



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 11:49 AM BST

PDB ID : 3IT8
Title : Crystal structure of TNF alpha complexed with a poxvirus MHC-related TNF binding protein
Authors : Yang, Z.; West Jr., A.P.; Bjorkman, P.J.
Deposited on : 2009-08-27
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

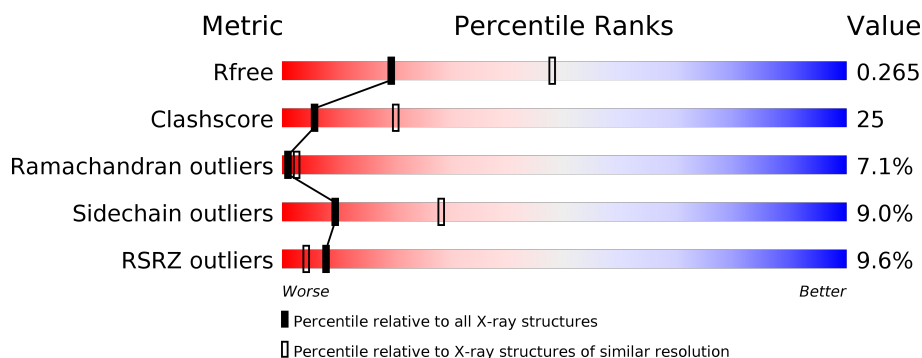
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	161	<div> <div>11%</div> <div> <div></div> <div>51%</div> <div>29%</div> <div>14%</div> <div>6%</div> </div> </div>
1	B	161	<div> <div>10%</div> <div> <div></div> <div>53%</div> <div>29%</div> <div>12%</div> <div>6%</div> </div> </div>
1	C	161	<div> <div>9%</div> <div> <div></div> <div>51%</div> <div>30%</div> <div>12%</div> <div>6%</div> </div> </div>
1	G	161	<div> <div>13%</div> <div> <div></div> <div>48%</div> <div>32%</div> <div>13%</div> <div>6%</div> </div> </div>
1	H	161	<div> <div>12%</div> <div> <div></div> <div>52%</div> <div>29%</div> <div>13%</div> <div>6%</div> </div> </div>
1	I	161	<div> <div>11%</div> <div> <div></div> <div>49%</div> <div>33%</div> <div>12%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	D	324	
2	E	324	
2	F	324	
2	J	324	
2	K	324	
2	L	324	

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	F	327	-	-	-	X
3	NAG	J	327	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22002 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 Tumor necrosis factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1190	760	207	221	2			
1	B	152	Total	C	N	O	S	0	0	0
			1190	760	207	221	2			
1	C	152	Total	C	N	O	S	0	0	0
			1190	760	207	221	2			
1	G	152	Total	C	N	O	S	0	0	0
			1190	760	207	221	2			
1	H	152	Total	C	N	O	S	0	0	0
			1190	760	207	221	2			
1	I	152	Total	C	N	O	S	0	0	0
			1190	760	207	221	2			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	expression tag	UNP P01375
A	-2	GLY	-	expression tag	UNP P01375
A	-1	SER	-	expression tag	UNP P01375
A	0	HIS	-	expression tag	UNP P01375
A	1	HIS	-	expression tag	UNP P01375
A	2	HIS	-	expression tag	UNP P01375
A	3	HIS	-	expression tag	UNP P01375
A	4	HIS	-	expression tag	UNP P01375
A	5	HIS	-	expression tag	UNP P01375
A	143	LEU	ASP	conflict	UNP P01375
B	-3	MET	-	expression tag	UNP P01375
B	-2	GLY	-	expression tag	UNP P01375
B	-1	SER	-	expression tag	UNP P01375
B	0	HIS	-	expression tag	UNP P01375
B	1	HIS	-	expression tag	UNP P01375
B	2	HIS	-	expression tag	UNP P01375
B	3	HIS	-	expression tag	UNP P01375

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	HIS	-	expression tag	UNP P01375
B	5	HIS	-	expression tag	UNP P01375
B	143	LEU	ASP	conflict	UNP P01375
C	-3	MET	-	expression tag	UNP P01375
C	-2	GLY	-	expression tag	UNP P01375
C	-1	SER	-	expression tag	UNP P01375
C	0	HIS	-	expression tag	UNP P01375
C	1	HIS	-	expression tag	UNP P01375
C	2	HIS	-	expression tag	UNP P01375
C	3	HIS	-	expression tag	UNP P01375
C	4	HIS	-	expression tag	UNP P01375
C	5	HIS	-	expression tag	UNP P01375
C	143	LEU	ASP	conflict	UNP P01375
G	-3	MET	-	expression tag	UNP P01375
G	-2	GLY	-	expression tag	UNP P01375
G	-1	SER	-	expression tag	UNP P01375
G	0	HIS	-	expression tag	UNP P01375
G	1	HIS	-	expression tag	UNP P01375
G	2	HIS	-	expression tag	UNP P01375
G	3	HIS	-	expression tag	UNP P01375
G	4	HIS	-	expression tag	UNP P01375
G	5	HIS	-	expression tag	UNP P01375
G	143	LEU	ASP	conflict	UNP P01375
H	-3	MET	-	expression tag	UNP P01375
H	-2	GLY	-	expression tag	UNP P01375
H	-1	SER	-	expression tag	UNP P01375
H	0	HIS	-	expression tag	UNP P01375
H	1	HIS	-	expression tag	UNP P01375
H	2	HIS	-	expression tag	UNP P01375
H	3	HIS	-	expression tag	UNP P01375
H	4	HIS	-	expression tag	UNP P01375
H	5	HIS	-	expression tag	UNP P01375
H	143	LEU	ASP	conflict	UNP P01375
I	-3	MET	-	expression tag	UNP P01375
I	-2	GLY	-	expression tag	UNP P01375
I	-1	SER	-	expression tag	UNP P01375
I	0	HIS	-	expression tag	UNP P01375
I	1	HIS	-	expression tag	UNP P01375
I	2	HIS	-	expression tag	UNP P01375
I	3	HIS	-	expression tag	UNP P01375
I	4	HIS	-	expression tag	UNP P01375
I	5	HIS	-	expression tag	UNP P01375

