILE:H	1.60	0.49
1:K:121:ILE:HG13	1:K:259:LYS:HE3	1.93	0.49
1:Q:316:LEU:HD12	2:R:104:ASN:OD1	2.13	0.49
2:P:19:ASP:HB2	2:P:36:ALA:HB2	1.95	0.49
1:E:201:TYR:CE2	1:E:248:ASN:HB2	2.48	0.49
1:A:201:TYR:CE2	1:A:248:ASN:HB2	2.47	0.49
2:H:38:LYS:O	2:H:42:GLN:HB2	2.13	0.49
1:A:74:PRO:HB3	1:A:141:TYR:HD1	1.77	0.49
1:K:307:LYS:HZ1	2:L:62:GLN:HB3	1.77	0.49
1:Q:223:VAL:C	1:Q:225:GLY:H	2.15	0.49
1:C:179:LEU:HD23	1:C:234:TRP:CB	2.39	0.49
1:Q:53:ASP:HA	1:Q:58:PRO:HD3	1.95	0.49
1:O:279:THR:OG1	1:O:287:ALA:HB1	2.12	0.49
1:E:238:LYS:O	1:E:239:PRO:C	2.50	0.49
1:A:143:GLY:HA3	1:Q:285:MET:HG2	1.94	0.49
1:K:45:LYS:HE2	1:K:312:ASN:O	2.12	0.49
1:Q:222:LYS:HG2	1:Q:227:SER:HB2	1.95	0.49
1:G:58:PRO:HB3	1:G:86:TYR:CZ	2.48	0.49
1:O:140:PRO:O	1:O:141:TYR:C	2.51	0.49
1:Q:200:THR:HG21	1:Q:250:ASN:N	2.27	0.49
1:G:238:LYS:HG3	1:G:239:PRO:HD2	1.94	0.49
1:I:201:TYR:CE2	1:I:248:ASN:HB2	2.48	0.49
1:I:45:LYS:HE2	1:I:312:ASN:O	2.13	0.49
1:E:79:PHE:O	1:E:80:ILE:CG1	2.61	0.48
1:E:304:GLU:HG2	2:F:63:PHE:HA	1.95	0.48
1:O:123:ILE:HD12	1:O:123:ILE:HA	1.68	0.48
1:Q:82:VAL:O	1:Q:83:GLU:N	2.33	0.48
2:B:117:ASN:HD21	2:D:4:GLY:N	2.11	0.48
1:K:298:HIS:ND1	1:K:299:PRO:HD2	2.28	0.48
2:P:94:TYR:O	2:P:95:ASN:C	2.50	0.48
1:Q:27:THR:CG2	1:Q:28:ILE:N	2.76	0.48
1:E:122:GLN:OE1	1:E:125:PRO:HB3	2.13	0.48
1:E:275:GLY:O	1:E:277:CYS:CB	2.52	0.48
1:A:27:THR:HG22	1:A:31:MET:N	2.26	0.48
1:Q:109:LYS:NZ	1:Q:267:ILE:HG21	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:202:ILE:H	1:M:213:LEU:HB2	1.78	0.48
1:A:13:ILE:HD11	2:B:149:MET:HG2	1.95	0.48
2:J:28:ASN:HD22	2:J:28:ASN:H	1.62	0.48
1:E:75:MET:CB	1:E:95:ASN:HD21	2.24	0.48
2:L:63:PHE:HD1	2:L:63:PHE:H	1.57	0.48
2:H:90:ASP:OD1	2:L:63:PHE:HE1	1.95	0.48
1:O:164:ILE:O	1:O:246:GLU:HA	2.14	0.48
1:Q:200:THR:HA	1:Q:248:ASN:HB3	1.95	0.48
1:Q:168:TYR:O	1:Q:242:ALA:HA	2.13	0.48
1:Q:116:ASN:O	1:Q:117:HIS:HB2	2.12	0.48
1:I:12:GLN:HB2	2:J:27:SER:OG	2.12	0.48
1:C:179:LEU:CD2	1:C:234:TRP:HB3	2.40	0.48
1:I:206:THR:HB	1:I:209:LEU:HB3	1.95	0.48
1:G:87:ILE:HB	1:G:267:ILE:HG13	1.96	0.48
3:O:1:NAG:H62	3:O:2:NAG:HN2	1.79	0.48
1:A:120:LYS:HG3	1:A:258:TYR:CE2	2.48	0.48
1:O:169:ASN:HB3	1:O:171:THR:HG23	1.96	0.48
2:D:28:ASN:HD22	2:D:28:ASN:H	1.61	0.48
2:N:150:GLU:O	2:N:154:ASN:CB	2.51	0.48
1:E:126:SER:CB	1:I:79:PHE:CZ	2.77	0.48
1:G:279:THR:CG2	1:G:287:ALA:HB1	2.42	0.48
1:I:238:LYS:HG3	1:I:239:PRO:HD2	1.96	0.48
1:O:23:GLU:HA	1:O:23:GLU:OE2	2.14	0.48
1:M:230:MET:HG2	1:M:232:PHE:CZ	2.49	0.48
2:N:46:ASP:O	2:N:50:ASN:HB2	2.14	0.48
2:P:153:ARG:O	2:P:154:ASN:C	2.52	0.48
2:R:14:TRP:HB3	2:R:34:TYR:CE2	2.49	0.48
2:D:63:PHE:H	2:D:63:PHE:HD1	1.60	0.48
1:A:45:LYS:HE2	1:A:312:ASN:O	2.13	0.48
1:Q:53(A):LEU:HG	1:Q:282:GLN:HB2	1.96	0.48
1:K:124:ILE:CG1	1:K:124:ILE:O	2.62	0.48
1:A:143:GLY:O	1:Q:272:LEU:HG	2.14	0.48
1:Q:220:ARG:NH1	1:Q:228:GLY:HA2	2.28	0.48
1:I:58:PRO:HB3	1:I:86:TYR:CZ	2.48	0.48
1:C:298:HIS:ND1	1:C:299:PRO:HD2	2.28	0.48
2:L:62:GLN:N	2:L:62:GLN:CD	2.68	0.48
2:P:150:GLU:C	2:P:154:ASN:HB2	2.34	0.48
1:I:123:ILE:HD11	1:I:168:TYR:CZ	2.48	0.48
2:R:166:ALA:O	2:R:170:ARG:HB2	2.13	0.48
2:H:81:ASN:HD22	2:J:80:LEU:HD13	1.79	0.48
1:A:304:GLU:HG2	2:B:63:PHE:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:123:ARG:HG3	2:N:138:PHE:HZ	1.78	0.47
2:P:72:ASN:HB2	2:P:75:ARG:HD2	1.95	0.47
2:N:71:ASN:C	2:N:71:ASN:OD1	2.52	0.47
1:A:80:ILE:HG22	1:A:80:ILE:O	2.14	0.47
1:O:206:THR:HB	1:O:208:THR:N	2.24	0.47
2:B:68:ARG:HH11	2:B:68:ARG:HB2	1.78	0.47
2:B:28:ASN:HD22	2:B:28:ASN:H	1.62	0.47
1:G:136:SER:O	1:G:145:SER:HB2	2.13	0.47
2:B:90:ASP:OD1	2:F:63:PHE:CE1	2.62	0.47
1:Q:11:ASP:HB2	2:R:140:PHE:CD1	2.48	0.47
2:H:62:GLN:N	2:H:62:GLN:CD	2.67	0.47
2:P:9:PHE:HD1	2:P:10:ILE:N	2.12	0.47
1:Q:247:SER:OG	1:Q:251:PHE:HB2	2.13	0.47
1:K:170:ASN:O	1:K:239:PRO:O	2.32	0.47
2:P:2:LEU:HB2	2:P:109:ASP:OD2	2.14	0.47
1:C:309:VAL:HG22	2:D:93:THR:HA	1.96	0.47
1:O:143:GLY:O	1:O:144:LYS:C	2.51	0.47
1:Q:75:MET:HE1	1:Q:140:PRO:HD2	1.95	0.47
2:R:169:LYS:HG3	2:R:169:LYS:O	2.14	0.47
1:Q:292:MET:HB3	1:Q:293:PRO:HD2	1.96	0.47
2:R:24:TYR:CE2	2:R:153:ARG:HG2	2.50	0.47
1:O:316:LEU:HD13	2:P:100:VAL:HG22	1.97	0.47
1:O:201:TYR:CE2	1:O:248:ASN:ND2	2.82	0.47
1:M:60:ILE:HG23	1:M:88:VAL:HB	1.97	0.47
1:O:226:GLN:NE2	1:O:228:GLY:H	2.11	0.47
1:E:181:GLY:C	1:E:182:ILE:HD13	2.35	0.47
1:K:27:THR:HG22	1:K:31:MET:N	2.21	0.47
1:M:307:LYS:HD3	1:M:307:LYS:HA	1.56	0.47
1:I:42:ILE:HD13	1:I:42:ILE:HA	1.68	0.47
2:H:125:GLN:HG2	2:H:157:TYR:HB3	1.96	0.47
1:K:307:LYS:HZ3	2:L:62:GLN:HB3	1.76	0.47
1:Q:82:VAL:C	1:Q:83:GLU:H	2.17	0.47
2:P:149:MET:HA	2:P:152:VAL:HG23	1.97	0.47
2:B:125:GLN:HG2	2:B:157:TYR:HB3	1.95	0.47
1:G:114:ARG:HH11	1:G:265:SER:HB3	1.79	0.47
1:C:62:ARG:H	1:C:62:ARG:HD3	1.80	0.47
1:A:174:GLU:N	1:A:174:GLU:OE2	2.45	0.47
1:M:154:LEU:HD12	1:M:251:PHE:HB3	1.97	0.47
2:R:169:LYS:O	2:R:169:LYS:CG	2.62	0.47
1:E:49:GLY:HA2	1:E:285:MET:O	2.15	0.47
1:K:27:THR:HG22	1:K:32:GLU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:123:ILE:HD12	1:K:123:ILE:HA	1.41	0.47
1:O:124:ILE:HD12	1:O:127:TRP:HZ2	1.80	0.47
2:B:68:ARG:NH1	2:B:68:ARG:HB2	2.30	0.47
1:I:307:LYS:HD2	2:J:92:TRP:CE2	2.49	0.47
1:O:64:CYS:SG	1:O:95:ASN:HB2	2.54	0.47
1:C:12:GLN:HB2	2:D:27:SER:OG	2.15	0.47
2:R:28:ASN:HB3	2:R:31:GLY:CA	2.45	0.47
1:I:316:LEU:HD13	2:J:100:VAL:HG22	1.95	0.47
2:D:123:ARG:HD2	2:D:132:GLU:OE1	2.15	0.47
2:B:81:ASN:HD22	2:D:80:LEU:HD13	1.79	0.47
1:A:181:GLY:O	1:A:182:ILE:HD13	2.13	0.47
1:E:123:ILE:HD11	1:E:168:TYR:CZ	2.49	0.47
1:K:279:THR:HB	1:K:281:CYS:H	1.80	0.47
1:K:72:GLY:HA3	1:K:149:ARG:H	1.79	0.47
1:C:45:LYS:HE2	1:C:312:ASN:O	2.14	0.47
2:B:38:LYS:O	2:B:42:GLN:HB2	2.14	0.47
1:O:220:ARG:HH11	1:O:229:ARG:HG2	1.79	0.47
1:A:59:LEU:CD1	1:A:80:ILE:HG23	2.42	0.47
2:L:59:MET:C	2:L:61:THR:H	2.19	0.47
1:Q:312:ASN:OD1	1:Q:312:ASN:N	2.47	0.47
2:P:41:THR:O	2:P:45:ILE:HG13	2.14	0.47
1:O:47:HIS:HB3	1:O:297:ILE:CD1	2.45	0.47
1:C:72:GLY:HA3	1:C:149:ARG:HB2	1.97	0.47
1:Q:18:HIS:CE1	2:R:18:VAL:HA	2.50	0.47
1:O:134:GLY:CA	1:O:155:ILE:HD13	2.45	0.46
1:M:172:ASN:OD1	1:M:259:LYS:HD3	2.15	0.46
1:O:36:VAL:HG12	1:O:38:HIS:H	1.78	0.46
3:G:1:NAG:H62	3:G:2:NAG:N2	2.30	0.46
1:A:216:ARG:O	1:A:220:ARG:NH2	2.48	0.46
1:E:137:SER:HA	1:E:145:SER:HB2	1.97	0.46
1:M:236:ILE:HD12	1:M:236:ILE:H	1.80	0.46
2:L:28:ASN:H	2:L:28:ASN:HD22	1.63	0.46
1:O:27:THR:HG22	1:O:28:ILE:N	2.31	0.46
1:C:181:GLY:O	1:C:182:ILE:HD13	2.15	0.46
2:N:30:GLN:HE22	2:N:145:ASP:HB2	1.80	0.46
1:M:200:THR:HA	1:M:248:ASN:CG	2.36	0.46
1:E:27:THR:HG22	1:E:32:GLU:N	2.30	0.46
1:Q:262:LYS:O	1:Q:262:LYS:CG	2.63	0.46
1:C:279:THR:CG2	1:C:287:ALA:HB1	2.41	0.46
1:O:124:ILE:HD12	1:O:127:TRP:CZ2	2.51	0.46
1:A:230:MET:SD	1:A:252:ILE:CD1	3.02	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ILE:HA	1:C:123:ILE:HD12	1.32	0.46
1:O:279:THR:HG21	1:O:287:ALA:HB1	1.97	0.46
1:O:60:ILE:CD1	1:O:274:TYR:HB2	2.45	0.46
2:P:169:LYS:HA	2:P:172:GLU:HB2	1.97	0.46
1:E:182:ILE:N	1:E:182:ILE:HD13	2.30	0.46
2:D:63:PHE:CE1	2:F:90:ASP:OD1	2.67	0.46
1:C:27:THR:HG22	1:C:31:MET:N	2.23	0.46
2:H:65:ALA:O	2:H:66:VAL:CG1	2.64	0.46
2:B:83:LYS:HD3	2:F:66:VAL:HG22	1.96	0.46
2:F:65:ALA:O	2:F:66:VAL:CG1	2.64	0.46
1:I:86:TYR:HA	1:I:113:SER:O	2.15	0.46
1:M:117:HIS:HB3	1:M:261:VAL:HG23	1.98	0.46
2:H:28:ASN:H	2:H:28:ASN:HD22	1.63	0.46
1:O:129:SER:HA	1:O:157:LYS:HD2	1.97	0.46
1:O:219:THR:HG22	1:O:220:ARG:N	2.27	0.46
1:C:307:LYS:HG2	2:D:59:MET:HE3	1.97	0.46
1:O:71:LEU:N	1:O:71:LEU:HD23	2.31	0.46
1:G:12:GLN:HA	2:H:138:PHE:O	2.16	0.46
1:M:96(A):LEU:HB3	1:M:98:TYR:O	2.15	0.46
1:I:75:MET:CB	1:I:95:ASN:ND2	2.63	0.46
2:P:91:VAL:HG12	2:P:92:TRP:N	2.30	0.46
1:K:123:ILE:HD11	1:K:168:TYR:CZ	2.51	0.46
2:P:141:TYR:O	2:P:169:LYS:HG2	2.15	0.46
1:O:149:ARG:HB3	1:O:149:ARG:HH11	1.80	0.46
1:G:66:VAL:HG23	1:G:89:GLU:OE2	2.16	0.46
1:G:200:THR:HG22	1:G:215:PRO:CD	2.46	0.46
2:H:63:PHE:CE1	2:J:90:ASP:OD1	2.66	0.46
2:D:62:GLN:CD	2:D:62:GLN:H	2.17	0.46
1:K:295:HIS:CD2	1:K:297:ILE:H	2.32	0.46
1:E:295:HIS:CD2	1:E:297:ILE:H	2.33	0.46
1:I:124:ILE:CD1	1:I:254:PRO:HG2	2.44	0.46
1:K:206:THR:HB	1:K:209:LEU:HB3	1.97	0.46
2:N:59:MET:O	2:N:61:THR:C	2.54	0.46
2:R:151:SER:HA	2:R:154:ASN:HB2	1.98	0.46
1:A:249:GLY:O	1:A:250:ASN:OD1	2.34	0.46
1:E:124:ILE:HG12	1:E:254:PRO:O	2.16	0.46
2:H:59:MET:C	2:H:61:THR:H	2.19	0.46
2:N:59:MET:CE	2:N:62:GLN:HG3	2.44	0.46
1:E:15:ILE:HD11	2:F:122:VAL:HG21	1.98	0.46
2:F:68:ARG:HH11	2:F:68:ARG:HB2	1.81	0.46
1:G:309:VAL:HG22	2:H:93:THR:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:136:SER:O	1:I:145:SER:HB2	2.15	0.46
1:I:17:TYR:CD1	2:J:13:GLY:HA3	2.51	0.46
1:E:186:ASN:HB3	1:E:190:GLU:OE2	2.16	0.46
2:R:111:HIS:HA	2:R:114:ASN:ND2	2.31	0.46
1:K:136:SER:O	1:K:145:SER:HB2	2.16	0.46
2:N:49:THR:HG22	2:N:53:ASN:HD21	1.80	0.46
1:M:125(A):LYS:O	1:M:125(B):SER:C	2.53	0.46
1:O:251:PHE:CZ	1:O:253:ALA:HA	2.51	0.46
1:M:275:GLY:O	1:M:276:ASN:C	2.53	0.46
1:I:178:VAL:O	1:I:234:TRP:HA	2.15	0.46
1:G:11:ASP:HB2	2:H:140:PHE:CD1	2.48	0.46
1:G:123:ILE:HA	1:G:123:ILE:HD12	1.36	0.46
1:O:37:THR:HG1	1:O:320:LEU:H	1.63	0.46
1:Q:39:ALA:O	1:Q:40:GLN:HB2	2.16	0.46
1:A:279:THR:CG2	1:A:287:ALA:HB1	2.43	0.45
1:Q:51:LEU:HD11	1:Q:88:VAL:HG21	1.98	0.45
1:K:87:ILE:HB	1:K:267:ILE:HG13	1.98	0.45
1:M:230:MET:SD	1:M:252:ILE:CD1	3.04	0.45
2:P:53:ASN:O	2:P:57:ASP:N	2.46	0.45
1:Q:50:LYS:O	1:Q:286:GLY:HA2	2.17	0.45
2:P:110:PHE:O	2:P:114:ASN:OD1	2.34	0.45
2:P:140:PHE:C	2:P:142:HIS:H	2.20	0.45