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Chain	Residue	Modelled	Actual	Comment	Reference
I	143	LEU	ASP	conflict	UNP P01375

- Molecule 2 is a protein called 2L protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	299	Total	C	N	O	S	0	0	0
			2419	1545	395	466	13			
2	E	299	Total	C	N	O	S	0	0	0
			2419	1545	395	466	13			
2	F	299	Total	C	N	O	S	0	0	0
			2419	1545	395	466	13			
2	J	299	Total	C	N	O	S	0	0	0
			2419	1545	395	466	13			
2	K	299	Total	C	N	O	S	0	0	0
			2419	1545	395	466	13			
2	L	299	Total	C	N	O	S	0	0	0
			2419	1545	395	466	13			

There are 48 discrepancies between the modelled and reference sequences:

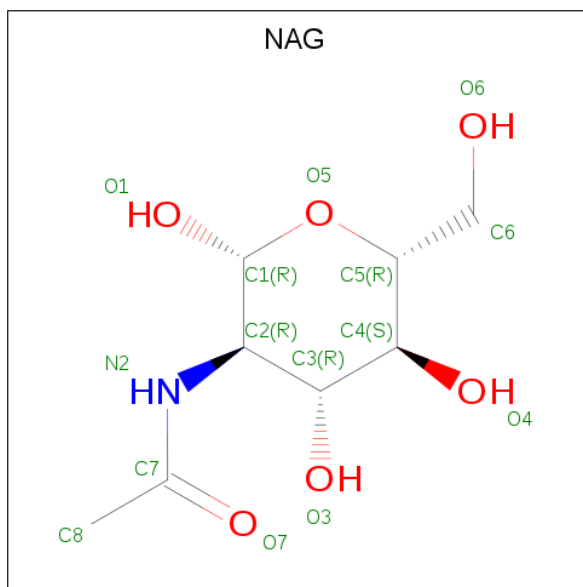
Chain	Residue	Modelled	Actual	Comment	Reference
D	317	GLY	-	expression tag	UNP Q9DHW0
D	318	SER	-	expression tag	UNP Q9DHW0
D	319	HIS	-	expression tag	UNP Q9DHW0
D	320	HIS	-	expression tag	UNP Q9DHW0
D	321	HIS	-	expression tag	UNP Q9DHW0
D	322	HIS	-	expression tag	UNP Q9DHW0
D	323	HIS	-	expression tag	UNP Q9DHW0
D	324	HIS	-	expression tag	UNP Q9DHW0
E	317	GLY	-	expression tag	UNP Q9DHW0
E	318	SER	-	expression tag	UNP Q9DHW0
E	319	HIS	-	expression tag	UNP Q9DHW0
E	320	HIS	-	expression tag	UNP Q9DHW0
E	321	HIS	-	expression tag	UNP Q9DHW0
E	322	HIS	-	expression tag	UNP Q9DHW0
E	323	HIS	-	expression tag	UNP Q9DHW0
E	324	HIS	-	expression tag	UNP Q9DHW0
F	317	GLY	-	expression tag	UNP Q9DHW0
F	318	SER	-	expression tag	UNP Q9DHW0
F	319	HIS	-	expression tag	UNP Q9DHW0
F	320	HIS	-	expression tag	UNP Q9DHW0
F	321	HIS	-	expression tag	UNP Q9DHW0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	322	HIS	-	expression tag	UNP Q9DHW0
F	323	HIS	-	expression tag	UNP Q9DHW0
F	324	HIS	-	expression tag	UNP Q9DHW0
J	317	GLY	-	expression tag	UNP Q9DHW0
J	318	SER	-	expression tag	UNP Q9DHW0
J	319	HIS	-	expression tag	UNP Q9DHW0
J	320	HIS	-	expression tag	UNP Q9DHW0
J	321	HIS	-	expression tag	UNP Q9DHW0
J	322	HIS	-	expression tag	UNP Q9DHW0
J	323	HIS	-	expression tag	UNP Q9DHW0
J	324	HIS	-	expression tag	UNP Q9DHW0
K	317	GLY	-	expression tag	UNP Q9DHW0
K	318	SER	-	expression tag	UNP Q9DHW0
K	319	HIS	-	expression tag	UNP Q9DHW0
K	320	HIS	-	expression tag	UNP Q9DHW0
K	321	HIS	-	expression tag	UNP Q9DHW0
K	322	HIS	-	expression tag	UNP Q9DHW0
K	323	HIS	-	expression tag	UNP Q9DHW0
K	324	HIS	-	expression tag	UNP Q9DHW0
L	317	GLY	-	expression tag	UNP Q9DHW0
L	318	SER	-	expression tag	UNP Q9DHW0
L	319	HIS	-	expression tag	UNP Q9DHW0
L	320	HIS	-	expression tag	UNP Q9DHW0
L	321	HIS	-	expression tag	UNP Q9DHW0
L	322	HIS	-	expression tag	UNP Q9DHW0
L	323	HIS	-	expression tag	UNP Q9DHW0
L	324	HIS	-	expression tag	UNP Q9DHW0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	J	1	Total	C	N	O	0	0
			14	8	1	5		
3	J	1	Total	C	N	O	0	0
			14	8	1	5		
3	J	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		
3	K	1	Total	C	N	O	0	0
			14	8	1	5		

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

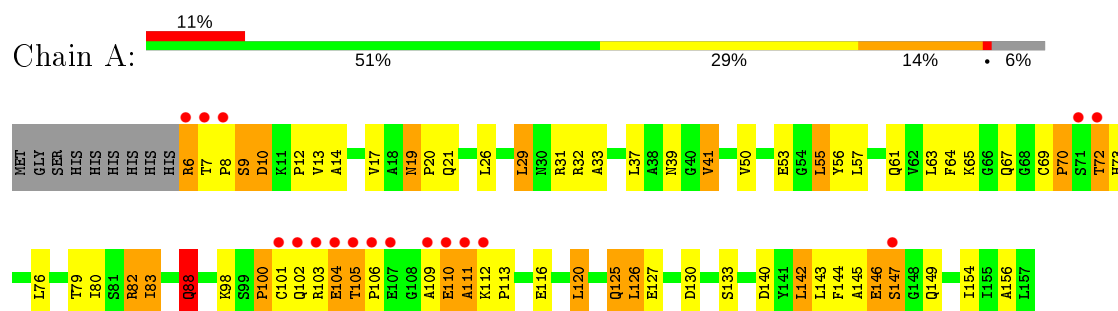
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	9	Total	O	0	0
			9	9		
4	C	10	Total	O	0	0
			10	10		
4	D	6	Total	O	0	0
			6	6		
4	E	7	Total	O	0	0
			7	7		
4	F	6	Total	O	0	0
			6	6		
4	G	10	Total	O	0	0
			10	10		
4	H	9	Total	O	0	0
			9	9		
4	I	11	Total	O	0	0
			11	11		
4	J	6	Total	O	0	0
			6	6		
4	K	6	Total	O	0	0
			6	6		
4	L	6	Total	O	0	0
			6	6		

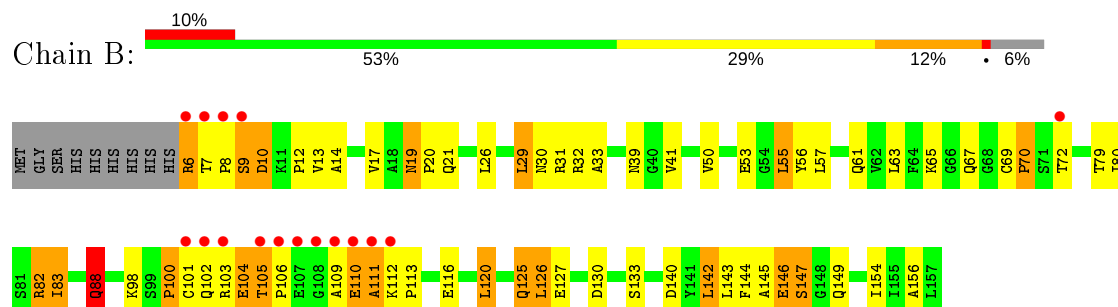
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