1:O:220:ARG:HB3	1:O:227:SER:HB2	1.98	0.45
1:K:79:PHE:HD1	1:K:80:ILE:N	2.14	0.45
1:A:179:LEU:HD23	1:A:234:TRP:CB	2.43	0.45
1:C:212:ARG:HB2	1:E:216:ARG:HG2	1.97	0.45
1:I:87:ILE:HD12	1:I:113:SER:HA	1.98	0.45
2:L:125:GLN:HG2	2:L:157:TYR:HB3	1.97	0.45
1:A:79:PHE:HD1	1:A:79:PHE:O	1.84	0.45
1:O:42:ILE:O	1:O:293:PRO:HD2	2.16	0.45
2:H:51:LYS:HG3	1:I:28:ILE:HG23	1.97	0.45
1:Q:281:CYS:SG	1:Q:288:ILE:HD12	2.55	0.45
1:C:49:GLY:HA2	1:C:285:MET:O	2.17	0.45
1:I:80:ILE:CG2	1:I:80:ILE:O	2.63	0.45
1:I:80:ILE:C	1:I:82:VAL:H	2.20	0.45
1:M:124:ILE:O	1:M:125:PRO:C	2.54	0.45
2:B:62:GLN:H	2:B:62:GLN:CD	2.18	0.45
1:M:222:LYS:HA	1:M:226:GLN:O	2.17	0.45
1:A:316:LEU:HD13	2:B:100:VAL:HG22	1.98	0.45
1:M:58:PRO:HB3	1:M:86:TYR:CE2	2.52	0.45
1:E:125:PRO:HG3	1:I:79:PHE:HA	1.12	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLY:HA3	1:A:149:ARG:HB2	1.98	0.45
1:O:234:TRP:O	1:O:235:THR:CB	2.64	0.45
1:Q:13:ILE:HD11	2:R:149:MET:HG2	1.98	0.45
1:G:201:TYR:CE2	1:G:248:ASN:HB2	2.51	0.45
3:M:1:NAG:H3	3:M:2:NAG:O5	2.17	0.45
1:M:62:ARG:NH2	1:M:77:ASP:OD1	2.49	0.45
1:C:78:GLU:O	1:C:80:ILE:N	2.49	0.45
1:G:216:ARG:O	1:G:220:ARG:NH2	2.49	0.45
1:G:137:SER:HA	1:G:145:SER:HB2	1.99	0.45
1:A:114:ARG:HH11	1:A:265:SER:HB3	1.82	0.45
1:O:190:GLU:C	1:O:192:THR:H	2.20	0.45
1:K:59:LEU:HD11	1:K:80:ILE:CG2	2.44	0.45
2:N:166:ALA:C	2:N:168:LEU:N	2.70	0.45
1:O:161:TYR:OH	1:O:164:ILE:HD11	2.16	0.45
1:M:15:ILE:HD12	1:M:15:ILE:N	2.31	0.45
2:N:26:HIS:O	2:N:32:SER:HB2	2.16	0.45
2:N:65:ALA:C	2:N:66:VAL:CG1	2.85	0.45
1:O:185:PRO:O	1:O:217:ILE:HG23	2.17	0.45
1:O:251:PHE:HE1	1:O:253:ALA:HA	1.75	0.45
2:N:59:MET:HB3	2:N:59:MET:HE2	1.78	0.45
1:Q:320:LEU:HA	2:R:108:LEU:CD2	2.46	0.45
2:N:159:TYR:HB3	2:N:160:PRO:CD	2.46	0.45
1:M:134:GLY:O	1:M:153:TRP:HB3	2.17	0.45
1:E:78:GLU:O	1:E:80:ILE:N	2.49	0.45
1:A:75:MET:HB2	1:A:95:ASN:HD21	1.72	0.45
1:Q:301:THR:OG1	1:Q:305:CYS:SG	2.61	0.45
1:O:49:GLY:HA2	1:O:285:MET:O	2.17	0.45
1:M:283:THR:HG23	1:M:298:HIS:HB3	1.97	0.45
1:K:137:SER:HA	1:K:145:SER:HB2	1.98	0.45
1:Q:206:THR:CG2	1:Q:207:SER:N	2.54	0.45
1:E:282:GLN:HG3	1:E:283:THR:N	2.32	0.45
2:D:59:MET:C	2:D:61:THR:H	2.20	0.45
1:O:42:ILE:HD13	1:O:42:ILE:HA	1.48	0.45
1:O:200:THR:CG2	1:O:250:ASN:HB2	2.45	0.45
1:G:156:LYS:HD2	1:G:196:GLN:HG2	1.99	0.45
1:E:201:TYR:HE1	1:E:246:GLU:HG2	1.82	0.45
1:M:202:ILE:HD12	1:M:202:ILE:N	2.32	0.44
1:Q:223:VAL:C	1:Q:225:GLY:N	2.70	0.44
1:K:279:THR:CG2	1:K:287:ALA:HB1	2.45	0.44
1:M:129:SER:HA	1:M:157:LYS:HD3	2.00	0.44
1:Q:164:ILE:O	1:Q:246:GLU:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:38:LYS:O	2:F:42:GLN:HB2	2.17	0.44
1:K:227:SER:HA	1:K:229:ARG:HH12	1.82	0.44
1:G:27:THR:HG22	1:G:32:GLU:N	2.30	0.44
4:A:3:NAG:H61	4:A:4:NAG:C1	2.48	0.44
1:E:320:LEU:HB3	2:F:111:HIS:CG	2.52	0.44
2:L:38:LYS:O	2:L:42:GLN:HB2	2.18	0.44
1:G:186:ASN:HB3	1:G:190:GLU:OE2	2.17	0.44
1:E:316:LEU:HD23	2:F:52:VAL:HG22	1.99	0.44
1:M:85:SER:O	1:M:114:ARG:NH1	2.51	0.44
2:R:95:ASN:O	2:R:99:LEU:CB	2.60	0.44
1:I:206:THR:HB	1:I:209:LEU:CB	2.47	0.44
1:G:307:LYS:HZ1	2:H:62:GLN:HB3	1.83	0.44
1:Q:139:CYS:SG	1:Q:147:PHE:HA	2.57	0.44
1:Q:48:ASN:OD1	1:Q:287:ALA:N	2.50	0.44
2:J:123:ARG:HD2	2:J:132:GLU:OE1	2.18	0.44
1:E:124:ILE:HA	1:E:125:PRO:HD2	1.68	0.44
1:C:59:LEU:CD1	1:C:80:ILE:HG23	2.44	0.44
1:G:27:THR:HG22	1:G:31:MET:N	2.25	0.44
1:M:283:THR:HB	1:M:286:GLY:H	1.81	0.44
1:Q:201:TYR:CD2	1:Q:248:ASN:HB2	2.53	0.44
1:O:70:LEU:HA	1:O:70:LEU:HD23	1.68	0.44
2:J:72:ASN:HB2	2:J:75:ARG:HD2	1.99	0.44
1:G:206:THR:HB	1:G:209:LEU:HB3	2.00	0.44
1:I:124:ILE:CG1	1:I:124:ILE:O	2.65	0.44
1:E:171:THR:CB	1:I:121:ILE:HD13	2.47	0.44
2:N:59:MET:CE	2:N:62:GLN:CG	2.95	0.44
1:A:307:LYS:NZ	2:B:62:GLN:HB3	2.32	0.44
1:I:230:MET:SD	1:I:252:ILE:HD11	2.57	0.44
1:O:25:VAL:CG1	1:O:26:ASP:N	2.80	0.44
1:I:186:ASN:HB3	1:I:190:GLU:OE2	2.17	0.44
1:O:160:THR:HG1	1:O:160:THR:CB	2.15	0.44
1:O:185:PRO:HG2	1:O:217:ILE:HG23	1.99	0.44
1:A:78:GLU:O	1:A:80:ILE:N	2.50	0.44
1:C:182:ILE:HD11	1:C:213:LEU:CD1	2.35	0.44
1:K:307:LYS:HG2	2:L:59:MET:HE1	1.99	0.44
1:M:144:LYS:HE3	1:M:144:LYS:HB3	1.80	0.44
2:B:66:VAL:HG22	2:D:83:LYS:HD3	2.00	0.44
2:D:38:LYS:O	2:D:42:GLN:HB2	2.18	0.44
1:M:104:ASP:HB2	1:M:234:TRP:HE1	1.83	0.44
1:K:200:THR:HG22	1:K:215:PRO:CD	2.48	0.44
1:M:152:VAL:N	1:M:253:ALA:O	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:182:ILE:CD1	1:Q:202:ILE:HG12	2.48	0.44
2:R:57:ASP:O	2:R:59:MET:N	2.47	0.44
1:C:174:GLU:OE2	1:C:174:GLU:N	2.51	0.44
1:A:159:SER:O	1:A:196:GLN:CG	2.58	0.44
1:M:37:THR:HG22	1:M:38:HIS:CD2	2.52	0.44
1:A:123:ILE:HG22	1:A:124:ILE:HG23	1.99	0.44
1:A:124:ILE:O	1:A:124:ILE:CG1	2.65	0.44
1:G:11:ASP:CB	2:H:140:PHE:HD1	2.28	0.44
1:E:307:LYS:HZ1	2:F:62:GLN:HB3	1.79	0.44
2:R:148:CYS:O	2:R:151:SER:OG	2.35	0.44
1:O:52:CYS:CA	1:O:277:CYS:HB3	2.45	0.44
1:Q:295:HIS:HD2	1:Q:297:ILE:HG12	1.82	0.44
2:F:19:ASP:HB3	2:F:36:ALA:HB3	2.00	0.44
2:F:123:ARG:HD2	2:F:132:GLU:OE1	2.17	0.44
1:M:11:ASP:N	1:M:11:ASP:OD2	2.51	0.44
1:E:79:PHE:O	1:E:80:ILE:HG12	2.18	0.44
1:G:79:PHE:O	1:G:80:ILE:CG1	2.66	0.44
1:Q:104:ASP:HB2	1:Q:234:TRP:NE1	2.27	0.44
1:M:245:PHE:CD1	1:M:245:PHE:N	2.85	0.44
1:O:112:LEU:HA	1:O:112:LEU:HD23	1.67	0.44
1:C:17:TYR:CD1	2:D:13:GLY:HA3	2.53	0.44
1:M:97:CYS:HB2	1:M:138:ALA:O	2.18	0.44
1:C:124:ILE:CD1	1:C:254:PRO:HG2	2.47	0.43
1:M:134:GLY:CA	1:M:153:TRP:HB3	2.48	0.43
2:R:45:ILE:HG13	2:R:45:ILE:H	1.63	0.43
1:Q:283:THR:HB	1:Q:286:GLY:O	2.18	0.43
2:F:145:ASP:O	2:F:148:CYS:HB3	2.17	0.43
1:K:154:LEU:O	1:K:155:ILE:HD12	2.17	0.43
1:O:307:LYS:HZ1	2:P:62:GLN:HB3	1.83	0.43
1:O:302:ILE:HA	2:P:65:ALA:O	2.18	0.43
1:I:121:ILE:HA	1:I:121:ILE:HD13	1.89	0.43
2:R:52:VAL:O	2:R:55:ILE:HB	2.18	0.43
1:C:120:LYS:HG3	1:C:258:TYR:CE2	2.52	0.43
1:G:293:PRO:HG2	1:G:294:PHE:CE1	2.53	0.43
2:N:5:ALA:HA	2:N:9:PHE:CD1	2.53	0.43
1:Q:20:ASN:N	1:Q:20:ASN:OD1	2.38	0.43
2:P:145:ASP:OD1	2:P:148:CYS:CB	2.54	0.43
1:A:79:PHE:O	1:A:80:ILE:CG1	2.66	0.43
1:O:285:MET:CE	1:O:285:MET:HA	2.49	0.43
1:A:295:HIS:HD2	1:A:297:ILE:H	1.66	0.43
1:O:182:ILE:CG2	1:O:215:PRO:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:307:LYS:HZ3	2:H:62:GLN:HB3	1.83	0.43
1:O:149:ARG:HH11	1:O:149:ARG:CG	2.32	0.43
1:C:115:ILE:HG21	1:C:118:PHE:HB2	2.01	0.43
1:C:97:CYS:O	1:C:224:ASN:ND2	2.50	0.43
1:K:114:ARG:HH11	1:K:265:SER:HB3	1.83	0.43
1:A:298:HIS:ND1	1:A:299:PRO:HD2	2.33	0.43
1:C:53(A):LEU:HD23	1:C:53(A):LEU:HA	1.63	0.43
1:I:320:LEU:N	1:I:320:LEU:HD23	2.33	0.43
1:I:59:LEU:CD1	1:I:80:ILE:HG23	2.44	0.43
2:P:144:CYS:SG	2:P:149:MET:HG2	2.58	0.43
2:R:28:ASN:HB3	2:R:31:GLY:HA3	2.00	0.43
1:E:120:LYS:HG3	1:E:258:TYR:CE2	2.54	0.43
1:Q:86:TYR:HA	1:Q:265:SER:CB	2.49	0.43
1:M:84:TRP:NE1	1:M:112:LEU:O	2.50	0.43
1:I:200:THR:HG22	1:I:215:PRO:CD	2.48	0.43
4:E:5:BMA:O4	1:Q:55:GLY:C	2.57	0.43
1:C:206:THR:HB	1:C:209:LEU:HB3	2.00	0.43
1:Q:200:THR:HG23	1:Q:249:GLY:N	2.29	0.43
2:R:151:SER:O	2:R:154:ASN:HB2	2.18	0.43
1:Q:295:HIS:CD2	1:Q:297:ILE:H	2.37	0.43
1:E:230:MET:SD	1:E:252:ILE:HD11	2.58	0.43
1:Q:142:GLN:HG3	1:Q:142:GLN:O	2.19	0.43
2:P:143:LYS:NZ	2:P:143:LYS:CD	2.82	0.43
2:N:30:GLN:NE2	2:N:145:ASP:HB2	2.33	0.43
1:Q:141:TYR:CG	1:Q:142:GLN:N	2.85	0.43
2:F:28:ASN:HD22	2:F:28:ASN:H	1.67	0.43
2:R:127:ARG:H	2:R:127:ARG:HD3	1.84	0.43
1:O:230:MET:HB3	1:O:232:PHE:CE1	2.53	0.43
1:G:124:ILE:CD1	1:G:254:PRO:HG2	2.47	0.43
1:M:230:MET:SD	1:M:252:ILE:HD11	2.58	0.43
2:R:18:VAL:O	2:R:18:VAL:HG12	2.18	0.43
1:G:25:VAL:HG13	2:H:104:ASN:ND2	2.33	0.43
2:R:88:PHE:O	2:R:92:TRP:HD1	2.01	0.43
1:Q:305:CYS:O	1:Q:307:LYS:N	2.51	0.43
1:C:297:ILE:H	1:C:297:ILE:HG12	1.70	0.43
1:M:279:THR:CG2	1:M:287:ALA:HB1	2.44	0.43
2:N:141:TYR:CD1	2:N:166:ALA:HB1	2.53	0.43
1:G:201:TYR:HE1	1:G:246:GLU:HG2	1.83	0.43
2:H:167:ARG:HD3	2:J:174:SER:HA	2.01	0.43
1:K:65:SER:OG	1:K:96:ASP:HA	2.19	0.43
1:M:202:ILE:HG12	1:M:251:PHE:HD1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:131:LYS:C	2:N:133:LEU:H	2.21	0.43
1:G:307:LYS:HD2	2:H:92:TRP:CE2	2.53	0.43
1:M:141:TYR:O	1:M:143:GLY:N	2.52	0.43
1:M:181:GLY:HA3	1:M:252:ILE:HB	2.01	0.43
2:P:140:PHE:HB3	2:P:142:HIS:O	2.18	0.43
1:M:147:PHE:CG	1:M:148:PHE:N	2.86	0.43
1:M:118:PHE:CE1	1:M:260:ILE:HD11	2.54	0.43
1:E:115:ILE:HG21	1:E:118:PHE:HB2	2.01	0.43
1:O:260:ILE:HG23	1:O:261:VAL:N	2.34	0.43
1:E:174:GLU:N	1:E:174:GLU:OE2	2.47	0.43
1:C:164:ILE:O	1:C:246:GLU:HA	2.19	0.42
1:O:266:THR:HG22	1:O:302:ILE:HD11	2.01	0.42
2:R:99:LEU:HD12	2:R:99:LEU:HA	1.86	0.42
1:O:291:SER:HB2	1:O:292:MET:HE2	2.00	0.42
1:O:231:GLU:O	1:O:233:PHE:CE1	2.72	0.42
2:R:70:PHE:HB2	2:R:78:GLU:HB2	2.01	0.42
2:N:44:ALA:O	2:N:45:ILE:C	2.57	0.42
2:R:84:MET:HE1	2:R:85:GLU:HG3	2.01	0.42
1:O:220:ARG:HD2	1:O:229:ARG:HG2	2.01	0.42
1:C:200:THR:HG23	1:C:201:TYR:N	2.34	0.42
1:Q:55:GLY:HA2	1:Q:278:ASN:HD21	1.84	0.42
1:O:42:ILE:HD12	2:P:56:ILE:HD11	2.01	0.42
1:G:207:SER:HA	1:I:229:ARG:NH2	2.34	0.42
2:P:26:HIS:CE1	2:P:32:SER:HA	2.54	0.42
1:M:19:ALA:HB1	1:M:322:ASN:HD21	1.84	0.42
3:M:3:NAG:C6	3:M:4:NAG:HN2	2.31	0.42
1:O:52:CYS:HB3	1:O:277:CYS:HB3	1.82	0.42
2:D:125:GLN:HG2	2:D:157:TYR:HB3	2.00	0.42
1:O:220:ARG:HH11	1:O:229:ARG:CG	2.33	0.42
1:G:178:VAL:O	1:G:234:TRP:HA	2.18	0.42
1:A:123:ILE:CG2	1:A:124:ILE:HG23	2.49	0.42
1:C:206:THR:HG23	1:C:207:SER:H	1.84	0.42
1:M:168:TYR:O	1:M:243:ILE:HG22	2.18	0.42
1:Q:122:GLN:HE21	1:Q:125:PRO:HA	1.84	0.42
2:R:155:GLY:C	2:R:157:TYR:H	2.22	0.42
2:N:37:ASP:C	2:N:39:GLU:N	2.70	0.42
1:M:12:GLN:HB2	2:N:27:SER:OG	2.19	0.42
2:H:123:ARG:HD2	2:H:132:GLU:OE1	2.20	0.42
2:N:84:MET:O	2:N:87:GLY:N	2.53	0.42
1:C:137:SER:HA	1:C:145:SER:HB2	2.01	0.42
1:O:173:GLN:HB2	1:O:173:GLN:HE21	1.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:186:ASN:HB2	1:O:227:SER:O	2.19	0.42
1:C:195:TYR:CE1	1:C:250:ASN:ND2	2.87	0.42
1:I:276:ASN:O	1:I:277:CYS:HB2	2.19	0.42
1:M:114:ARG:HD2	1:M:264(A):ASP:O	2.20	0.42
1:E:136:SER:O	1:E:145:SER:HB2	2.20	0.42
1:M:118:PHE:HE1	1:M:260:ILE:HD11	1.84	0.42
1:K:106:GLU:OE2	2:L:71:ASN:HB3	2.19	0.42
1:I:13:ILE:HA	2:J:25:HIS:O	2.20	0.42
1:E:106:GLU:OE2	2:F:71:ASN:HB3	2.20	0.42
1:E:12:GLN:HG2	2:F:138:PHE:O	2.19	0.42
2:D:19:ASP:HB3	2:D:36:ALA:HB3	2.02	0.42
1:K:59:LEU:CD1	1:K:80:ILE:HG23	2.46	0.42
1:Q:293:PRO:HB2	1:Q:294:PHE:HD1	1.84	0.42
1:O:38:HIS:HB2	1:O:319:GLY:H	1.84	0.42
2:B:173:ILE:O	2:F:167:ARG:NH1	2.53	0.42
1:O:32:GLU:HB3	1:O:35:VAL:HG21	2.01	0.42
1:O:146:SER:HG	1:O:147:PHE:H	1.64	0.42
2:N:28:ASN:H	2:N:28:ASN:HD22	1.67	0.42
1:E:178:VAL:O	1:E:234:TRP:HA	2.19	0.42
1:M:123:ILE:HG23	1:M:124:ILE:N	2.35	0.42
1:K:124:ILE:HA	1:K:125:PRO:HD2	1.87	0.42
1:A:229:ARG:NH2	1:E:207:SER:HA	2.29	0.42
1:E:171:THR:HB	1:I:121:ILE:CD1	2.48	0.42
1:O:61:LEU:HB3	1:O:64:CYS:O	2.18	0.42
1:M:77:ASP:HB2	1:M:79:PHE:H	1.82	0.42
1:I:115:ILE:HG21	1:I:118:PHE:HB2	2.01	0.42
2:N:38:LYS:NZ	2:N:38:LYS:HD2	2.34	0.42
2:B:59:MET:HG3	2:D:94:TYR:CD1	2.55	0.42
1:M:170:ASN:OD1	1:M:171:THR:N	2.53	0.42
1:C:79:PHE:O	1:C:80:ILE:CG1	2.68	0.42
1:G:304:GLU:HG2	2:H:63:PHE:HA	2.01	0.42
2:B:167:ARG:NH1	2:D:173:ILE:O	2.52	0.42
1:A:206:THR:HB	1:A:209:LEU:N	2.28	0.42
2:F:68:ARG:NH1	2:F:68:ARG:HB2	2.35	0.42
1:Q:295:HIS:CD2	1:Q:297:ILE:HG12	2.55	0.42
1:M:115:ILE:HG21	1:M:118:PHE:HB2	2.02	0.42
2:N:17:MET:HG3	2:N:34:TYR:HB3	2.02	0.42
2:L:123:ARG:HD2	2:L:132:GLU:OE1	2.19	0.42
1:G:115:ILE:HG21	1:G:118:PHE:HB2	2.01	0.42
1:K:174:GLU:N	1:K:174:GLU:OE2	2.52	0.42
1:G:15:ILE:HD13	2:H:119:TYR:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:181:GLY:O	1:I:182:ILE:HD13	2.20	0.42
1:E:11:ASP:OD2	2:F:144:CYS:N	2.52	0.42
1:G:49:GLY:HA2	1:G:285:MET:O	2.20	0.42
1:A:297:ILE:H	1:A:297:ILE:HG12	1.71	0.42
1:G:159:SER:C	1:G:196:GLN:HG3	2.40	0.42
1:Q:60:ILE:HA	1:Q:88:VAL:HB	2.01	0.42
1:E:156:LYS:HD2	1:E:196:GLN:HG2	2.02	0.42
1:O:108:LEU:HD22	1:O:234:TRP:CD1	2.55	0.42
1:C:227:SER:HA	1:C:229:ARG:HH12	1.85	0.42
1:A:75:MET:CB	1:A:95:ASN:HD21	2.30	0.42
1:G:295:HIS:CD2	1:G:297:ILE:H	2.36	0.42
1:E:87:ILE:HB	1:E:267:ILE:HG13	2.01	0.42
1:O:292:MET:HB3	1:O:293:PRO:HD2	2.01	0.42
1:G:72:GLY:HA3	1:G:149:ARG:H	1.84	0.42
1:K:206:THR:HG23	1:K:207:SER:H	1.84	0.42
1:M:294:PHE:HA	1:M:307:LYS:O	2.20	0.42
1:M:141:TYR:CB	1:M:146:SER:HB2	2.49	0.42
1:Q:220:ARG:HD2	1:Q:227:SER:O	2.20	0.42
1:Q:184:HIS:HA	1:Q:185:PRO:HD3	1.63	0.42
2:N:95:ASN:O	2:N:99:LEU:HB2	2.20	0.42
2:N:128:ASP:O	2:N:170:ARG:NH1	2.53	0.42
2:R:121:LYS:O	2:R:125:GLN:HB2	2.20	0.42
1:K:178:VAL:O	1:K:234:TRP:HA	2.20	0.41
1:G:18:HIS:N	2:H:21:TRP:O	2.48	0.41
1:A:238:LYS:O	1:A:239:PRO:C	2.57	0.41
1:Q:170:ASN:ND2	1:Q:238:LYS:O	2.52	0.41
2:P:155:GLY:O	2:P:157:TYR:N	2.49	0.41
2:D:167:ARG:NH1	2:F:173:ILE:O	2.53	0.41
1:E:123:ILE:HD12	1:E:123:ILE:HA	1.46	0.41
1:K:201:TYR:CE1	1:K:246:GLU:HG2	2.54	0.41
1:Q:251:PHE:HE2	1:Q:253:ALA:HB2	1.83	0.41
1:O:190:GLU:OE2	1:O:190:GLU:HA	2.20	0.41
1:K:120:LYS:HG3	1:K:258:TYR:CE2	2.54	0.41
2:N:143:LYS:N	2:N:143:LYS:HD3	2.22	0.41
1:I:124:ILE:HA	1:I:125:PRO:HD2	1.82	0.41
1:M:161:TYR:CE2	1:M:249:GLY:HA2	2.55	0.41
2:H:117:ASN:ND2	2:J:4:GLY:CA	2.84	0.41
1:M:125(A):LYS:HG3	1:M:132:ALA:HB1	2.02	0.41
1:A:309:VAL:HG22	2:B:93:THR:HA	2.01	0.41
2:P:59:MET:HB3	2:P:59:MET:HE2	1.97	0.41
2:R:1:GLY:HA3	2:R:8:GLY:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:75:MET:H	1:Q:75:MET:HG2	1.51	0.41
1:E:185:PRO:HG3	1:E:191:GLN:HG2	2.02	0.41
2:L:145:ASP:O	2:L:148:CYS:HB3	2.20	0.41
4:E:5:BMA:H62	1:Q:278:ASN:HD21	1.86	0.41
1:K:49:GLY:HA2	1:K:285:MET:O	2.20	0.41
2:N:143:LYS:CD	2:N:143:LYS:H	2.21	0.41
1:O:42:ILE:CD1	2:P:56:ILE:HD11	2.51	0.41
2:N:117:ASN:HA	2:N:117:ASN:HD22	1.65	0.41
2:D:81:ASN:HD22	2:F:80:LEU:CD1	2.30	0.41
1:M:161:TYR:HB2	1:M:196:GLN:HG3	2.02	0.41
1:M:144:LYS:HG2	1:M:145:SER:N	2.36	0.41
1:I:68:GLY:O	1:I:71:LEU:O	2.39	0.41
1:C:201:TYR:CE1	1:C:246:GLU:HG2	2.52	0.41
1:M:266:THR:HG23	1:M:302:ILE:HD11	2.01	0.41
1:A:206:THR:HB	1:A:209:LEU:HB3	2.02	0.41
1:G:266:THR:HB	2:H:66:VAL:HB	2.02	0.41
2:R:24:TYR:N	2:R:24:TYR:CD1	2.89	0.41
1:Q:147:PHE:CG	1:Q:148:PHE:N	2.89	0.41
1:K:86:TYR:HA	1:K:113:SER:O	2.21	0.41
1:K:238:LYS:O	1:K:239:PRO:C	2.58	0.41
1:A:99:PRO:HB3	1:A:223:VAL:CG1	2.51	0.41
2:R:43:LYS:HA	2:R:46:ASP:HB2	2.02	0.41
2:F:59:MET:O	2:F:61:THR:CA	2.66	0.41
1:O:152:VAL:N	1:O:253:ALA:O	2.54	0.41
2:N:132:GLU:C	2:N:134:GLY:H	2.23	0.41
2:R:26:HIS:CD2	2:R:153:ARG:HH22	2.39	0.41
1:A:86:TYR:HA	1:A:113:SER:O	2.20	0.41
1:M:99:PRO:HD2	1:M:226:GLN:HG3	2.02	0.41
1:C:66:VAL:HG23	1:C:89:GLU:OE2	2.21	0.41
1:E:11:ASP:HB2	2:F:140:PHE:HB2	2.02	0.41
1:E:276:ASN:O	1:E:277:CYS:HB2	2.20	0.41
1:M:48:ASN:HD21	1:M:287:ALA:HB3	1.85	0.41
1:K:72:GLY:HA3	1:K:149:ARG:HB2	2.02	0.41
2:J:66:VAL:HG22	2:L:83:LYS:HD3	2.03	0.41
1:I:262:LYS:NZ	1:I:264(A):ASP:OD1	2.39	0.41
2:N:80:LEU:HD12	2:N:80:LEU:HA	1.92	0.41
2:N:72:ASN:HA	2:N:75:ARG:HG3	2.02	0.41
1:O:184:HIS:HA	1:O:185:PRO:HD2	1.88	0.41
1:C:141:TYR:CE2	1:C:142:GLN:CG	3.03	0.41
1:O:147:PHE:O	1:O:148:PHE:C	2.59	0.41
1:O:251:PHE:CD1	1:O:251:PHE:C	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:119:GLU:O	1:M:259:LYS:N	2.53	0.41
2:H:63:PHE:H	2:H:63:PHE:HD1	1.59	0.41
1:I:275:GLY:O	1:I:277:CYS:CB	2.58	0.41
1:I:295:HIS:HD2	1:I:297:ILE:H	1.68	0.41
1:I:297:ILE:HG12	1:I:297:ILE:H	1.64	0.41
1:O:266:THR:HG23	1:O:267:ILE:N	2.36	0.41
1:M:295:HIS:CD2	1:M:297:ILE:HG12	2.56	0.41
2:P:21:TRP:HB2	2:P:41:THR:HG23	2.02	0.41
1:E:206:THR:HB	1:E:209:LEU:CB	2.50	0.41
1:C:86:TYR:HA	1:C:113:SER:O	2.20	0.41
2:N:59:MET:O	2:N:61:THR:O	2.38	0.41
1:O:86:TYR:HA	1:O:113:SER:O	2.21	0.41
1:O:127:TRP:HZ3	1:O:164:ILE:HD13	1.86	0.41
1:O:70:LEU:O	1:O:258:TYR:OH	2.37	0.41
1:Q:80:ILE:C	1:Q:82:VAL:N	2.74	0.41
1:M:293:PRO:HG2	1:M:294:PHE:CE1	2.56	0.41
2:H:110:PHE:CD1	2:J:2:LEU:HD21	2.56	0.41
1:M:176:LEU:O	1:M:237:LEU:N	2.54	0.41
1:M:232:PHE:C	1:M:233:PHE:CD1	2.94	0.41
1:O:117:HIS:H	1:O:261:VAL:HB	1.86	0.41
1:I:197:ASN:HA	1:I:198:PRO:HD3	1.96	0.41
1:K:293:PRO:HG2	1:K:294:PHE:CE1	2.56	0.41
1:G:185:PRO:HG3	1:G:191:GLN:HG2	2.03	0.41
2:N:125:GLN:HE21	2:N:125:GLN:HB2	1.71	0.41
1:I:187:ASP:C	1:I:187:ASP:OD2	2.60	0.41
1:G:185:PRO:HG2	1:G:217:ILE:HG13	2.02	0.41
2:R:66:VAL:HB	2:R:67:GLY:H	1.62	0.41
1:C:320:LEU:HD23	1:C:320:LEU:N	2.36	0.41
1:M:130:HIS:NE2	1:M:162:PRO:HD2	2.35	0.41
1:E:149:ARG:NH1	1:I:142:GLN:OE1	2.54	0.41
1:G:75:MET:CB	1:G:95:ASN:HD21	2.28	0.41
2:R:29:GLU:O	2:R:30:GLN:CB	2.69	0.41
2:N:28:ASN:HB2	2:N:144:CYS:O	2.20	0.41
1:I:72:GLY:HA3	1:I:149:ARG:H	1.86	0.41
1:E:100:GLY:HA3	1:E:230:MET:O	2.21	0.41
1:A:167:SER:CB	1:A:244:ASN:OD1	2.69	0.41
1:Q:161:TYR:C	1:Q:161:TYR:CD2	2.95	0.41
2:N:15:GLN:HA	2:N:15:GLN:HE21	1.86	0.41
2:P:98:LEU:HA	2:P:98:LEU:HD23	1.77	0.41
1:O:155:ILE:CG2	1:O:156:LYS:N	2.84	0.40
1:E:81:ASN:HB2	1:I:144:LYS:HZ3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:LEU:CD1	1:G:80:ILE:HG23	2.45	0.40
1:E:27:THR:HG23	2:F:105:GLU:HB2	2.04	0.40
1:E:266:THR:HB	2:F:66:VAL:HB	2.03	0.40
2:F:65:ALA:O	2:F:66:VAL:HG13	2.21	0.40
2:R:63:PHE:H	2:R:63:PHE:HD1	1.68	0.40
1:G:131:GLU:HB2	1:G:155:ILE:O	2.19	0.40
2:D:159:TYR:N	2:D:160:PRO:HD2	2.37	0.40
2:D:98:LEU:HA	2:D:98:LEU:HD23	1.84	0.40
1:E:59:LEU:CD1	1:E:80:ILE:HG23	2.45	0.40
1:O:27:THR:HG23	2:P:105:GLU:CB	2.50	0.40
1:A:282:GLN:HG3	1:A:283:THR:N	2.37	0.40
1:C:241:ASP:CG	1:C:242:ALA:H	2.25	0.40
1:I:206:THR:HG23	1:I:207:SER:H	1.86	0.40
2:P:120:ASP:O	2:P:124:LEU:HD12	2.22	0.40
2:P:141:TYR:HB2	2:P:166:ALA:HB1	2.02	0.40
2:H:145:ASP:O	2:H:148:CYS:HB3	2.21	0.40
2:L:19:ASP:HB3	2:L:36:ALA:HB3	2.03	0.40
1:K:249:GLY:O	1:K:250:ASN:OD1	2.39	0.40
2:R:127:ARG:HB2	2:R:127:ARG:NH1	2.18	0.40
1:O:295:HIS:HB3	1:O:306:PRO:HG2	2.04	0.40
2:L:145:ASP:H	2:L:148:CYS:HB3	1.86	0.40
1:M:150:ASN:HA	1:M:256:TYR:HD1	1.86	0.40
2:R:126:LEU:O	2:R:126:LEU:HD12	2.21	0.40
1:E:272:LEU:HD23	1:M:171:THR:HG21	1.98	0.40
1:M:126:SER:O	1:M:127:TRP:CD1	2.75	0.40
1:O:182:ILE:HA	1:O:182:ILE:HD13	1.93	0.40
1:K:237:LEU:CD1	1:K:241:ASP:HB3	2.52	0.40
2:B:62:GLN:NE2	2:B:62:GLN:H	2.19	0.40
2:D:65:ALA:C	2:D:66:VAL:CG1	2.89	0.40
1:I:307:LYS:HD2	2:J:92:TRP:CZ2	2.57	0.40
1:M:62:ARG:HH11	1:M:62:ARG:H	1.69	0.40
2:N:16:GLY:HA3	2:N:34:TYR:CZ	2.56	0.40
1:K:12:GLN:HB2	2:L:27:SER:OG	2.22	0.40
1:I:99:PRO:HB3	1:I:223:VAL:CG1	2.52	0.40
2:H:159:TYR:N	2:H:160:PRO:HD2	2.36	0.40
1:C:200:THR:HG22	1:C:215:PRO:CD	2.51	0.40
1:M:284:PRO:HD3	1:M:300:LEU:O	2.22	0.40
1:Q:109:LYS:HZ1	2:R:69:GLU:HG2	1.87	0.40
1:Q:58:PRO:HG2	1:Q:60:ILE:HD11	2.03	0.40
2:N:65:ALA:C	2:N:66:VAL:HG13	2.41	0.40
2:R:162:TYR:O	2:R:163:SER:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:ARG:HD2	2:B:132:GLU:OE1	2.22	0.40
2:B:98:LEU:HD23	2:B:98:LEU:HA	1.91	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:GLU:OE2	1:K:142:GLN:OE1[3_455]	1.69	0.51
1:C:142:GLN:OE1	1:G:78:GLU:OE2[2_555]	1.87	0.33
1:C:79:PHE:CE2	1:G:125(B):SER:C[2_555]	1.94	0.26
1:C:142:GLN:OE1	1:G:149:ARG:NH1[2_555]	2.17	0.03
1:A:125(B):SER:C	1:K:79:PHE:CE2[3_455]	2.18	0.02