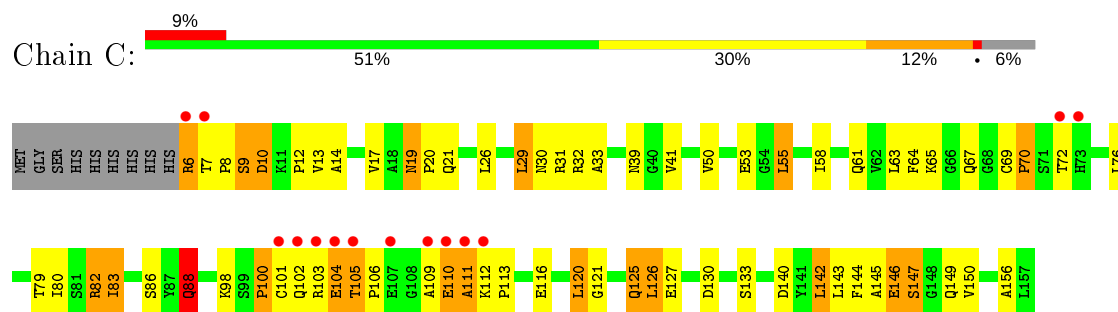
- Molecule 1: Tumor necrosis factor



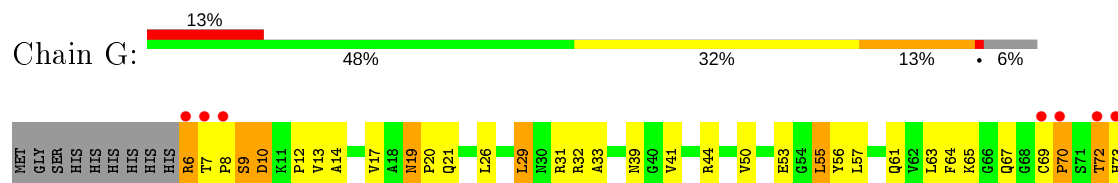
- Molecule 1: Tumor necrosis factor

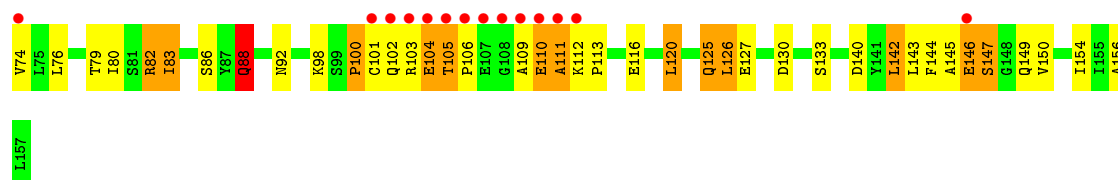


- Molecule 1: Tumor necrosis factor

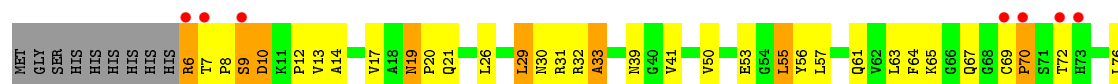


- Molecule 1: Tumor necrosis factor

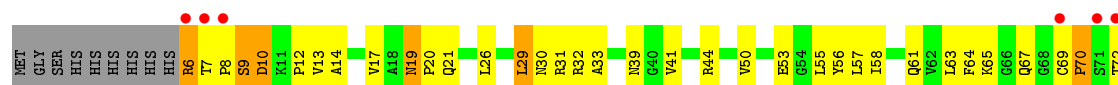




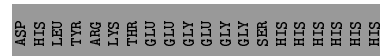
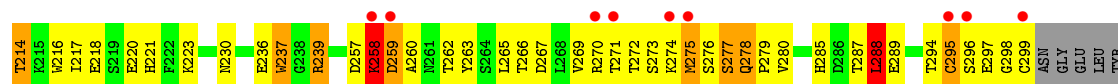
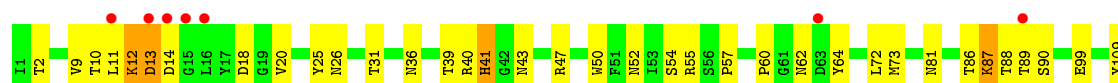
• Molecule 1: Tumor necrosis factor