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	320/334 (96%)	289 (90%)	25 (8%)	6 (2%)	10	40
1	C	320/334 (96%)	290 (91%)	26 (8%)	4 (1%)	15	51
1	E	320/334 (96%)	289 (90%)	25 (8%)	6 (2%)	10	40
1	G	320/334 (96%)	285 (89%)	31 (10%)	4 (1%)	15	51
1	I	320/334 (96%)	285 (89%)	29 (9%)	6 (2%)	10	40
1	K	320/334 (96%)	287 (90%)	28 (9%)	5 (2%)	12	45
1	M	320/334 (96%)	255 (80%)	52 (16%)	13 (4%)	3	17
1	O	320/334 (96%)	248 (78%)	57 (18%)	15 (5%)	3	15
1	Q	320/334 (96%)	237 (74%)	63 (20%)	20 (6%)	2	8
2	B	173/181 (96%)	161 (93%)	10 (6%)	2 (1%)	16	53
2	D	173/181 (96%)	164 (95%)	7 (4%)	2 (1%)	16	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	173/181 (96%)	162 (94%)	9 (5%)	2 (1%)	16	53
2	H	173/181 (96%)	162 (94%)	8 (5%)	3 (2%)	11	43
2	J	173/181 (96%)	163 (94%)	8 (5%)	2 (1%)	16	53
2	L	173/181 (96%)	164 (95%)	7 (4%)	2 (1%)	16	53
2	N	173/181 (96%)	132 (76%)	35 (20%)	6 (4%)	4	22
2	P	173/181 (96%)	126 (73%)	37 (21%)	10 (6%)	2	10
2	R	173/181 (96%)	124 (72%)	29 (17%)	20 (12%)	0	2
All	All	4437/4635 (96%)	3823 (86%)	486 (11%)	128 (3%)	6	27

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	ASN
2	B	127	ARG
2	D	60	ASN
2	D	127	ARG
1	E	80	ILE
2	F	60	ASN
2	F	127	ARG
1	G	80	ILE
2	H	60	ASN
2	H	127	ARG
2	J	60	ASN
2	J	127	ARG
1	K	80	ILE
2	L	60	ASN
2	L	127	ARG
1	M	133(A)	LEU
1	M	142	GLN
1	M	145	SER
2	N	38	LYS
2	N	60	ASN
2	N	133	LEU
1	O	158	ASN
2	P	60	ASN
2	P	151	SER
2	P	153	ARG
2	P	154	ASN
1	Q	91	ALA
1	Q	226	GLN

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Mol	Chain	Res	Type
1	Q	307	LYS
2	R	63	PHE
2	R	74	GLU
2	R	163	SER
1	A	79	PHE
1	A	80	ILE
1	C	79	PHE
1	C	80	ILE
1	E	79	PHE
1	G	79	PHE
1	I	79	PHE
1	M	113	SER
1	M	147	PHE
1	M	150	ASN
1	O	134	GLY
1	O	144	LYS
1	O	235	THR
1	O	239	PRO
2	P	152	VAL
1	Q	71	LEU
1	Q	96(A)	LEU
1	Q	142	GLN
1	Q	158	ASN
1	Q	249	GLY
1	Q	281	CYS
2	R	8	GLY
2	R	30	GLN
2	R	39	GLU
2	R	59	MET
2	R	154	ASN
2	R	157	TYR
1	C	277	CYS
1	E	277	CYS
1	G	277	CYS
1	M	144	LYS
1	M	249	GLY
1	M	276	ASN
2	N	167	ARG
1	O	96	ASP
1	O	133(A)	LEU
2	P	150	GLU
1	Q	81	ASN

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Mol	Chain	Res	Type
1	Q	82(A)	PRO
1	Q	83	GLU
1	Q	299	PRO
1	Q	306	PRO
2	R	60	ASN
2	R	161	GLN
2	R	174	SER
1	A	277	CYS
1	I	80	ILE
1	I	277	CYS
1	K	277	CYS
1	M	214	VAL
1	O	62	ARG
1	O	141	TYR
1	Q	45	LYS
1	Q	80	ILE
1	E	81	ASN
1	I	265	SER
1	K	146	SER
1	K	265	SER
1	M	54	ASP
2	N	132	GLU
1	O	99	PRO
1	O	106	GLU
1	O	224	ASN
1	O	236	ILE
1	O	289	ASN
1	Q	21	SER
1	Q	117	HIS
1	Q	262	LYS
2	R	29	GLU
1	A	81	ASN
1	A	239	PRO
1	A	265	SER
1	C	239	PRO
1	I	239	PRO
2	P	156	THR
2	R	17	MET
2	R	49	THR
2	R	66	VAL
2	R	127	ARG
2	R	134	GLY

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Mol	Chain	Res	Type
1	E	239	PRO
2	P	8	GLY
1	K	239	PRO
2	N	16	GLY
1	Q	25	VAL
1	E	249	GLY
1	M	298	HIS
2	P	66	VAL
1	G	249	GLY
2	H	66	VAL
1	M	123	ILE
1	O	93	PRO
2	R	18	VAL
2	R	173	ILE
1	I	249	GLY
2	P	160	PRO

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	289/300 (96%)	257 (89%)	32 (11%)	8	27
1	C	289/300 (96%)	260 (90%)	29 (10%)	9	32
1	E	289/300 (96%)	257 (89%)	32 (11%)	8	27
1	G	289/300 (96%)	258 (89%)	31 (11%)	8	29
1	I	289/300 (96%)	256 (89%)	33 (11%)	7	26
1	K	289/300 (96%)	255 (88%)	34 (12%)	6	24
1	M	289/300 (96%)	239 (83%)	50 (17%)	2	10
1	O	289/300 (96%)	246 (85%)	43 (15%)	4	15
1	Q	289/300 (96%)	238 (82%)	51 (18%)	2	10
2	B	149/155 (96%)	135 (91%)	14 (9%)	11	36
2	D	149/155 (96%)	135 (91%)	14 (9%)	11	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	149/155 (96%)	135 (91%)	14 (9%)	11	36
2	H	149/155 (96%)	134 (90%)	15 (10%)	9	32
2	J	149/155 (96%)	135 (91%)	14 (9%)	11	36
2	L	149/155 (96%)	135 (91%)	14 (9%)	11	36
2	N	149/155 (96%)	121 (81%)	28 (19%)	2	8
2	P	149/155 (96%)	121 (81%)	28 (19%)	2	8
2	R	149/155 (96%)	125 (84%)	24 (16%)	3	12
All	All	3942/4095 (96%)	3442 (87%)	500 (13%)	5	21

All (500) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	27	THR
1	A	28	ILE
1	A	35(A)	THR
1	A	37	THR
1	A	42	ILE
1	A	62	ARG
1	A	75	MET
1	A	78	GLU
1	A	79	PHE
1	A	82	VAL
1	A	101	ASP
1	A	114	ARG
1	A	123	ILE
1	A	124	ILE
1	A	136	SER
1	A	151	VAL
1	A	160	THR
1	A	163	THR
1	A	176	LEU
1	A	197	ASN
1	A	200	THR
1	A	208	THR
1	A	211	GLN
1	A	217	ILE
1	A	230	MET
1	A	235	THR
1	A	238	LYS

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Mol	Chain	Res	Type
1	A	239	PRO
1	A	297	ILE
1	A	309	VAL
1	A	320	LEU
2	B	28	ASN
2	B	30	GLN
2	B	34	TYR
2	B	62	GLN
2	B	63	PHE
2	B	68	ARG
2	B	69	GLU
2	B	72	ASN
2	B	89	LEU
2	B	126	LEU
2	B	127	ARG
2	B	156	THR
2	B	169	LYS
2	B	172	GLU
1	C	25	VAL
1	C	27	THR
1	C	28	ILE
1	C	35(A)	THR
1	C	37	THR
1	C	42	ILE
1	C	62	ARG
1	C	75	MET
1	C	79	PHE
1	C	114	ARG
1	C	123	ILE
1	C	124	ILE
1	C	136	SER
1	C	151	VAL
1	C	160	THR
1	C	163	THR
1	C	169	ASN
1	C	176	LEU
1	C	191	GLN
1	C	200	THR
1	C	208	THR
1	C	211	GLN
1	C	217	ILE
1	C	230	MET

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Mol	Chain	Res	Type
1	C	235	THR
1	C	239	PRO
1	C	297	ILE
1	C	309	VAL
1	C	320	LEU
2	D	28	ASN
2	D	30	GLN
2	D	34	TYR
2	D	62	GLN
2	D	63	PHE
2	D	68	ARG
2	D	69	GLU
2	D	72	ASN
2	D	89	LEU
2	D	126	LEU
2	D	127	ARG
2	D	156	THR
2	D	169	LYS
2	D	172	GLU
1	E	25	VAL
1	E	27	THR
1	E	28	ILE
1	E	35(A)	THR
1	E	37	THR
1	E	42	ILE
1	E	62	ARG
1	E	75	MET
1	E	78	GLU
1	E	79	PHE
1	E	82	VAL
1	E	114	ARG
1	E	123	ILE
1	E	124	ILE
1	E	136	SER
1	E	151	VAL
1	E	160	THR
1	E	163	THR
1	E	173	GLN
1	E	176	LEU
1	E	197	ASN
1	E	200	THR
1	E	208	THR

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Mol	Chain	Res	Type
1	E	211	GLN
1	E	217	ILE
1	E	230	MET
1	E	235	THR
1	E	238	LYS
1	E	239	PRO
1	E	297	ILE
1	E	309	VAL
1	E	320	LEU
2	F	28	ASN
2	F	30	GLN
2	F	34	TYR
2	F	62	GLN
2	F	63	PHE
2	F	68	ARG
2	F	69	GLU
2	F	72	ASN
2	F	89	LEU
2	F	126	LEU
2	F	127	ARG
2	F	156	THR
2	F	169	LYS
2	F	172	GLU
1	G	25	VAL
1	G	27	THR
1	G	28	ILE
1	G	35(A)	THR
1	G	37	THR
1	G	42	ILE
1	G	62	ARG
1	G	75	MET
1	G	78	GLU
1	G	79	PHE
1	G	82	VAL
1	G	114	ARG
1	G	123	ILE
1	G	124	ILE
1	G	136	SER
1	G	151	VAL
1	G	160	THR
1	G	163	THR
1	G	169	ASN

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Mol	Chain	Res	Type
1	G	176	LEU
1	G	197	ASN
1	G	200	THR
1	G	208	THR
1	G	211	GLN
1	G	217	ILE
1	G	230	MET
1	G	235	THR
1	G	238	LYS
1	G	297	ILE
1	G	309	VAL
1	G	320	LEU
2	H	28	ASN
2	H	30	GLN
2	H	34	TYR
2	H	62	GLN
2	H	63	PHE
2	H	64	GLU
2	H	68	ARG
2	H	69	GLU
2	H	72	ASN
2	H	89	LEU
2	H	126	LEU
2	H	127	ARG
2	H	156	THR
2	H	169	LYS
2	H	172	GLU
1	I	25	VAL
1	I	27	THR
1	I	28	ILE
1	I	35(A)	THR
1	I	37	THR
1	I	42	ILE
1	I	62	ARG
1	I	75	MET
1	I	78	GLU
1	I	79	PHE
1	I	80	ILE
1	I	82	VAL
1	I	114	ARG
1	I	123	ILE
1	I	124	ILE

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Mol	Chain	Res	Type
1	I	136	SER
1	I	151	VAL
1	I	160	THR
1	I	163	THR
1	I	169	ASN
1	I	173	GLN
1	I	176	LEU
1	I	191	GLN
1	I	197	ASN
1	I	200	THR
1	I	208	THR
1	I	211	GLN
1	I	217	ILE
1	I	230	MET
1	I	235	THR
1	I	297	ILE
1	I	309	VAL
1	I	320	LEU
2	J	28	ASN
2	J	30	GLN
2	J	34	TYR
2	J	62	GLN
2	J	63	PHE
2	J	68	ARG
2	J	69	GLU
2	J	72	ASN
2	J	89	LEU
2	J	126	LEU
2	J	127	ARG
2	J	156	THR
2	J	169	LYS
2	J	172	GLU
1	K	25	VAL
1	K	27	THR
1	K	28	ILE
1	K	35(A)	THR
1	K	37	THR
1	K	42	ILE
1	K	62	ARG
1	K	75	MET
1	K	78	GLU
1	K	79	PHE

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Mol	Chain	Res	Type
1	K	80	ILE
1	K	101	ASP
1	K	114	ARG
1	K	123	ILE
1	K	136	SER
1	K	151	VAL
1	K	160	THR
1	K	163	THR
1	K	169	ASN
1	K	173	GLN
1	K	176	LEU
1	K	197	ASN
1	K	200	THR
1	K	208	THR
1	K	211	GLN
1	K	217	ILE
1	K	230	MET
1	K	235	THR
1	K	238	LYS
1	K	239	PRO
1	K	264(A)	ASP
1	K	297	ILE
1	K	309	VAL
1	K	320	LEU
2	L	28	ASN
2	L	30	GLN
2	L	34	TYR
2	L	62	GLN
2	L	63	PHE
2	L	68	ARG
2	L	69	GLU
2	L	72	ASN
2	L	89	LEU
2	L	126	LEU
2	L	127	ARG
2	L	156	THR
2	L	169	LYS
2	L	172	GLU
1	M	11	ASP
1	M	27	THR
1	M	42	ILE
1	M	53(A)	LEU

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Mol	Chain	Res	Type
1	M	54	ASP
1	M	62	ARG
1	M	70	LEU
1	M	77	ASP
1	M	78	GLU
1	M	82	VAL
1	M	92	ASN
1	M	102	PHE
1	M	111	LEU
1	M	121	ILE
1	M	124	ILE
1	M	125(B)	SER
1	M	126	SER
1	M	133(A)	LEU
1	M	144	LYS
1	M	156	LYS
1	M	160	THR
1	M	164	ILE
1	M	171	THR
1	M	172	ASN
1	M	173	GLN
1	M	174	GLU
1	M	192	THR
1	M	196	GLN
1	M	197	ASN
1	M	207	SER
1	M	211	GLN
1	M	214	VAL
1	M	216	ARG
1	M	217	ILE
1	M	221	SER
1	M	222	LYS
1	M	224	ASN
1	M	238	LYS
1	M	248	ASN
1	M	255	GLU
1	M	265	SER
1	M	267	ILE
1	M	272	LEU
1	M	277	CYS
1	M	309	VAL
1	M	312	ASN

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Mol	Chain	Res	Type
1	M	313	ARG
1	M	320	LEU
1	M	322	ASN
1	M	323	SER
2	N	9	PHE
2	N	15	GLN
2	N	18	VAL
2	N	19	ASP
2	N	22	TYR
2	N	24	TYR
2	N	28	ASN
2	N	30	GLN
2	N	41	THR
2	N	48	VAL
2	N	50	ASN
2	N	60	ASN
2	N	62	GLN
2	N	63	PHE
2	N	82	LYS
2	N	112	ASP
2	N	113	SER
2	N	117	ASN
2	N	125	GLN
2	N	126	LEU
2	N	127	ARG
2	N	143	LYS
2	N	145	ASP
2	N	149	MET
2	N	156	THR
2	N	158	ASP
2	N	164	GLU
2	N	174	SER
1	O	22	THR
1	O	42	ILE
1	O	57	LYS
1	O	62	ARG
1	O	63	ASP
1	O	71	LEU
1	O	77	ASP
1	O	80	ILE
1	O	82	VAL
1	O	96(A)	LEU

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Mol	Chain	Res	Type
1	O	102	PHE
1	O	111	LEU
1	O	114	ARG
1	O	121	ILE
1	O	123	ILE
1	O	125(B)	SER
1	O	130	HIS
1	O	149	ARG
1	O	152	VAL
1	O	160	THR
1	O	163	THR
1	O	171	THR
1	O	172	ASN
1	O	173	GLN
1	O	187	ASP
1	O	191	GLN
1	O	197	ASN
1	O	199	THR
1	O	206	THR
1	O	209	LEU
1	O	214	VAL
1	O	216	ARG
1	O	230	MET
1	O	248	ASN
1	O	251	PHE
1	O	260	ILE
1	O	266	THR
1	O	273	GLU
1	O	277	CYS
1	O	285	MET
1	O	309	VAL
1	O	320	LEU
1	O	322	ASN
2	P	9	PHE
2	P	10	ILE
2	P	27	SER
2	P	28	ASN
2	P	30	GLN
2	P	32	SER
2	P	34	TYR
2	P	55	ILE
2	P	59	MET

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Mol	Chain	Res	Type
2	P	61	THR
2	P	62	GLN
2	P	63	PHE
2	P	69	GLU
2	P	72	ASN
2	P	103	GLU
2	P	112	ASP
2	P	121	LYS
2	P	124	LEU
2	P	125	GLN
2	P	127	ARG
2	P	128	ASP
2	P	131	LYS
2	P	147	GLU
2	P	153	ARG
2	P	158	ASP
2	P	164	GLU
2	P	172	GLU
2	P	173	ILE
1	Q	11	ASP
1	Q	17	TYR
1	Q	20	ASN
1	Q	23	GLU
1	Q	25	VAL
1	Q	44	GLU
1	Q	46	LYS
1	Q	48	ASN
1	Q	51	LEU
1	Q	52	CYS
1	Q	57	LYS
1	Q	61	LEU
1	Q	62	ARG
1	Q	75	MET
1	Q	85	SER
1	Q	95	ASN
1	Q	102	PHE
1	Q	115	ILE
1	Q	118	PHE
1	Q	124	ILE
1	Q	125(B)	SER
1	Q	127	TRP
1	Q	133(A)	LEU

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Mol	Chain	Res	Type
1	Q	135	VAL
1	Q	151	VAL
1	Q	161	TYR
1	Q	169	ASN
1	Q	170	ASN
1	Q	175	ASP
1	Q	176	LEU
1	Q	186	ASN
1	Q	191	GLN
1	Q	195	TYR
1	Q	199	THR
1	Q	211	GLN
1	Q	223	VAL
1	Q	236	ILE
1	Q	238	LYS
1	Q	260	ILE
1	Q	262	LYS
1	Q	272	LEU
1	Q	277	CYS
1	Q	281	CYS
1	Q	295	HIS
1	Q	302	ILE
1	Q	304	GLU
1	Q	310	LYS
1	Q	312	ASN
1	Q	315	VAL
1	Q	320	LEU
1	Q	322	ASN
2	R	3	PHE
2	R	21	TRP
2	R	22	TYR
2	R	24	TYR
2	R	30	GLN
2	R	43	LYS
2	R	59	MET
2	R	62	GLN
2	R	63	PHE
2	R	66	VAL
2	R	69	GLU
2	R	80	LEU
2	R	95	ASN
2	R	98	LEU

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Mol	Chain	Res	Type
2	R	106	ARG
2	R	112	ASP
2	R	113	SER
2	R	121	LYS
2	R	126	LEU
2	R	127	ARG
2	R	131	LYS
2	R	161	GLN
2	R	164	GLU
2	R	167	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	GLN
2	B	79	ASN
2	B	81	ASN
2	B	117	ASN
1	C	38	HIS
1	C	295	HIS
1	C	322	ASN
2	D	15	GLN
2	D	79	ASN
2	D	81	ASN
2	D	117	ASN
1	E	47	HIS
1	E	295	HIS
2	F	79	ASN
2	F	81	ASN
2	F	117	ASN
1	G	295	HIS
1	G	322	ASN
2	H	79	ASN
2	H	81	ASN
2	H	117	ASN
1	I	38	HIS
1	I	322	ASN
2	J	15	GLN
2	J	79	ASN
2	J	81	ASN
2	J	117	ASN
1	K	226	GLN