• Molecule 1: Tumor necrosis factor

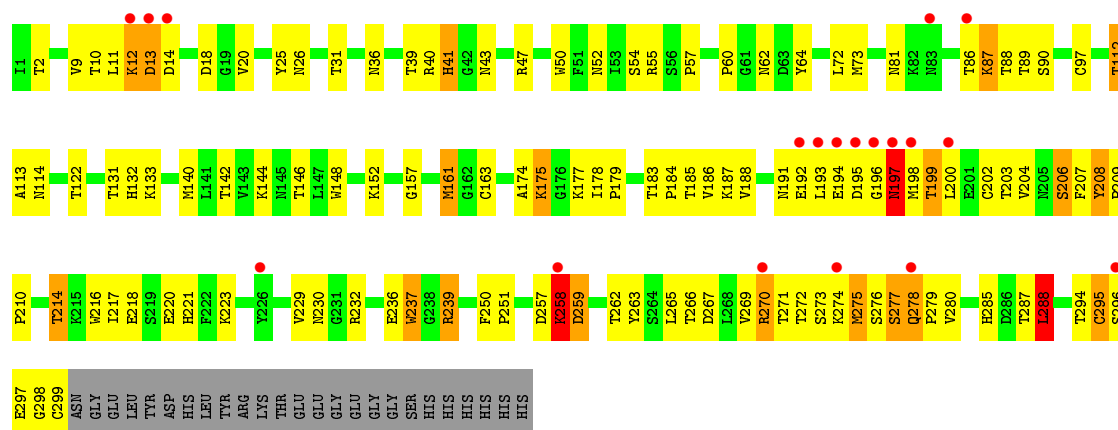


• Molecule 2: 2L protein

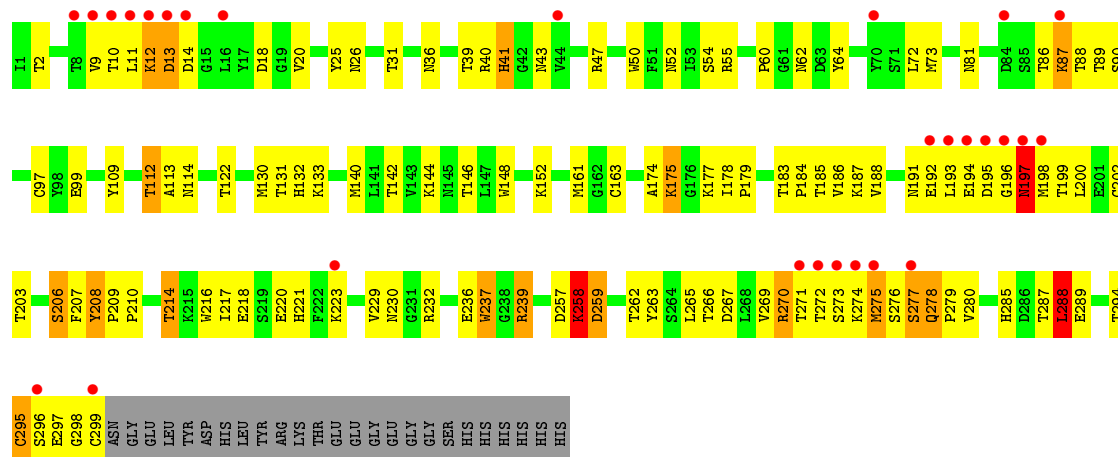


• Molecule 2: 2L protein

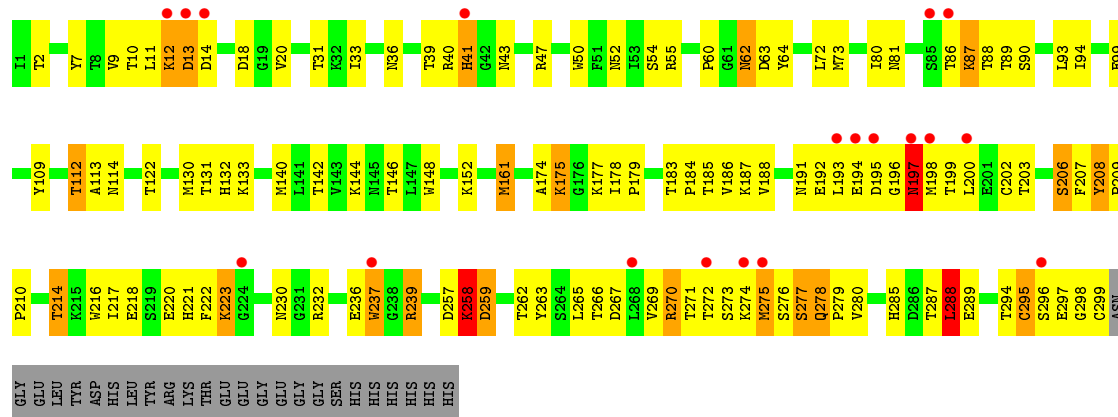




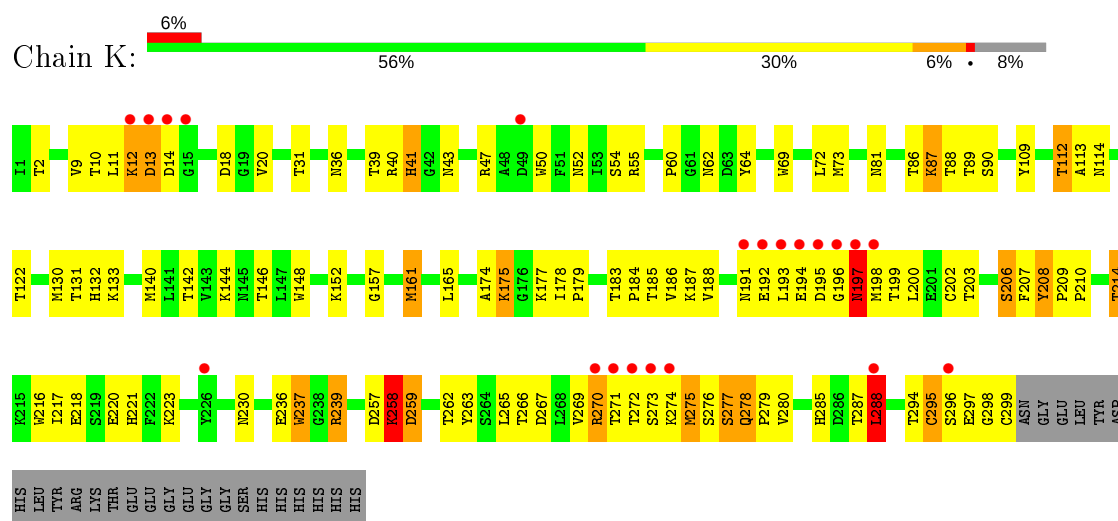
• Molecule 2: 2L protein



• Molecule 2: 2L protein



• Molecule 2: 2L protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.66Å 170.29Å 122.00Å 90.00° 92.04° 90.00°	Depositor
Resolution (Å)	38.77 – 2.80 45.07 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (38.77-2.80) 96.9 (45.07-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.266 0.239 , 0.265	Depositor DCC
R_{free} test set	5139 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.795	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22002	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.93% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	0/1217	0.68	0/1656
1	B	0.39	0/1217	0.69	0/1656
1	C	0.39	0/1217	0.68	0/1656
1	G	0.39	0/1217	0.69	0/1656
1	H	0.37	0/1217	0.68	0/1656
1	I	0.38	0/1217	0.68	0/1656
2	D	0.43	0/2487	0.69	2/3374 (0.1%)
2	E	0.41	0/2487	0.68	2/3374 (0.1%)
2	F	0.38	0/2487	0.68	2/3374 (0.1%)
2	J	0.43	0/2487	0.68	2/3374 (0.1%)
2	K	0.42	0/2487	0.68	2/3374 (0.1%)