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Mol	Chain	Res	Type
1	K	295	HIS
1	K	322	ASN
2	L	79	ASN
2	L	81	ASN
1	M	110	HIS
1	M	117	HIS
1	M	172	ASN
1	M	191	GLN
1	M	226	GLN
1	M	250	ASN
1	M	295	HIS
1	M	312	ASN
2	N	15	GLN
2	N	26	HIS
2	N	30	GLN
2	N	53	ASN
2	N	117	ASN
2	N	125	GLN
2	N	135	ASN
1	O	38	HIS
1	O	117	HIS
1	O	172	ASN
1	O	173	GLN
1	O	211	GLN
1	O	224	ASN
1	O	226	GLN
1	O	248	ASN
1	O	282	GLN
1	O	322	ASN
2	P	53	ASN
2	P	79	ASN
2	P	117	ASN
2	P	129	ASN
1	Q	24	GLN
1	Q	92	ASN
1	Q	95	ASN
1	Q	116	ASN
1	Q	122	GLN
1	Q	170	ASN
1	Q	276	ASN
1	Q	278	ASN
2	R	15	GLN

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Mol	Chain	Res	Type
2	R	26	HIS
2	R	28	ASN
2	R	30	GLN
2	R	42	GLN
2	R	81	ASN
2	R	114	ASN
2	R	135	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

35 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	1	1,3	14,14,15	0.61	0	15,19,21	1.74	4 (26%)
3	NAG	A	2	3	14,14,15	0.93	1 (7%)	15,19,21	0.74	0
4	NAG	A	3	1,4	14,14,15	0.68	0	15,19,21	1.33	1 (6%)
4	NAG	A	4	4	14,14,15	0.74	0	15,19,21	1.76	3 (20%)
4	BMA	A	5	4	11,11,12	0.69	0	14,15,17	1.51	2 (14%)
3	NAG	C	1	1,3	14,14,15	0.69	0	15,19,21	2.92	5 (33%)
3	NAG	C	2	3	14,14,15	0.60	0	15,19,21	1.51	1 (6%)
3	NAG	C	3	1,3	14,14,15	0.85	1 (7%)	15,19,21	2.38	3 (20%)
3	NAG	C	4	3	14,14,15	0.58	0	15,19,21	1.89	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	1,3	14,14,15	0.58	0	15,19,21	1.88	4 (26%)
3	NAG	E	2	3	14,14,15	0.92	1 (7%)	15,19,21	1.79	2 (13%)
4	NAG	E	3	1,4	14,14,15	0.63	0	15,19,21	1.08	1 (6%)
4	NAG	E	4	4	14,14,15	0.57	0	15,19,21	1.35	3 (20%)
4	BMA	E	5	4	11,11,12	0.85	0	14,15,17	2.71	4 (28%)
3	NAG	G	1	1,3	14,14,15	0.66	1 (7%)	15,19,21	1.22	1 (6%)
3	NAG	G	2	3	14,14,15	1.01	1 (7%)	15,19,21	1.46	2 (13%)
4	NAG	G	3	1,4	14,14,15	0.77	0	15,19,21	1.92	3 (20%)
4	NAG	G	4	4	14,14,15	0.73	0	15,19,21	1.46	2 (13%)
4	BMA	G	5	4	11,11,12	0.54	0	14,15,17	2.60	1 (7%)
3	NAG	I	1	1,3	14,14,15	0.80	1 (7%)	15,19,21	2.84	5 (33%)
3	NAG	I	2	3	14,14,15	0.81	1 (7%)	15,19,21	1.53	3 (20%)
3	NAG	I	3	1,3	14,14,15	0.82	1 (7%)	15,19,21	1.55	4 (26%)
3	NAG	I	4	3	14,14,15	0.63	0	15,19,21	1.23	1 (6%)
3	NAG	K	1	1,3	14,14,15	0.75	0	15,19,21	2.21	5 (33%)
3	NAG	K	2	3	14,14,15	1.03	1 (7%)	15,19,21	2.69	5 (33%)
3	NAG	K	3	1,3	14,14,15	0.70	0	15,19,21	1.86	2 (13%)
3	NAG	K	4	3	14,14,15	0.52	0	15,19,21	1.32	2 (13%)
3	NAG	M	1	1,3	14,14,15	0.79	0	15,19,21	1.86	4 (26%)
3	NAG	M	2	3	14,14,15	0.94	1 (7%)	15,19,21	1.14	0
3	NAG	M	3	1,3	14,14,15	0.91	1 (7%)	15,19,21	1.30	1 (6%)
3	NAG	M	4	3	14,14,15	0.86	0	15,19,21	2.20	4 (26%)
3	NAG	O	1	1,3	14,14,15	0.91	1 (7%)	15,19,21	1.94	4 (26%)
3	NAG	O	2	3	14,14,15	1.24	1 (7%)	15,19,21	1.84	2 (13%)
3	NAG	O	3	1,3	14,14,15	0.71	0	15,19,21	2.48	4 (26%)
3	NAG	O	4	3	14,14,15	0.88	1 (7%)	15,19,21	1.21	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
3	NAG	A	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2	3	-	0/6/23/26	0/1/1/1
4	NAG	A	3	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	4	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BMA	A	5	4	-	0/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	NAG	C	3	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	4	3	-	0/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	0/6/23/26	0/1/1/1
4	NAG	E	3	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	E	4	4	-	0/6/23/26	0/1/1/1
4	BMA	E	5	4	-	0/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	1/6/23/26	0/1/1/1
4	NAG	G	3	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	4	4	-	0/6/23/26	0/1/1/1
4	BMA	G	5	4	-	0/2/19/22	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	3	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	I	4	3	-	0/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	K	3	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	K	4	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	M	2	3	-	1/6/23/26	0/1/1/1
3	NAG	M	3	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	M	4	3	-	2/6/23/26	0/1/1/1
3	NAG	O	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	O	2	3	-	0/6/23/26	0/1/1/1
3	NAG	O	3	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	O	4	3	-	1/6/23/26	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	NAG	O5-C1	-2.11	1.40	1.43
3	G	1	NAG	C1-C2	2.01	1.55	1.52
3	I	2	NAG	C1-C2	2.16	1.55	1.52
3	I	3	NAG	C1-C2	2.23	1.55	1.52
3	I	1	NAG	C1-C2	2.34	1.55	1.52
3	O	4	NAG	C1-C2	2.35	1.55	1.52
3	E	2	NAG	C1-C2	2.58	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	3	NAG	C1-C2	2.61	1.56	1.52
3	K	2	NAG	C1-C2	2.71	1.56	1.52
3	O	1	NAG	C1-C2	2.85	1.56	1.52
3	G	2	NAG	C1-C2	2.85	1.56	1.52
3	M	2	NAG	C1-C2	2.86	1.56	1.52
3	A	2	NAG	C1-C2	2.95	1.56	1.52
3	O	2	NAG	C1-C2	3.86	1.57	1.52

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	NAG	C1-O5-C5	-6.18	104.40	112.25
3	O	3	NAG	C4-C3-C2	-5.58	102.56	111.23
3	C	4	NAG	C2-N2-C7	-5.36	116.16	123.04
3	C	3	NAG	C2-N2-C7	-4.91	116.73	123.04
4	A	4	NAG	C1-O5-C5	-4.82	106.13	112.25
3	E	1	NAG	C2-N2-C7	-4.66	117.06	123.04
3	O	1	NAG	C3-C4-C5	-4.04	103.15	110.20
3	O	3	NAG	C2-N2-C7	-3.87	118.06	123.04
3	C	1	NAG	C4-C3-C2	-3.64	105.57	111.23
3	I	1	NAG	C4-C3-C2	-3.42	105.91	111.23
4	G	4	NAG	C2-N2-C7	-3.38	118.70	123.04
3	M	4	NAG	C1-O5-C5	-3.32	108.03	112.25
3	A	1	NAG	C4-C3-C2	-3.20	106.26	111.23
3	O	1	NAG	C4-C3-C2	-3.17	106.30	111.23
4	A	3	NAG	C1-O5-C5	-3.16	108.23	112.25
3	M	3	NAG	C3-C4-C5	-3.03	104.91	110.20
4	G	3	NAG	C2-N2-C7	-2.85	119.38	123.04
3	I	4	NAG	C3-C4-C5	-2.76	105.39	110.20
3	I	3	NAG	C3-C2-N2	-2.55	104.44	110.56
4	A	4	NAG	O3-C3-C2	-2.48	104.20	109.11
3	C	1	NAG	C3-C4-C5	-2.39	106.03	110.20
3	E	1	NAG	C3-C4-C5	-2.32	106.15	110.20
3	K	1	NAG	O4-C4-C5	-2.26	103.26	109.24
3	I	1	NAG	C3-C4-C5	-2.11	106.53	110.20
3	I	3	NAG	O7-C7-C8	-2.08	118.25	122.06
4	G	3	NAG	O4-C4-C3	-2.05	105.73	110.34
3	G	2	NAG	O5-C5-C6	2.03	111.74	107.35
3	I	1	NAG	O3-C3-C4	2.08	115.02	110.34
3	M	1	NAG	C3-C2-N2	2.09	115.56	110.56
4	A	5	BMA	O5-C1-C2	2.14	114.33	110.86
3	E	1	NAG	O5-C5-C6	2.14	111.98	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	4	NAG	O4-C4-C5	2.15	114.95	109.24
3	C	4	NAG	C3-C4-C5	2.18	113.99	110.20
4	A	4	NAG	O5-C5-C6	2.18	112.07	107.35
4	E	5	BMA	C2-C3-C4	2.26	114.87	111.04
3	A	1	NAG	C2-N2-C7	2.30	125.99	123.04
3	C	1	NAG	O4-C4-C5	2.32	115.38	109.24
4	E	4	NAG	C1-O5-C5	2.32	115.19	112.25
3	I	2	NAG	C4-C3-C2	2.41	114.98	111.23
3	O	1	NAG	O4-C4-C5	2.44	115.71	109.24
3	I	2	NAG	C3-C4-C5	2.51	114.57	110.20
4	E	4	NAG	C3-C4-C5	2.53	114.62	110.20
3	M	1	NAG	C4-C3-C2	2.60	115.27	111.23
3	I	3	NAG	C3-C4-C5	2.72	114.94	110.20
3	O	3	NAG	O4-C4-C5	2.74	116.50	109.24
3	O	1	NAG	C1-O5-C5	2.76	115.76	112.25
3	C	3	NAG	C8-C7-N2	2.80	121.47	116.11
3	K	1	NAG	O5-C5-C6	2.82	113.45	107.35
3	C	1	NAG	O3-C3-C2	2.82	114.71	109.11
3	I	1	NAG	O4-C4-C3	2.89	116.83	110.34
3	A	1	NAG	C1-O5-C5	2.91	115.94	112.25
3	G	1	NAG	C1-O5-C5	2.91	115.94	112.25
4	E	3	NAG	C1-O5-C5	2.95	116.00	112.25
3	A	1	NAG	C3-C2-N2	2.98	117.70	110.56
3	M	1	NAG	C1-O5-C5	3.04	116.11	112.25
3	G	2	NAG	C2-N2-C7	3.09	127.01	123.04
4	E	4	NAG	C4-C3-C2	3.15	116.12	111.23
3	M	4	NAG	C3-C4-C5	3.17	115.72	110.20
3	I	3	NAG	C2-N2-C7	3.26	127.22	123.04
3	K	3	NAG	C1-O5-C5	3.31	116.45	112.25
3	O	4	NAG	C4-C3-C2	3.34	116.42	111.23
3	O	2	NAG	C2-N2-C7	3.36	127.36	123.04
4	G	4	NAG	C4-C3-C2	3.42	116.54	111.23
3	K	1	NAG	C3-C4-C5	3.52	116.33	110.20
3	C	4	NAG	C1-O5-C5	3.55	116.75	112.25
3	K	2	NAG	C4-C3-C2	3.57	116.78	111.23
3	E	2	NAG	C4-C3-C2	3.59	116.82	111.23
3	K	2	NAG	C2-N2-C7	3.60	127.67	123.04
4	E	5	BMA	O5-C1-C2	3.60	116.70	110.86
3	K	2	NAG	O5-C5-C6	3.67	115.29	107.35
3	K	1	NAG	C4-C3-C2	3.67	116.93	111.23
3	K	4	NAG	C1-O5-C5	3.72	116.97	112.25
3	M	4	NAG	C4-C3-C2	3.84	117.20	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	1	NAG	C2-N2-C7	3.92	128.07	123.04
3	E	1	NAG	C1-O5-C5	4.06	117.40	112.25
3	I	2	NAG	C1-O5-C5	4.11	117.46	112.25
4	A	5	BMA	C1-O5-C5	4.15	117.51	112.25
3	K	2	NAG	C3-C4-C5	4.39	117.85	110.20
3	K	3	NAG	C2-N2-C7	4.49	128.81	123.04
3	C	2	NAG	C3-C4-C5	4.56	118.15	110.20
3	O	2	NAG	C1-O5-C5	4.81	118.36	112.25
3	M	4	NAG	C2-N2-C7	4.96	129.41	123.04
3	E	2	NAG	C2-N2-C7	4.99	129.44	123.04
4	G	3	NAG	C1-O5-C5	5.00	118.59	112.25
4	E	5	BMA	C1-O5-C5	5.32	119.00	112.25
3	K	1	NAG	C1-O5-C5	5.42	119.12	112.25
3	O	3	NAG	C1-O5-C5	5.65	119.42	112.25
3	K	2	NAG	C1-O5-C5	6.63	120.66	112.25
4	E	5	BMA	C1-C2-C3	6.91	117.71	109.54
3	I	1	NAG	C1-O5-C5	8.73	123.33	112.25
3	C	1	NAG	C1-O5-C5	9.04	123.73	112.25
4	G	5	BMA	C1-O5-C5	9.22	123.95	112.25

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	3	NAG	C1
3	I	3	NAG	C1
3	C	3	NAG	C1
4	A	3	NAG	C1
3	O	3	NAG	C1
3	M	3	NAG	C1
3	K	3	NAG	C1

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	O7-C7-N2-C2
3	M	2	NAG	O7-C7-N2-C2
3	O	4	NAG	O7-C7-N2-C2
3	M	4	NAG	C8-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
3	M	4	NAG	O7-C7-N2-C2

There are no ring outliers.

15 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	NAG	1	0
3	A	2	NAG	1	0
4	A	3	NAG	1	0
4	A	4	NAG	3	0
3	C	1	NAG	1	0
4	E	5	BMA	3	0
3	G	1	NAG	2	0
3	G	2	NAG	2	0
3	I	1	NAG	1	0
3	M	1	NAG	1	0
3	M	2	NAG	1	0
3	M	3	NAG	2	0
3	M	4	NAG	3	0
3	O	1	NAG	2	0
3	O	2	NAG	1	0

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	322/334 (96%)	1.31	55 (17%) 2 1	70, 71, 72, 73	0
1	C	322/334 (96%)	1.21	49 (15%) 3 1	70, 71, 72, 73	0
1	E	322/334 (96%)	1.38	48 (14%) 3 1	70, 71, 72, 73	0
1	G	322/334 (96%)	1.34	41 (12%) 5 2	70, 71, 72, 73	0
1	I	322/334 (96%)	1.30	53 (16%) 2 1	70, 71, 72, 73	0
1	K	322/334 (96%)	1.40	61 (18%) 2 1	70, 71, 72, 74	0
1	M	322/334 (96%)	2.24	154 (47%) 0 0	54, 67, 75, 84	0
1	O	322/334 (96%)	2.10	140 (43%) 0 0	57, 68, 76, 83	0
1	Q	322/334 (96%)	3.62	231 (71%) 0 0	63, 72, 81, 86	0
2	B	175/181 (96%)	2.32	73 (41%) 0 0	70, 71, 72, 73	0
2	D	175/181 (96%)	2.67	90 (51%) 0 0	70, 71, 72, 73	0
2	F	175/181 (96%)	2.59	77 (44%) 0 0	70, 71, 72, 73	0
2	H	175/181 (96%)	2.83	90 (51%) 0 0	70, 71, 72, 73	0
2	J	175/181 (96%)	2.57	86 (49%) 0 0	70, 71, 72, 73	0
2	L	175/181 (96%)	2.83	89 (50%) 0 0	70, 71, 72, 73	0
2	N	175/181 (96%)	2.06	68 (38%) 0 0	55, 71, 82, 87	0
2	P	175/181 (96%)	2.16	65 (37%) 0 0	58, 68, 80, 82	0
2	R	175/181 (96%)	3.99	123 (70%) 0 0	60, 70, 85, 87	0
All	All	4473/4635 (96%)	2.08	1593 (35%) 0 0	54, 71, 77, 87	0

All (1593) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	324	PRO	21.9
2	R	134	GLY	20.1
1	I	16	GLY	18.2

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Mol	Chain	Res	Type	RSRZ
1	Q	324	PRO	17.9
1	Q	323	SER	16.2
1	A	324	PRO	15.5
2	R	175	SER	14.1
1	K	16	GLY	14.1
2	F	160	PRO	14.0
2	L	138	PHE	13.9
2	D	138	PHE	13.4
2	R	64	GLU	13.0
2	L	175	SER	12.7
2	J	8	GLY	12.7
2	H	22	TYR	12.5
2	J	142	HIS	12.4
2	R	65	ALA	12.1
1	E	13	ILE	11.9
1	E	324	PRO	11.6
2	H	164	GLU	11.6
2	J	157	TYR	11.5
1	Q	267	ILE	11.5
2	L	160	PRO	11.3
1	C	324	PRO	11.2
2	H	6	ILE	11.2
1	Q	281	CYS	11.1
2	R	133	LEU	11.0
2	H	140	PHE	10.9
2	F	140	PHE	10.9
1	E	10	GLY	10.8
1	O	324	PRO	10.7
2	B	8	GLY	10.7
2	D	29	GLU	10.7
2	F	167	ARG	10.5
2	D	139	GLU	10.5
2	F	175	SER	10.4
2	L	19	ASP	10.3
1	Q	198	PRO	10.1
1	G	14	CYS	10.1
2	R	63	PHE	10.0
1	Q	309	VAL	10.0
2	B	2	LEU	10.0
2	F	159	TYR	9.9
1	Q	276	ASN	9.9
2	R	35	ALA	9.8

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Mol	Chain	Res	Type	RSRZ
2	J	29	GLU	9.8
2	R	168	LEU	9.7
2	R	129	ASN	9.7
1	M	324	PRO	9.7
1	Q	82(A)	PRO	9.7
2	R	160	PRO	9.6
1	Q	322	ASN	9.3
1	Q	60	ILE	9.3
2	R	130	ALA	9.1
2	J	7	ALA	9.1
1	Q	167	SER	9.0
2	P	174	SER	9.0
2	R	156	THR	9.0
2	R	147	GLU	8.9
2	L	174	SER	8.9
1	Q	262	LYS	8.9
1	Q	26	ASP	8.9
1	Q	303	GLY	8.9
2	R	19	ASP	8.8
1	M	189	ALA	8.8
2	R	144	CYS	8.7
2	L	157	TYR	8.7
2	J	23	GLY	8.7
2	N	174	SER	8.7
2	R	158	ASP	8.7
1	Q	254	PRO	8.6
2	R	17	MET	8.6
2	L	139	GLU	8.6
2	F	139	GLU	8.6
1	E	80	ILE	8.6
2	H	18	VAL	8.6
2	L	25	HIS	8.5
2	B	29	GLU	8.4
2	P	175	SER	8.4
2	J	174	SER	8.3
2	L	156	THR	8.3
2	R	27	SER	8.2
1	O	188	ALA	8.2
1	Q	151	VAL	8.2
2	R	138	PHE	8.2
1	O	51	LEU	8.2
2	D	167	ARG	8.1

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Mol	Chain	Res	Type	RSRZ
2	H	141	TYR	8.1
1	Q	296	ASN	8.1
2	B	147	GLU	8.0
2	L	141	TYR	8.0
1	Q	176	LEU	8.0
2	R	146	ASN	7.9
2	D	23	GLY	7.9
1	Q	304	GLU	7.9
2	R	14	TRP	7.9
2	F	142	HIS	7.8
2	R	73	LEU	7.8
1	O	192	THR	7.8
1	Q	58	PRO	7.8
1	Q	256	TYR	7.8
2	R	174	SER	7.7
1	I	15	ILE	7.7
1	A	16	GLY	7.7
2	R	143	LYS	7.7
1	Q	125(B)	SER	7.7
2	H	157	TYR	7.6
2	H	1	GLY	7.6
1	Q	133	SER	7.6
1	Q	76	CYS	7.6
1	Q	133(A)	LEU	7.6
2	R	125	GLN	7.6
1	Q	52	CYS	7.6
2	R	28	ASN	7.5
2	F	22	TYR	7.5
1	O	248	ASN	7.5
1	M	10	GLY	7.5
1	Q	61	LEU	7.4
2	F	29	GLU	7.4
2	H	32	SER	7.4
1	Q	150	ASN	7.4
2	P	5	ALA	7.4
2	D	170	ARG	7.4
2	L	1	GLY	7.4
1	K	79	PHE	7.3
1	Q	38	HIS	7.3
2	P	173	ILE	7.3
1	K	55	GLY	7.3
2	R	135	ASN	7.2

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Mol	Chain	Res	Type	RSRZ
1	Q	82	VAL	7.2
1	Q	64	CYS	7.2
2	H	147	GLU	7.2
2	B	1	GLY	7.2
1	Q	302	ILE	7.1
1	Q	18	HIS	7.1
1	Q	68	GLY	7.1
1	O	156	LYS	7.1
2	R	23	GLY	7.1
2	H	16	GLY	7.0
1	O	127	TRP	7.0
2	D	1	GLY	7.0
1	Q	282	GLN	7.0
1	M	166	ARG	7.0
1	M	174	GLU	7.0
2	N	173	ILE	7.0
2	R	145	ASP	7.0
2	F	138	PHE	7.0
2	H	8	GLY	6.9
1	Q	129	SER	6.9
1	E	12	GLN	6.9
2	B	144	CYS	6.9
1	O	10	GLY	6.9
2	P	28	ASN	6.9
2	H	5	ALA	6.8
1	C	79	PHE	6.8
1	Q	79	PHE	6.8
2	L	24	TYR	6.8
2	J	1	GLY	6.8
2	J	173	ILE	6.8
1	Q	155	ILE	6.7
1	Q	170	ASN	6.7
2	F	143	LYS	6.7
2	R	29	GLU	6.7
2	J	175	SER	6.7
2	H	138	PHE	6.7
2	F	8	GLY	6.6
2	H	9	PHE	6.6
2	L	140	PHE	6.6
2	H	10	ILE	6.6
2	N	172	GLU	6.6
1	O	152	VAL	6.6

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Mol	Chain	Res	Type	RSRZ
2	F	141	TYR	6.6
2	B	30	GLN	6.6
1	O	80	ILE	6.6
2	J	6	ILE	6.6
2	R	163	SER	6.6
1	Q	258	TYR	6.5
1	K	324	PRO	6.5
1	Q	118	PHE	6.5
1	M	12	GLN	6.5
1	Q	25	VAL	6.4
2	H	21	TRP	6.4
2	H	163	SER	6.4
2	L	22	TYR	6.4
2	H	132	GLU	6.4
2	D	9	PHE	6.4
2	P	156	THR	6.3
2	L	163	SER	6.3
1	E	76	CYS	6.3
2	F	148	CYS	6.3
2	L	130	ALA	6.3
2	F	174	SER	6.3
2	N	139	GLU	6.3
1	M	199	THR	6.3
2	R	7	ALA	6.3
1	G	12	GLN	6.3
1	I	324	PRO	6.3
1	Q	288	ILE	6.3
1	M	55	GLY	6.3
1	E	11	ASP	6.2
1	Q	305	CYS	6.2
2	R	148	CYS	6.2
1	Q	188	ALA	6.2
2	D	35	ALA	6.2
2	J	168	LEU	6.2
2	D	25	HIS	6.2
2	P	145	ASP	6.2
1	Q	128	SER	6.2
2	J	27	SER	6.2
2	J	3	PHE	6.2
2	B	18	VAL	6.2
1	Q	253	ALA	6.1
2	N	7	ALA	6.1

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Mol	Chain	Res	Type	RSRZ
1	G	13	ILE	6.1
1	M	154	LEU	6.1
2	N	175	SER	6.1
1	E	17	TYR	6.1
1	E	78	GLU	6.1
1	Q	237	LEU	6.1
2	L	32	SER	6.1
2	H	29	GLU	6.1
2	P	166	ALA	6.1
2	L	28	ASN	6.1
1	Q	13	ILE	6.1
1	O	79	PHE	6.1
2	B	28	ASN	6.1
2	R	150	GLU	6.1
1	M	188	ALA	6.1
2	H	137	CYS	6.0
1	Q	144	LYS	6.0
2	H	17	MET	6.0
2	L	4	GLY	6.0
2	D	174	SER	6.0
2	J	139	GLU	6.0
2	B	23	GLY	6.0
1	O	141	TYR	6.0
2	L	164	GLU	5.9
2	B	60	ASN	5.9
2	F	157	TYR	5.9
1	A	323	SER	5.9
1	Q	171	THR	5.9
2	F	144	CYS	5.9
1	M	64	CYS	5.9
2	F	145	ASP	5.9
2	H	36	ALA	5.9
2	D	22	TYR	5.9
1	Q	131	GLU	5.8
2	N	125	GLN	5.8
2	R	132	GLU	5.8
2	P	142	HIS	5.8
2	L	8	GLY	5.8
1	K	12	GLN	5.8
1	Q	219	THR	5.8
2	B	7	ALA	5.8
1	M	81	ASN	5.7

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Mol	Chain	Res	Type	RSRZ
1	M	209	LEU	5.7
1	Q	194	LEU	5.7
2	L	149	MET	5.7
2	P	168	LEU	5.7
1	G	15	ILE	5.7
1	K	276	ASN	5.7
1	O	158	ASN	5.7
1	M	128	SER	5.7
2	L	166	ALA	5.7
2	J	25	HIS	5.7
1	O	133(A)	LEU	5.7
1	Q	130	HIS	5.7
2	H	175	SER	5.6
2	H	142	HIS	5.6
1	O	252	ILE	5.6
2	L	137	CYS	5.6
2	N	162	TYR	5.6
1	K	15	ILE	5.6
2	H	143	LYS	5.6
2	L	27	SER	5.6
1	M	129	SER	5.6
1	M	158	ASN	5.6
2	R	18	VAL	5.6
1	Q	307	LYS	5.6
1	E	318	THR	5.6
2	D	132	GLU	5.6
2	H	14	TRP	5.6
2	L	9	PHE	5.6
2	J	131	LYS	5.5
2	F	26	HIS	5.5
2	R	12	GLY	5.5
2	P	141	TYR	5.5
1	A	14	CYS	5.5
1	M	256	TYR	5.5
1	K	11	ASP	5.5
2	R	8	GLY	5.5
2	D	141	TYR	5.4
2	D	19	ASP	5.4
2	J	144	CYS	5.4
1	Q	318	THR	5.4
2	D	155	GLY	5.4
2	J	143	LYS	5.4

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Mol	Chain	Res	Type	RSRZ
2	H	167	ARG	5.4
1	M	200	THR	5.4
1	M	322	ASN	5.4
2	F	16	GLY	5.4
1	Q	63	ASP	5.4
1	Q	263	LYS	5.4
1	Q	88	VAL	5.4
2	D	144	CYS	5.4
2	N	17	MET	5.4
1	C	322	ASN	5.4
2	H	139	GLU	5.4
1	Q	46	LYS	5.3
2	D	163	SER	5.3
1	Q	308	TYR	5.3
2	P	139	GLU	5.3
2	J	28	ASN	5.3
2	L	167	ARG	5.3
2	N	145	ASP	5.3
1	Q	260	ILE	5.3
1	I	20	ASN	5.3
2	R	20	GLY	5.3
2	J	132	GLU	5.3
1	I	323	SER	5.3
1	Q	195	TYR	5.3
2	L	162	TYR	5.3
1	K	81	ASN	5.3
2	H	31	GLY	5.3
1	I	12	GLN	5.3
1	M	79	PHE	5.3
1	Q	252	ILE	5.3
2	F	161	GLN	5.3
2	J	18	VAL	5.3
2	N	27	SER	5.3
1	M	77	ASP	5.2
1	G	10	GLY	5.2
1	M	192	THR	5.2
1	G	17	TYR	5.2
1	O	13	ILE	5.2
2	B	168	LEU	5.2
2	N	144	CYS	5.2
1	E	15	ILE	5.2
1	K	17	TYR	5.2

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Mol	Chain	Res	Type	RSRZ
1	K	14	CYS	5.2
1	K	13	ILE	5.2
2	D	124	LEU	5.2
1	Q	310	LYS	5.2
2	R	149	MET	5.2
1	Q	62	ARG	5.2
2	H	26	HIS	5.2
2	R	162	TYR	5.1
2	L	144	CYS	5.1
2	L	7	ALA	5.1
2	R	5	ALA	5.1
2	R	157	TYR	5.1
1	O	68	GLY	5.1
2	L	170	ARG	5.1
2	R	141	TYR	5.1
1	G	20	ASN	5.1
1	O	98	TYR	5.1
2	P	8	GLY	5.1
2	R	40	SER	5.1
2	R	159	TYR	5.1
1	A	290	SER	5.1
1	G	78	GLU	5.1
1	Q	152	VAL	5.1
2	R	4	GLY	5.0
2	J	2	LEU	5.0
1	M	187	ASP	5.0
1	Q	266	THR	5.0
1	Q	285	MET	5.0
1	C	289	ASN	5.0
2	D	131	LYS	5.0
1	Q	236	ILE	5.0
1	G	318	THR	5.0
1	Q	53	ASP	5.0
2	L	171	GLU	5.0
1	O	48	ASN	5.0
1	M	201	TYR	5.0
2	L	142	HIS	4.9
2	D	168	LEU	4.9
1	Q	228	GLY	4.9
1	A	22	THR	4.9
2	B	146	ASN	4.9
2	F	149	MET	4.9

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Mol	Chain	Res	Type	RSRZ
1	M	17	TYR	4.9
1	O	283	THR	4.9
2	P	125	GLN	4.9
1	I	11	ASP	4.9
1	Q	286	GLY	4.9
2	D	60	ASN	4.9
2	F	156	THR	4.9
1	O	129	SER	4.9
2	H	173	ILE	4.8
1	Q	255	GLU	4.8
1	M	205	GLY	4.8
1	Q	42	ILE	4.8
1	C	14	CYS	4.8
2	J	137	CYS	4.8
2	R	3	PHE	4.8
1	Q	291	SER	4.8
1	M	283	THR	4.8
2	P	134	GLY	4.8
1	O	81	ASN	4.8
1	O	201	TYR	4.8
2	D	143	LYS	4.8
2	N	28	ASN	4.8
2	F	128	ASP	4.8
2	B	31	GLY	4.7
2	D	3	PHE	4.7
2	D	175	SER	4.7
2	P	18	VAL	4.7
2	B	157	TYR	4.7
2	R	46	ASP	4.7
1	I	21	SER	4.7
2	R	11	GLU	4.7
2	J	162	TYR	4.7
2	N	5	ALA	4.7
2	P	45	ILE	4.7
2	R	136	GLY	4.7
2	D	171	GLU	4.7
2	R	41	THR	4.7
1	K	19(A)	ASN	4.7
2	D	159	TYR	4.7
2	P	147	GLU	4.7
1	C	13	ILE	4.7
1	M	48	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
1	Q	197	ASN	4.7
1	Q	290	SER	4.7
1	M	122	GLN	4.6
2	N	140	PHE	4.6
2	B	22	TYR	4.6
2	H	165	GLU	4.6
2	H	155	GLY	4.6
2	R	126	LEU	4.6
2	R	173	ILE	4.6
1	Q	244	ASN	4.6
2	D	27	SER	4.6
1	Q	84	TRP	4.6
1	Q	127	TRP	4.6
1	M	91	ALA	4.6
1	I	322	ASN	4.6
2	F	170	ARG	4.6
1	G	21	SER	4.6
2	F	3	PHE	4.6
1	G	80	ILE	4.6
1	M	184	HIS	4.6
1	O	117	HIS	4.6
2	R	49	THR	4.6
2	R	16	GLY	4.6
2	R	170	ARG	4.6
2	L	60	ASN	4.6
2	F	164	GLU	4.6
2	F	2	LEU	4.6
2	R	50	ASN	4.6
1	M	133(A)	LEU	4.6
1	O	54	ASP	4.5
2	R	22	TYR	4.5
1	M	221	SER	4.5
1	Q	23	GLU	4.5
1	K	20	ASN	4.5
1	O	322	ASN	4.5
1	C	323	SER	4.5
2	D	34	TYR	4.5
2	F	12	GLY	4.5
2	L	29	GLU	4.5
2	J	166	ALA	4.5
1	M	225	GLY	4.5
2	H	35	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	K	323	SER	4.5
2	J	133	LEU	4.5
1	A	13	ILE	4.5
1	Q	168	TYR	4.5
2	R	128	ASP	4.5
2	P	144	CYS	4.5
2	R	137	CYS	4.5
1	M	198	PRO	4.5
1	A	322	ASN	4.5
1	O	253	ALA	4.5
2	H	160	PRO	4.5
2	R	21	TRP	4.5
1	Q	274	TYR	4.4
2	N	154	ASN	4.4
1	O	160	THR	4.4
2	D	8	GLY	4.4
2	F	163	SER	4.4
1	Q	77	ASP	4.4
1	Q	81	ASN	4.4
2	R	123	ARG	4.4
2	R	172	GLU	4.4
2	H	144	CYS	4.4
1	I	51	LEU	4.4
1	Q	182	ILE	4.4
2	F	147	GLU	4.4
2	H	172	GLU	4.4
2	P	46	ASP	4.4
2	N	1	GLY	4.4
2	H	161	GLN	4.4
1	Q	116	ASN	4.4
1	Q	83	GLU	4.4
1	A	21	SER	4.4
2	L	152	VAL	4.4
2	J	30	GLN	4.4
1	C	15	ILE	4.4
1	G	76	CYS	4.4
1	Q	39	ALA	4.4
1	Q	292	MET	4.3
1	O	251	PHE	4.3
1	M	76	CYS	4.3
2	L	148	CYS	4.3
2	B	162	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
2	D	156	THR	4.3
2	L	127	ARG	4.3
1	Q	230	MET	4.3
2	D	4	GLY	4.3
1	O	163	THR	4.3
2	H	156	THR	4.3
1	Q	113	SER	4.3
1	Q	229	ARG	4.3
2	F	158	ASP	4.3
2	F	27	SER	4.3
1	Q	157	LYS	4.3
2	R	118	LEU	4.3
1	O	140	PRO	4.3
1	Q	208	THR	4.3
1	Q	259	LYS	4.3
1	O	225	GLY	4.2
1	M	41	ASP	4.2
2	F	28	ASN	4.2
1	Q	269	LYS	4.2
2	D	31	GLY	4.2
1	I	141	TYR	4.2
2	N	133	LEU	4.2
2	N	160	PRO	4.2
1	G	16	GLY	4.2
2	N	134	GLY	4.2
1	E	79	PHE	4.2
2	B	6	ILE	4.2
2	P	30	GLN	4.2
1	Q	24	GLN	4.2
2	L	21	TRP	4.2
2	R	36	ALA	4.2
1	Q	19(A)	ASN	4.2
1	O	184	HIS	4.2
1	M	208	THR	4.2
2	N	141	TYR	4.2
2	B	38	LYS	4.2
2	R	53	ASN	4.2
1	O	112	LEU	4.2
1	M	210	ASN	4.2
2	N	45	ILE	4.2
1	Q	265	SER	4.2
2	D	164	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
1	Q	15	ILE	4.2
2	F	38	LYS	4.2
2	R	45	ILE	4.2
2	R	31	GLY	4.2
1	M	116	ASN	4.1
2	N	8	GLY	4.1
1	Q	75	MET	4.1
1	A	23	GLU	4.1
2	J	136	GLY	4.1
2	R	61	THR	4.1
1	A	143	GLY	4.1
1	Q	97	CYS	4.1
1	M	194	LEU	4.1
1	O	189	ALA	4.1
1	Q	193	LYS	4.1
1	Q	261	VAL	4.1
2	J	138	PHE	4.1
1	M	246	GLU	4.1
1	Q	126	SER	4.1
2	D	24	TYR	4.1
2	N	34	TYR	4.1
1	I	79	PHE	4.1
1	Q	191	GLN	4.1
2	H	130	ALA	4.1
1	E	141	TYR	4.1
1	O	161	TYR	4.1
2	B	158	ASP	4.1
2	D	146	ASN	4.1
2	B	3	PHE	4.1
2	P	140	PHE	4.1
2	J	22	TYR	4.1
1	E	186	ASN	4.1
1	Q	174	GLU	4.1
2	J	172	GLU	4.1
1	C	16	GLY	4.0
2	R	155	GLY	4.0
2	B	131	LYS	4.0
2	L	5	ALA	4.0
2	D	2	LEU	4.0
2	D	32	SER	4.0
2	P	159	TYR	4.0
2	H	19	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	Q	153	TRP	4.0
1	Q	319	GLY	4.0
1	Q	67	ALA	4.0
1	Q	270	SER	4.0
2	P	167	ARG	4.0
2	N	132	GLU	4.0
2	H	131	LYS	4.0
1	Q	295	HIS	4.0
2	N	163	SER	4.0
1	C	55	GLY	4.0
1	Q	143	GLY	4.0
1	M	186	ASN	4.0
2	J	135	ASN	4.0
2	R	161	GLN	4.0
2	J	117	ASN	4.0
1	O	199	THR	4.0
1	Q	49	GLY	4.0
2	J	4	GLY	4.0
1	O	128	SER	4.0
1	O	285	MET	4.0
2	R	127	ARG	4.0
1	O	214	VAL	4.0
1	Q	199	THR	4.0
2	D	122	VAL	4.0
2	R	171	GLU	4.0
2	P	133	LEU	4.0
2	D	61	THR	4.0
1	M	242	ALA	4.0
1	O	132	ALA	4.0
2	B	145	ASP	4.0
2	J	147	GLU	3.9
1	M	51	LEU	3.9
2	J	171	GLU	3.9
1	E	132	ALA	3.9
1	M	86	TYR	3.9
2	J	26	HIS	3.9
2	P	35	ALA	3.9
1	M	14	CYS	3.9
1	O	159	SER	3.9
2	F	6	ILE	3.9
1	O	77	ASP	3.9
1	Q	279	THR	3.9