2	L	0.36	0/2487	0.67	2/3374 (0.1%)
All	All	0.40	0/22224	0.68	12/30180 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	288	LEU	CA-CB-CG	9.00	136.00	115.30
2	J	288	LEU	CA-CB-CG	8.99	135.97	115.30
2	E	288	LEU	CA-CB-CG	8.95	135.88	115.30
2	D	288	LEU	CA-CB-CG	8.91	135.80	115.30
2	L	288	LEU	CA-CB-CG	8.75	135.43	115.30
2	F	288	LEU	CA-CB-CG	8.56	134.98	115.30
2	L	236	GLU	N-CA-C	5.86	126.82	111.00
2	J	236	GLU	N-CA-C	5.86	126.82	111.00
2	D	236	GLU	N-CA-C	5.83	126.73	111.00
2	F	236	GLU	N-CA-C	5.82	126.72	111.00
2	K	236	GLU	N-CA-C	5.81	126.69	111.00
2	E	236	GLU	N-CA-C	5.76	126.56	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1190	0	1192	76	0
1	B	1190	0	1192	71	0
1	C	1190	0	1192	73	0
1	G	1190	0	1192	84	0
1	H	1190	0	1192	74	0
1	I	1190	0	1192	78	0
2	D	2419	0	2309	103	1
2	E	2419	0	2309	115	0
2	F	2419	0	2308	113	0
2	J	2419	0	2308	118	1
2	K	2419	0	2309	113	0
2	L	2419	0	2308	116	0
3	D	42	0	39	3	0
3	E	42	0	39	4	0
3	F	42	0	39	5	0
3	J	42	0	39	3	0
3	K	42	0	39	4	0
3	L	42	0	39	6	0
4	A	10	0	0	0	0
4	B	9	0	0	0	0
4	C	10	0	0	0	0
4	D	6	0	0	0	0
4	E	7	0	0	0	0
4	F	6	0	0	0	0
4	G	10	0	0	0	0
4	H	9	0	0	0	0
4	I	11	0	0	0	0
4	J	6	0	0	0	0
4	K	6	0	0	0	0
4	L	6	0	0	0	0
All	All	22002	0	21237	1094	1

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 25.

All (1094) 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)
2:L:50:TRP:HB3	2:L:177:LYS:HD2	1.30	1.09
2:J:50:TRP:HB3	2:J:177:LYS:HD2	1.32	1.08
2:K:50:TRP:HB3	2:K:177:LYS:HD2	1.32	1.07
2:F:50:TRP:HB3	2:F:177:LYS:HD2	1.31	1.07
2:L:112:THR:HG22	2:L:114:ASN:H	1.18	1.07
2:E:50:TRP:HB3	2:E:177:LYS:HD2	1.32	1.06
2:E:112:THR:HG22	2:E:114:ASN:H	1.19	1.05
2:F:112:THR:HG22	2:F:114:ASN:H	1.17	1.05
2:D:50:TRP:HB3	2:D:177:LYS:HD2	1.34	1.04
1:G:44:ARG:NH1	2:J:232:ARG:HH22	1.56	1.03
2:J:112:THR:HG22	2:J:114:ASN:H	1.19	1.03
2:K:112:THR:HG22	2:K:114:ASN:H	1.22	1.02
2:D:112:THR:HG22	2:D:114:ASN:H	1.19	1.02
2:E:148:TRP:HE1	2:E:152:LYS:HE3	1.31	0.94
2:J:148:TRP:HE1	2:J:152:LYS:HE3	1.35	0.92
2:F:148:TRP:HE1	2:F:152:LYS:HE3	1.34	0.91
2:K:148:TRP:HE1	2:K:152:LYS:HE3	1.35	0.91
1:G:112:LYS:HE2	1:I:103:ARG:HH21	1.35	0.90
2:L:148:TRP:HE1	2:L:152:LYS:HE3	1.36	0.89
2:D:148:TRP:HE1	2:D:152:LYS:HE3	1.37	0.89
2:D:148:TRP:NE1	2:D:152:LYS:HE3	1.89	0.88
2:E:148:TRP:NE1	2:E:152:LYS:HE3	1.87	0.87
2:J:148:TRP:NE1	2:J:152:LYS:HE3	1.89	0.87
2:F:148:TRP:NE1	2:F:152:LYS:HE3	1.90	0.87
1:G:44:ARG:HH12	2:J:232:ARG:HH22	1.19	0.86
2:K:148:TRP:NE1	2:K:152:LYS:HE3	1.90	0.86
2:L:148:TRP:NE1	2:L:152:LYS:HE3	1.91	0.85
2:L:112:THR:CG2	2:L:114:ASN:H	1.92	0.82
2:J:112:THR:CG2	2:J:114:ASN:H	1.91	0.82
2:F:112:THR:HG22	2:F:114:ASN:N	1.95	0.82
2:F:112:THR:CG2	2:F:114:ASN:H	1.93	0.82
1:I:69:CYS:HB2	1:I:106:PRO:HD3	1.63	0.81
2:J:112:THR:HG22	2:J:114:ASN:N	1.96	0.81
2:D:88:THR:HG21	2:D:112:THR:HG23	1.63	0.81
1:G:44:ARG:NH1	2:J:232:ARG:NH2	2.28	0.81
2:D:112:THR:HG22	2:D:114:ASN:N	1.96	0.81
2:E:112:THR:CG2	2:E:114:ASN:H	1.93	0.81
2:L:112:THR:HG22	2:L:114:ASN:N	1.95	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:69:CYS:HB2	1:H:106:PRO:HD3	1.63	0.80
1:B:69:CYS:HB2	1:B:106:PRO:HD3	1.64	0.80
1:G:88:GLN:HE21	1:G:88:GLN:H	1.29	0.80
1:G:88:GLN:HE21	1:G:88:GLN:N	1.81	0.79
2:F:88:THR:HG21	2:F:112:THR:HG23	1.63	0.79
2:J:239:ARG:HB3	2:J:239:ARG:HH11	1.48	0.79
2:J:10:THR:HG23	2:J:90:SER:HB3	1.63	0.79
2:F:239:ARG:HB3	2:F:239:ARG:HH11	1.48	0.79
2:E:88:THR:HG21	2:E:112:THR:HG23	1.65	0.79
1:A:69:CYS:HB2	1:A:106:PRO:HD3	1.63	0.79
2:F:10:THR:HG23	2:F:90:SER:HB3	1.64	0.79
1:B:112:LYS:HE2	1:C:103:ARG:HH21	1.48	0.78
2:L:88:THR:HG21	2:L:112:THR:HG23	1.65	0.78
2:K:10:THR:HG23	2:K:90:SER:HB3	1.65	0.78
1:G:69:CYS:HB2	1:G:106:PRO:HD3	1.65	0.78
1:C:88:GLN:HE21	1:C:88:GLN:H	1.32	0.78
2:D:112:THR:CG2	2:D:114:ASN:H	1.94	0.78
2:K:112:THR:HG22	2:K:114:ASN:N	1.98	0.78
1:C:69:CYS:HB2	1:C:106:PRO:HD3	1.65	0.78
2:K:112:THR:CG2	2:K:114:ASN:H	1.95	0.78
2:K:88:THR:HG21	2:K:112:THR:HG23	1.65	0.77
1:A:88:GLN:HE21	1:A:88:GLN:H	1.32	0.77
1:B:88:GLN:HE21	1:B:88:GLN:H	1.32	0.77
2:E:112:THR:HG22	2:E:114:ASN:N	1.96	0.77
2:E:239:ARG:HB3	2:E:239:ARG:HH11	1.49	0.77
2:D:10:THR:HG23	2:D:90:SER:HB3	1.64	0.77
1:H:88:GLN:H	1:H:88:GLN:HE21	1.31	0.77
1:I:88:GLN:HE21	1:I:88:GLN:N	1.82	0.77
2:L:10:THR:HG23	2:L:90:SER:HB3	1.65	0.77
2:F:184:PRO:HB3	2:F:207:PHE:HB3	1.67	0.77
1:B:88:GLN:HE21	1:B:88:GLN:N	1.83	0.76
1:C:88:GLN:HE21	1:C:88:GLN:N	1.84	0.76