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Mol	Chain	Res	Type	RSRZ
2	L	159	TYR	3.9
2	H	133	LEU	3.9
2	H	13	GLY	3.9
2	H	148	CYS	3.9
1	Q	242	ALA	3.9
2	B	27	SER	3.9
1	Q	45	LYS	3.9
2	D	137	CYS	3.9
2	F	14	TRP	3.9
1	G	11	ASP	3.9
1	C	141	TYR	3.9
1	M	145	SER	3.9
2	D	130	ALA	3.9
2	F	7	ALA	3.9
1	M	143	GLY	3.9
2	B	155	GLY	3.9
2	D	173	ILE	3.9
2	J	61	THR	3.9
2	B	5	ALA	3.9
2	D	134	GLY	3.9
1	O	206	THR	3.9
2	P	162	TYR	3.9
2	F	60	ASN	3.8
2	B	136	GLY	3.8
1	M	219	THR	3.8
1	O	75	MET	3.8
1	Q	192	THR	3.8
1	C	12	GLN	3.8
2	D	157	TYR	3.8
2	D	28	ASN	3.8
2	R	154	ASN	3.8
2	L	16	GLY	3.8
2	F	133	LEU	3.8
2	B	138	PHE	3.8
1	I	290	SER	3.8
2	L	36	ALA	3.8
2	R	32	SER	3.8
1	I	289	ASN	3.8
2	P	158	ASP	3.8
1	E	21	SER	3.8
1	M	190	GLU	3.8
2	P	160	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	143	LYS	3.8
2	H	34	TYR	3.8
1	Q	43	LEU	3.8
2	R	56	ILE	3.8
1	O	310	LYS	3.8
2	N	42	GLN	3.8
2	P	42	GLN	3.8
1	O	155	ILE	3.8
2	R	58	LYS	3.8
1	M	142	GLN	3.8
2	B	141	TYR	3.8
1	M	59	LEU	3.8
2	F	18	VAL	3.8
1	C	20	ASN	3.8
2	R	72	ASN	3.8
2	R	113	SER	3.8
1	K	10	GLY	3.8
1	M	278	ASN	3.7
1	O	154	LEU	3.7
2	D	109	ASP	3.7
1	M	227	SER	3.7
2	B	172	GLU	3.7
2	N	32	SER	3.7
2	D	128	ASP	3.7
1	Q	80	ILE	3.7
2	F	137	CYS	3.7
2	B	165	GLU	3.7
1	C	186	ASN	3.7
1	I	240	ASN	3.7
2	D	160	PRO	3.7
1	E	54	ASP	3.7
2	L	117	ASN	3.7
1	Q	53(A)	LEU	3.7
2	R	140	PHE	3.7
2	P	164	GLU	3.7
2	J	12	GLY	3.7
1	M	257	ALA	3.7
1	M	277	CYS	3.7
1	Q	189	ALA	3.7
2	B	156	THR	3.7
1	Q	313	ARG	3.7
2	P	21	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
2	L	151	SER	3.7
2	P	27	SER	3.7
1	Q	117	HIS	3.7
2	H	159	TYR	3.7
2	P	34	TYR	3.7
2	B	173	ILE	3.7
2	P	165	GLU	3.6
1	Q	102	PHE	3.6
1	O	133	SER	3.6
1	Q	140	PRO	3.6
2	D	158	ASP	3.6
1	K	292	MET	3.6
1	G	159	SER	3.6
2	R	37	ASP	3.6
2	R	79	ASN	3.6
1	K	160	THR	3.6
1	Q	211	GLN	3.6
1	Q	47	HIS	3.6
2	P	126	LEU	3.6
2	L	161	GLN	3.6
1	I	14	CYS	3.6
1	Q	158	ASN	3.6
1	M	323	SER	3.6
1	O	256	TYR	3.6
2	P	24	TYR	3.6
1	Q	57	LYS	3.6
1	M	254	PRO	3.6
1	K	322	ASN	3.6
1	O	153	TRP	3.6
1	A	33	LYS	3.6
2	J	109	ASP	3.6
2	J	165	GLU	3.6
2	P	19	ASP	3.6
2	P	172	GLU	3.6
1	E	158	ASN	3.6
1	O	95	ASN	3.6
1	M	127	TRP	3.6
1	O	71	LEU	3.6
2	R	1	GLY	3.6
1	I	40	GLN	3.6
1	Q	246	GLU	3.6
1	I	60	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	O	41	ASP	3.6
2	L	41	THR	3.6
2	B	21	TRP	3.6
1	C	17	TYR	3.6
2	D	135	ASN	3.6
1	Q	283	THR	3.5
2	R	107	THR	3.5
1	A	80	ILE	3.5
1	K	80	ILE	3.5
2	P	14	TRP	3.5
2	L	145	ASP	3.5
1	G	31	MET	3.5
2	F	17	MET	3.5
2	P	13	GLY	3.5
1	Q	111	LEU	3.5
2	L	168	LEU	3.5
2	R	89	LEU	3.5
1	Q	138	ALA	3.5
2	B	4	GLY	3.5
1	C	19(A)	ASN	3.5
1	E	322	ASN	3.5
2	D	140	PHE	3.5
1	M	37	THR	3.5
2	J	167	ARG	3.5
1	O	194	LEU	3.5
1	Q	173	GLN	3.5
1	C	22	THR	3.5
1	M	121	ILE	3.5
1	Q	72	GLY	3.5
2	H	23	GLY	3.5
2	N	3	PHE	3.5
2	D	72	ASN	3.5
1	Q	241	ASP	3.5
1	O	67	ALA	3.5
1	Q	12	GLN	3.5
1	Q	11	ASP	3.5
1	A	24	GLN	3.5
2	B	142	HIS	3.5
2	P	111	HIS	3.5
1	Q	85	SER	3.5
2	H	33	GLY	3.5
2	N	16	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
2	N	159	TYR	3.5
1	E	276	ASN	3.4
2	J	60	ASN	3.4
2	J	120	ASP	3.4
1	M	230	MET	3.4
2	H	2	LEU	3.4
1	A	10	GLY	3.4
1	Q	184	HIS	3.4
2	L	33	GLY	3.4
2	N	6	ILE	3.4
1	M	240	ASN	3.4
2	B	10	ILE	3.4
2	B	175	SER	3.4
1	M	191	GLN	3.4
1	O	191	GLN	3.4
2	H	118	LEU	3.4
2	J	38	LYS	3.4
1	A	318	THR	3.4
2	H	158	ASP	3.4
1	A	292	MET	3.4
1	Q	300	LEU	3.4
2	H	168	LEU	3.4
1	A	141	TYR	3.4
2	F	1	GLY	3.4
1	Q	27	THR	3.4
2	H	166	ALA	3.4
1	Q	312	ASN	3.4
1	G	323	SER	3.4
1	M	159	SER	3.4
1	Q	55	GLY	3.4
2	H	4	GLY	3.4
2	N	61	THR	3.4
1	Q	20	ASN	3.4
1	K	142	GLN	3.4
2	J	113	SER	3.4
2	J	149	MET	3.4
2	N	170	ARG	3.4
2	P	170	ARG	3.4
2	F	152	VAL	3.4
2	F	132	GLU	3.4
1	O	224	ASN	3.4
1	Q	115	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
2	J	24	TYR	3.4
1	A	101	ASP	3.4
2	R	26	HIS	3.4
1	M	20	ASN	3.4
1	O	205	GLY	3.3
2	J	155	GLY	3.3
1	E	14	CYS	3.3
2	F	10	ILE	3.3
2	D	166	ALA	3.3
1	M	241	ASP	3.3
1	Q	165	LYS	3.3
2	D	142	HIS	3.3
2	N	25	HIS	3.3
2	P	26	HIS	3.3
2	N	60	ASN	3.3
1	O	66	VAL	3.3
1	K	21	SER	3.3
1	Q	212	ARG	3.3
1	M	67	ALA	3.3
2	L	147	GLU	3.3
2	N	147	GLU	3.3
2	N	168	LEU	3.3
2	D	151	SER	3.3
2	J	140	PHE	3.3
2	L	3	PHE	3.3
2	D	161	GLN	3.3
1	O	40	GLN	3.3
2	N	161	GLN	3.3
2	R	116	LYS	3.3
2	R	139	GLU	3.3
1	I	142	GLN	3.3
2	F	168	LEU	3.3
2	D	21	TRP	3.3
2	F	25	HIS	3.3
1	M	95	ASN	3.3
1	G	317	ALA	3.3
2	F	9	PHE	3.3
1	O	86	TYR	3.3
2	N	21	TRP	3.3
1	G	33	LYS	3.3
2	B	17	MET	3.3
2	L	169	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	M	193	LYS	3.3
1	Q	56	VAL	3.3
2	R	9	PHE	3.3
1	M	163	THR	3.3
1	O	185	PRO	3.3
1	Q	203	SER	3.3
2	R	24	TYR	3.3
2	L	165	GLU	3.2
1	I	292	MET	3.2
2	J	106	ARG	3.2
1	O	284	PRO	3.2
2	F	127	ARG	3.2
1	M	108	LEU	3.2
1	O	174	GLU	3.2
1	Q	227	SER	3.2
2	J	32	SER	3.2
1	M	214	VAL	3.2
1	C	80	ILE	3.2
1	M	60	ILE	3.2
1	M	101	ASP	3.2
2	R	52	VAL	3.2
2	R	121	LYS	3.2
2	B	114	ASN	3.2
1	O	65	SER	3.2
1	Q	311	SER	3.2
1	Q	35(A)	THR	3.2
2	R	39	GLU	3.2
1	C	290	SER	3.2
1	O	241	ASP	3.2
1	O	186	ASN	3.2
1	Q	94	VAL	3.2
1	Q	287	ALA	3.2
1	M	217	ILE	3.2
1	E	290	SER	3.2
1	Q	65	SER	3.2
2	P	22	TYR	3.2
2	R	119	TYR	3.2
2	B	25	HIS	3.2
1	M	54	ASP	3.2
1	O	62	ARG	3.1
1	Q	178	VAL	3.1
2	H	28	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	Q	297	ILE	3.1
1	I	291	SER	3.1
1	M	125(B)	SER	3.1
2	F	32	SER	3.1
1	E	77	ASP	3.1
1	O	157	LYS	3.1
1	E	20	ASN	3.1
1	I	81	ASN	3.1
1	O	14	CYS	3.1
2	H	7	ALA	3.1
2	P	60	ASN	3.1
2	H	30	GLN	3.1
2	N	41	THR	3.1
1	C	145	SER	3.1
2	B	112	ASP	3.1
1	M	139	CYS	3.1
1	K	25	VAL	3.1
2	H	3	PHE	3.1
2	H	127	ARG	3.1
2	H	146	ASN	3.1
2	R	84	MET	3.1
1	O	60	ILE	3.1
1	Q	169	ASN	3.1
2	L	146	ASN	3.1
1	I	26	ASP	3.1
1	Q	321	ARG	3.1
1	M	13	ILE	3.1
1	O	142	GLN	3.1
1	K	132	ALA	3.1
2	L	14	TRP	3.1
1	A	15	ILE	3.1
1	Q	78	GLU	3.1
1	C	276	ASN	3.1
1	O	275	GLY	3.1
1	M	291	SER	3.1
1	O	146	SER	3.1
1	Q	137	SER	3.1
2	B	9	PHE	3.1
2	H	152	VAL	3.1
2	N	36	ALA	3.1
1	E	320	LEU	3.1
2	L	2	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	O	212	ARG	3.0
2	F	124	LEU	3.0
2	H	153	ARG	3.0
2	L	34	TYR	3.0
2	N	46	ASP	3.0
2	P	161	GLN	3.0
2	F	155	GLY	3.0
1	M	87	ILE	3.0
2	P	40	SER	3.0
2	P	4	GLY	3.0
1	C	144	LYS	3.0
2	H	171	GLU	3.0
2	F	166	ALA	3.0
2	N	26	HIS	3.0
1	M	152	VAL	3.0
2	L	37	ASP	3.0
2	R	86	ASP	3.0
2	D	33	GLY	3.0
2	D	5	ALA	3.0
2	P	72	ASN	3.0
1	Q	163	THR	3.0
1	Q	132	ALA	3.0
2	H	60	ASN	3.0
2	H	111	HIS	3.0
2	N	165	GLU	3.0
1	K	290	SER	3.0
1	M	11	ASP	3.0
1	Q	196	GLN	3.0
1	Q	264	GLY	3.0
2	L	45	ILE	3.0
1	Q	280	LYS	3.0
1	I	279	THR	2.9
2	B	35	ALA	2.9
1	M	119	GLU	2.9
2	B	125	GLN	2.9
2	L	30	GLN	2.9
1	Q	34	ASN	2.9
1	M	183	HIS	2.9
1	O	193	LYS	2.9
2	L	26	HIS	2.9
2	D	119	TYR	2.9
1	M	52	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	R	151	SER	2.9
1	O	166	ARG	2.9
1	K	46	LYS	2.9
2	F	111	HIS	2.9
1	Q	86	TYR	2.9
2	L	23	GLY	2.9
2	R	66	VAL	2.9
2	F	33	GLY	2.9
2	L	38	LYS	2.9
1	I	241	ASP	2.9
2	R	30	GLN	2.9
2	B	106	ARG	2.9
2	H	117	ASN	2.9
2	N	171	GLU	2.9
2	L	18	VAL	2.9
1	M	290	SER	2.9
2	R	42	GLN	2.9
1	I	276	ASN	2.9
1	M	287	ALA	2.9
2	N	4	GLY	2.9
1	E	25	VAL	2.9
2	J	21	TRP	2.9
1	O	219	THR	2.9
1	Q	240	ASN	2.9
1	O	52	CYS	2.9
1	O	144	LYS	2.9
1	O	151	VAL	2.9
2	P	15	GLN	2.9
2	J	112	ASP	2.9
1	Q	272	LEU	2.9
2	D	45	ILE	2.9
2	J	34	TYR	2.8
1	O	176	LEU	2.8
1	Q	73	ASN	2.8
2	B	117	ASN	2.8
2	J	5	ALA	2.8
1	G	25	VAL	2.8
2	R	74	GLU	2.8
2	N	119	TYR	2.8
1	O	237	LEU	2.8
2	D	101	LEU	2.8
2	N	138	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	23	GLU	2.8
1	I	52	CYS	2.8
1	O	82	VAL	2.8
1	Q	214	VAL	2.8
2	D	152	VAL	2.8
2	J	11	GLU	2.8
2	J	164	GLU	2.8
2	R	62	GLN	2.8
2	N	167	ARG	2.8
2	F	24	TYR	2.8
2	F	120	ASP	2.8
2	N	142	HIS	2.8
1	Q	103	ASN	2.8
1	M	175	ASP	2.8
2	H	24	TYR	2.8
1	Q	145	SER	2.8
1	K	186	ASN	2.8
2	B	129	ASN	2.8
2	R	124	LEU	2.8
1	G	281	CYS	2.8
2	N	148	CYS	2.8
2	B	154	ASN	2.8
2	P	138	PHE	2.8
1	K	173	GLN	2.8
1	M	167	SER	2.8
1	I	174	GLU	2.8
1	O	202	ILE	2.8
1	Q	271	GLU	2.8
2	D	162	TYR	2.8
2	L	119	TYR	2.8
1	A	75	MET	2.8
1	A	142	GLN	2.8
1	M	185	PRO	2.8
2	D	30	GLN	2.8
1	I	315	VAL	2.8
2	L	43	LYS	2.8
1	K	288	ILE	2.8
1	O	20	ASN	2.8
1	O	210	ASN	2.8
1	O	246	GLU	2.8
2	D	136	GLY	2.8
2	H	11	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
2	P	146	ASN	2.8
1	C	279	THR	2.8
1	G	141	TYR	2.8
2	J	163	SER	2.7
2	H	12	GLY	2.7
2	N	33	GLY	2.7
1	I	19(A)	ASN	2.7
1	Q	187	ASP	2.7
2	H	114	ASN	2.7
1	M	231	GLU	2.7
2	R	142	HIS	2.7
1	O	216	ARG	2.7
1	O	250	ASN	2.7
1	K	141	TYR	2.7
2	F	35	ALA	2.7
1	K	266	THR	2.7
1	Q	235	THR	2.7
2	J	102	MET	2.7
2	R	164	GLU	2.7
1	G	320	LEU	2.7
1	Q	70	LEU	2.7
2	H	27	SER	2.7
2	L	35	ALA	2.7
1	Q	301	THR	2.7
2	F	171	GLU	2.7
1	O	69	TRP	2.7
2	H	66	VAL	2.7
2	H	38	LYS	2.7
1	M	213	LEU	2.7
1	O	187	ASP	2.7
1	Q	224	ASN	2.7
2	H	170	ARG	2.7
2	P	29	GLU	2.7
1	Q	201	TYR	2.7
2	L	136	GLY	2.7
1	O	215	PRO	2.7
1	M	179	LEU	2.7
1	O	97	CYS	2.7
2	B	137	CYS	2.7
1	O	183	HIS	2.7
1	C	282	GLN	2.7
1	O	12	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	13	GLY	2.7
1	A	158	ASN	2.7
1	A	35(A)	THR	2.7
1	A	314	LEU	2.7
1	K	283	THR	2.7
1	I	87	ILE	2.7
1	Q	273	GLU	2.7
2	B	14	TRP	2.7
2	P	6	ILE	2.7
1	M	133	SER	2.7
2	F	146	ASN	2.7
2	F	34	TYR	2.7
1	O	101	ASP	2.7
1	K	287	ALA	2.7
1	E	323	SER	2.7
1	Q	142	GLN	2.7
1	K	52	CYS	2.6
1	M	141	TYR	2.6
2	B	149	MET	2.6
2	J	9	PHE	2.6
1	Q	121	ILE	2.6
1	Q	239	PRO	2.6
1	O	226	GLN	2.6
1	K	275	GLY	2.6
2	P	25	HIS	2.6
1	Q	233	PHE	2.6
1	K	41	ASP	2.6
1	O	277	CYS	2.6
1	A	27	THR	2.6
1	I	173	GLN	2.6
1	G	18	HIS	2.6
2	R	54	SER	2.6
2	L	132	GLU	2.6
2	J	101	LEU	2.6
2	N	81	ASN	2.6
2	R	71	ASN	2.6
2	H	119	TYR	2.6
2	J	19	ASP	2.6
1	I	22	THR	2.6
1	I	27	THR	2.6
1	C	94	VAL	2.6
1	C	177	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	92	ASN	2.6
1	I	17	TYR	2.6
1	O	218	ALA	2.6
2	B	109	ASP	2.6
2	F	134	GLY	2.6
1	I	82	VAL	2.6
2	J	170	ARG	2.6
2	B	113	SER	2.6
2	B	174	SER	2.6
1	A	87	ILE	2.6
2	R	6	ILE	2.6
1	M	100	GLY	2.6
1	O	63	ASP	2.6
1	O	134	GLY	2.6
2	D	120	ASP	2.6
2	N	164	GLU	2.6
1	C	199	THR	2.6
1	K	279	THR	2.6
2	F	66	VAL	2.6
1	M	267	ILE	2.6
1	O	76	CYS	2.6
1	K	53	ASP	2.6
1	O	17	TYR	2.6
1	Q	222	LYS	2.6
2	J	116	LYS	2.6
1	E	304	GLU	2.6
1	M	80	ILE	2.6
1	Q	48	ASN	2.6
1	Q	107	GLU	2.6
2	H	149	MET	2.6
2	J	31	GLY	2.6
2	L	155	GLY	2.6
2	P	10	ILE	2.6
1	M	144	LYS	2.6
1	G	149	ARG	2.6
1	Q	114	ARG	2.6
2	D	36	ALA	2.6
1	M	93	PRO	2.6
2	B	34	TYR	2.6
2	B	140	PHE	2.5
2	H	25	HIS	2.5
2	P	163	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	158	ASN	2.5
2	H	37	ASP	2.5
2	P	154	ASN	2.5
1	O	99	PRO	2.5
1	E	35	VAL	2.5
1	M	112	LEU	2.5
2	R	2	LEU	2.5
2	L	61	THR	2.5
1	E	291	SER	2.5
1	M	103	ASN	2.5
1	M	168	TYR	2.5
1	M	204	VAL	2.5
2	N	157	TYR	2.5
2	J	111	HIS	2.5
1	O	208	THR	2.5
1	Q	317	ALA	2.5
1	I	277	CYS	2.5
1	O	113	SER	2.5
1	A	48	ASN	2.5
1	C	69	TRP	2.5
2	F	5	ALA	2.5
2	N	30	GLN	2.5
1	Q	207	SER	2.5
2	H	162	TYR	2.5
2	P	148	CYS	2.5
1	E	18	HIS	2.5
1	A	11	ASP	2.5
1	E	128	SER	2.5
1	I	160	THR	2.5
1	E	16	GLY	2.5
1	M	244	ASN	2.5
1	G	316	LEU	2.5
1	O	139	CYS	2.5
1	M	115	ILE	2.5
1	Q	202	ILE	2.5
2	F	125	GLN	2.5
2	B	11	GLU	2.5
2	L	11	GLU	2.5
1	M	104	ASP	2.5
1	E	35(A)	THR	2.5
1	M	82	VAL	2.5
1	O	200	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	19(A)	ASN	2.5
1	E	140	PRO	2.5
1	G	143	GLY	2.5
1	Q	16	GLY	2.5
1	Q	275	GLY	2.5
1	O	287	ALA	2.5
2	J	145	ASP	2.5
1	G	73	ASN	2.5
2	H	108	LEU	2.5
1	K	122	GLN	2.5
2	N	130	ALA	2.5
2	F	21	TRP	2.5
1	E	292	MET	2.5
2	J	110	PHE	2.5
1	O	167	SER	2.4
1	O	290	SER	2.4
1	K	24	GLN	2.4
1	M	195	TYR	2.4
2	R	131	LYS	2.4
1	Q	147	PHE	2.4
2	D	66	VAL	2.4
2	F	4	GLY	2.4
1	C	81	ASN	2.4
1	O	50	LYS	2.4
1	M	202	ILE	2.4
1	M	68	GLY	2.4
1	M	84	TRP	2.4
1	A	78	GLU	2.4
1	M	156	LYS	2.4
1	E	142	GLN	2.4
1	E	317	ALA	2.4
1	G	289	ASN	2.4
2	D	10	ILE	2.4
1	M	47	HIS	2.4
2	P	106	ARG	2.4
1	E	33	LYS	2.4
1	Q	119	GLU	2.4
2	B	84	MET	2.4
1	M	137	SER	2.4
1	M	207	SER	2.4
2	L	10	ILE	2.4
2	R	44	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	186	ASN	2.4
2	D	16	GLY	2.4
1	Q	277	CYS	2.4
1	K	82	VAL	2.4
1	Q	69	TRP	2.4
1	M	265	SER	2.4
2	N	22	TYR	2.4
1	M	32	GLU	2.4
2	J	150	GLU	2.4
2	L	150	GLU	2.4
1	M	135	VAL	2.4
2	B	115	VAL	2.4
1	C	31	MET	2.4
1	Q	179	LEU	2.4
2	L	17	MET	2.4
1	I	13	ILE	2.4
1	I	144	LYS	2.4
1	M	165	LYS	2.4
2	R	166	ALA	2.4
1	O	227	SER	2.4
2	L	40	SER	2.4
1	M	232	PHE	2.4
2	D	172	GLU	2.4
2	H	110	PHE	2.4
1	A	144	LYS	2.4
1	I	46	LYS	2.4
1	K	282	GLN	2.4
1	O	190	GLU	2.4
2	L	101	LEU	2.4
1	A	28	ILE	2.4
2	J	10	ILE	2.4
1	A	19(A)	ASN	2.4
1	K	291	SER	2.4
1	I	105	TYR	2.4
2	B	107	THR	2.4
1	A	40	GLN	2.3
1	M	125(A)	LYS	2.3
1	K	88	VAL	2.3
1	M	73	ASN	2.3
1	O	137	SER	2.3
1	O	204	VAL	2.3
1	M	176	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	J	156	THR	2.3
1	C	19	ALA	2.3
2	D	6	ILE	2.3
1	E	81	ASN	2.3
1	I	65	SER	2.3
1	O	116	ASN	2.3
2	D	104	ASN	2.3
1	M	22	THR	2.3
1	M	134	GLY	2.3
1	M	218	ALA	2.3
1	A	221	SER	2.3
1	G	95	ASN	2.3
1	M	173	GLN	2.3
1	O	53(A)	LEU	2.3
2	F	95	ASN	2.3
2	N	156	THR	2.3
1	A	217	ILE	2.3
1	A	131	GLU	2.3
1	M	269	LYS	2.3
1	Q	122	GLN	2.3
2	D	108	LEU	2.3
1	A	319	GLY	2.3
2	D	107	THR	2.3
1	C	246	GLU	2.3
1	K	194	LEU	2.3
1	Q	101	ASP	2.3
1	E	149	ARG	2.3
2	B	111	HIS	2.3
2	D	95	ASN	2.3
2	J	104	ASN	2.3
1	I	171	THR	2.3
1	K	22	THR	2.3
1	K	174	GLU	2.3
2	B	164	GLU	2.3
2	L	39	GLU	2.3
1	O	82(A)	PRO	2.3
2	L	91	VAL	2.3
2	D	106	ARG	2.3
2	D	112	ASP	2.3
1	E	34	ASN	2.3
1	G	22	THR	2.3
1	O	36	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	R	91	VAL	2.3
2	B	90	ASP	2.3
2	H	124	LEU	2.3
1	M	136	SER	2.3
1	A	232	PHE	2.3
2	D	165	GLU	2.3
2	N	29	GLU	2.3
1	M	160	THR	2.3
1	Q	35	VAL	2.3
1	A	282	GLN	2.3
1	I	50	LYS	2.3
2	L	121	LYS	2.3
1	C	130	HIS	2.2
1	E	113	SER	2.2
2	F	113	SER	2.2
2	J	141	TYR	2.2
2	P	17	MET	2.2
1	A	281	CYS	2.2
1	O	55	GLY	2.2
1	O	282	GLN	2.2
1	Q	234	TRP	2.2
1	Q	299	PRO	2.2
2	R	25	HIS	2.2
1	K	285	MET	2.2
2	P	149	MET	2.2
1	C	10	GLY	2.2
1	Q	22	THR	2.2
1	A	119	GLU	2.2
1	C	52	CYS	2.2
1	K	166	ARG	2.2
1	K	218	ALA	2.2
1	K	277	CYS	2.2
1	G	65	SER	2.2
1	K	296	ASN	2.2
1	I	25	VAL	2.2
1	C	142	GLN	2.2
1	Q	177	LEU	2.2
2	R	169	LYS	2.2
1	A	277	CYS	2.2
1	G	124	ILE	2.2
1	A	289	ASN	2.2
1	I	312	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	130	HIS	2.2
1	G	319	GLY	2.2
1	Q	220	ARG	2.2
2	H	134	GLY	2.2
2	J	13	GLY	2.2
2	J	125	GLN	2.2
1	C	54	ASP	2.2
1	M	284	PRO	2.2
1	M	220	ARG	2.2
1	Q	149	ARG	2.2
1	C	274	TYR	2.2
1	K	94	VAL	2.2
1	M	94	VAL	2.2
1	O	178	VAL	2.2
1	Q	156	LYS	2.2
2	P	11	GLU	2.2
2	R	122	VAL	2.2
1	Q	134	GLY	2.2
2	B	132	GLU	2.2
2	F	162	TYR	2.2
2	L	94	TYR	2.2
1	M	146	SER	2.2
1	Q	112	LEU	2.2
1	Q	19	ALA	2.2
1	C	160	THR	2.2
2	L	143	LYS	2.2
1	Q	249	GLY	2.2
1	A	176	LEU	2.2
1	K	116	ASN	2.2
1	M	40	GLN	2.2
1	Q	51	LEU	2.2
2	J	146	ASN	2.2
2	L	133	LEU	2.2
1	C	39	ALA	2.2
1	I	321	ARG	2.2
2	D	7	ALA	2.2
2	L	113	SER	2.2
1	I	97	CYS	2.2
1	O	198	PRO	2.2
1	Q	190	GLU	2.2
2	R	67	GLY	2.2
1	C	40	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	282	GLN	2.2
1	C	98	TYR	2.2
1	I	84	TRP	2.2
2	H	100	VAL	2.2
1	K	289	ASN	2.2
2	J	94	TYR	2.2
1	G	125(A)	LYS	2.1
1	C	74	PRO	2.1
1	E	55	GLY	2.1
1	O	267	ILE	2.1
2	F	31	GLY	2.1
2	J	107	THR	2.1
1	M	237	LEU	2.1
2	R	108	LEU	2.1
1	G	248	ASN	2.1
2	F	96	ALA	2.1
1	O	87	ILE	2.1
1	Q	87	ILE	2.1
2	J	67	GLY	2.1
1	A	18	HIS	2.1
2	R	94	TYR	2.1
1	O	83	GLU	2.1
1	O	203	SER	2.1
1	Q	21	SER	2.1
2	D	123	ARG	2.1
2	F	118	LEU	2.1
1	G	322	ASN	2.1
1	O	233	PHE	2.1
1	Q	289	ASN	2.1
2	D	94	TYR	2.1
1	A	291	SER	2.1
2	H	113	SER	2.1
1	A	160	THR	2.1
1	K	286	GLY	2.1
1	O	286	GLY	2.1
2	B	43	LYS	2.1
1	K	265	SER	2.1
1	O	162	PRO	2.1
2	L	102	MET	2.1
1	M	117	HIS	2.1
1	K	303	GLY	2.1
1	M	250	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	R	81	ASN	2.1
2	R	10	ILE	2.1
1	A	62	ARG	2.1
2	N	106	ARG	2.1
1	A	61	LEU	2.1
1	C	277	CYS	2.1
1	C	292	MET	2.1
2	B	166	ALA	2.1
1	K	158	ASN	2.1
1	K	274	TYR	2.1
2	F	40	SER	2.1
1	C	140	PRO	2.1
1	K	176	LEU	2.1
1	O	209	LEU	2.1
1	E	139	CYS	2.1
1	Q	268	MET	2.1
1	M	212	ARG	2.1
2	H	128	ASP	2.1
1	Q	98	TYR	2.1
2	L	107	THR	2.1
2	D	11	GLU	2.1
2	P	157	TYR	2.1
1	E	172	ASN	2.1
1	A	70	LEU	2.1
1	Q	213	LEU	2.1
1	A	125(A)	LYS	2.0
1	C	50	LYS	2.0
1	G	54	ASP	2.0
2	L	128	ASP	2.0
1	M	97	CYS	2.0
1	O	217	ILE	2.0
2	N	94	TYR	2.0
1	G	19(A)	ASN	2.0
2	B	15	GLN	2.0
2	N	135	ASN	2.0
1	M	71	LEU	2.0
2	D	127	ARG	2.0
2	J	98	LEU	2.0
1	M	82(A)	PRO	2.0
2	B	160	PRO	2.0
2	D	96	ALA	2.0
1	M	222	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	Q	90	LYS	2.0
1	O	38	HIS	2.0
1	Q	175	ASP	2.0
2	L	172	GLU	2.0
1	A	267	ILE	2.0
1	A	20	ASN	2.0
2	D	117	ASN	2.0
1	I	272	LEU	2.0
2	R	48	VAL	2.0
1	O	74	PRO	2.0
2	B	87	GLY	2.0
2	F	13	GLY	2.0
2	H	136	GLY	2.0
1	Q	264(A)	ASP	2.0
2	N	37	ASP	2.0
2	N	24	TYR	2.0
1	O	278	ASN	2.0
2	D	121	LYS	2.0
2	H	101	LEU	2.0
2	J	114	ASN	2.0
2	N	129	ASN	2.0
1	I	113	SER	2.0
1	M	247	SER	2.0
1	M	251	PHE	2.0
1	O	145	SER	2.0
1	O	323	SER	2.0
1	A	32	GLU	2.0
2	B	39	GLU	2.0
1	M	69	TRP	2.0
1	C	272	LEU	2.0
1	M	151	VAL	2.0
1	E	319	GLY	2.0
2	J	44	ALA	2.0
2	J	72	ASN	2.0
2	J	154	ASN	2.0
2	N	166	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	O	3	14/15	0.67	0.48	4.93	87,91,94,99	0
3	NAG	K	3	14/15	0.84	0.29	2.38	61,71,74,80	0
3	NAG	C	3	14/15	0.73	0.33	1.64	70,73,77,78	0
4	NAG	E	3	14/15	0.81	0.33	1.06	79,81,84,89	0
3	NAG	I	3	14/15	0.79	0.30	-0.27	64,72,76,79	0
4	BMA	E	5	11/12	0.46	0.47	-0.32	105,106,107,107	0
3	NAG	M	3	14/15	0.78	0.41	-0.52	82,85,87,89	0
4	NAG	G	3	14/15	0.85	0.22	-1.04	67,69,73,78	0
4	NAG	A	3	14/15	0.88	0.20	-2.12	57,64,69,75	0
4	NAG	G	4	14/15	0.64	0.37	-	82,85,88,91	0
3	NAG	I	1	14/15	0.64	0.42	-	90,97,100,103	0
3	NAG	K	1	14/15	0.62	0.44	-	90,97,100,106	0
4	BMA	G	5	11/12	0.53	0.59	-	94,96,97,97	0
4	BMA	A	5	11/12	0.31	0.56	-	96,100,101,102	0
3	NAG	I	4	14/15	0.70	0.44	-	82,85,88,88	0
3	NAG	G	2	14/15	0.62	0.46	-	103,106,107,108	0
3	NAG	C	4	14/15	0.75	0.54	-	80,82,86,86	0
3	NAG	K	4	14/15	0.74	0.49	-	82,84,85,87	0
3	NAG	O	4	14/15	0.46	0.52	-	104,106,111,112	0
3	NAG	A	2	14/15	0.63	0.56	-	97,100,103,104	0
3	NAG	C	1	14/15	0.77	0.43	-	85,91,92,94	0
3	NAG	K	2	14/15	0.46	0.44	-	109,112,114,115	0
3	NAG	O	1	14/15	0.60	0.40	-	99,104,107,113	0
3	NAG	I	2	14/15	0.62	0.69	-	107,108,109,110	0
3	NAG	M	4	14/15	0.51	0.33	-	92,93,94,94	0
3	NAG	C	2	14/15	0.70	0.51	-	94,95,97,97	0
3	NAG	G	1	14/15	0.80	0.35	-	87,91,94,100	0
3	NAG	M	1	14/15	0.73	0.50	-	92,98,102,105	0
4	NAG	A	4	14/15	0.69	0.41	-	80,84,88,92	0
3	NAG	M	2	14/15	0.58	0.63	-	109,110,110,110	0
4	NAG	E	4	14/15	0.61	0.40	-	94,97,100,103	0
3	NAG	O	2	14/15	0.07	0.68	-	115,117,118,118	0
3	NAG	A	1	14/15	0.70	0.48	-	87,93,97,98	0
3	NAG	E	1	14/15	0.71	0.36	-	87,91,96,102	0
3	NAG	E	2	14/15	0.28	0.49	-	108,111,113,113	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.