1:A:70:PRO:O	1:A:105:THR:HG22	1.86	0.76
2:D:239:ARG:HB3	2:D:239:ARG:HH11	1.51	0.76
1:H:70:PRO:O	1:H:105:THR:HG22	1.86	0.76
2:K:239:ARG:HB3	2:K:239:ARG:HH11	1.51	0.76
1:I:88:GLN:HE21	1:I:88:GLN:H	1.32	0.75
2:L:239:ARG:HB3	2:L:239:ARG:HH11	1.51	0.75
2:F:192:GLU:HG2	2:F:198:MET:HA	1.66	0.75
2:J:88:THR:HG21	2:J:112:THR:HG23	1.67	0.75
2:E:10:THR:HG23	2:E:90:SER:HB3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:88:GLN:HE21	1:H:88:GLN:N	1.84	0.75
2:J:296:SER:C	2:J:298:GLY:H	1.89	0.75
1:H:65:LYS:HD2	1:H:143:LEU:HD22	1.68	0.74
1:A:88:GLN:N	1:A:88:GLN:HE21	1.85	0.74
2:D:184:PRO:HB3	2:D:207:PHE:HB3	1.69	0.74
1:B:70:PRO:O	1:B:105:THR:HG22	1.87	0.74
2:J:192:GLU:HG2	2:J:198:MET:HA	1.69	0.74
3:E:326:NAG:H3	3:E:326:NAG:H83	1.69	0.74
1:H:125:GLN:NE2	1:I:8:PRO:HA	2.03	0.74
1:I:65:LYS:HD2	1:I:143:LEU:HD22	1.70	0.74
1:G:65:LYS:HD2	1:G:143:LEU:HD22	1.70	0.74
2:L:192:GLU:HG2	2:L:198:MET:HA	1.69	0.74
1:C:65:LYS:HD2	1:C:143:LEU:HD22	1.68	0.74
2:E:192:GLU:HG2	2:E:198:MET:HA	1.68	0.74
2:K:188:VAL:O	2:K:299:CYS:SG	2.45	0.74
1:C:70:PRO:O	1:C:105:THR:HG22	1.88	0.74
1:I:70:PRO:O	1:I:105:THR:HG22	1.87	0.74
2:J:184:PRO:HB3	2:J:207:PHE:HB3	1.70	0.73
1:B:65:LYS:HD2	1:B:143:LEU:HD22	1.70	0.73
2:D:257:ASP:OD1	2:D:262:THR:HG23	1.88	0.73
2:J:188:VAL:O	2:J:299:CYS:SG	2.47	0.73
1:G:70:PRO:O	1:G:105:THR:HG22	1.88	0.73
2:E:296:SER:C	2:E:298:GLY:H	1.91	0.73
1:I:50:VAL:HG21	1:I:126:LEU:HD23	1.71	0.73
2:L:188:VAL:O	2:L:299:CYS:SG	2.47	0.73
1:H:19:ASN:CA	1:H:29:LEU:HD11	2.19	0.73
2:J:280:VAL:HG23	2:J:294:THR:HG22	1.70	0.73
2:J:73:MET:HG2	2:J:140:MET:CE	2.19	0.72
2:F:296:SER:C	2:F:298:GLY:H	1.91	0.72
2:L:184:PRO:HB3	2:L:207:PHE:HB3	1.71	0.72
2:K:55:ARG:HD3	3:K:326:NAG:H82	1.70	0.72
1:A:65:LYS:HD2	1:A:143:LEU:HD22	1.71	0.72
2:L:73:MET:HG2	2:L:140:MET:CE	2.20	0.72
2:E:184:PRO:HB3	2:E:207:PHE:HB3	1.72	0.72
2:K:192:GLU:HG2	2:K:198:MET:HA	1.70	0.72
1:G:112:LYS:HE2	1:I:103:ARG:NH2	2.04	0.72
2:K:296:SER:C	2:K:298:GLY:H	1.91	0.72
2:E:257:ASP:OD1	2:E:262:THR:HG23	1.90	0.72
2:L:257:ASP:OD1	2:L:262:THR:HG23	1.89	0.72
1:A:19:ASN:CA	1:A:29:LEU:HD11	2.20	0.72
2:L:131:THR:HG22	2:L:133:LYS:H	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:73:MET:HG2	2:E:140:MET:CE	2.20	0.71
2:D:296:SER:C	2:D:298:GLY:H	1.92	0.71
2:E:188:VAL:O	2:E:299:CYS:SG	2.48	0.71
2:L:296:SER:C	2:L:298:GLY:H	1.91	0.71
2:K:257:ASP:OD1	2:K:262:THR:HG23	1.91	0.71
2:F:188:VAL:O	2:F:299:CYS:SG	2.49	0.71
2:K:200:LEU:HD21	2:K:296:SER:OG	1.90	0.71
2:D:188:VAL:O	2:D:299:CYS:SG	2.48	0.71
2:F:257:ASP:OD1	2:F:262:THR:HG23	1.91	0.71
2:F:73:MET:HG2	2:F:140:MET:CE	2.21	0.71
2:J:131:THR:HG22	2:J:133:LYS:H	1.56	0.71
2:E:73:MET:HG2	2:E:140:MET:HE2	1.73	0.71
1:G:100:PRO:HG2	1:G:101:CYS:H	1.56	0.71
2:D:192:GLU:HG2	2:D:198:MET:HA	1.71	0.70
2:L:200:LEU:HD21	2:L:296:SER:OG	1.91	0.70
1:G:19:ASN:CA	1:G:29:LEU:HD11	2.22	0.70
2:K:131:THR:HG22	2:K:133:LYS:H	1.56	0.70
2:E:200:LEU:HD21	2:E:296:SER:OG	1.91	0.70
1:B:19:ASN:CA	1:B:29:LEU:HD11	2.22	0.70
2:F:200:LEU:HD21	2:F:296:SER:OG	1.91	0.70
2:F:131:THR:HG22	2:F:133:LYS:H	1.56	0.70
2:F:191:ASN:O	2:F:192:GLU:HG3	1.92	0.69
1:B:8:PRO:O	1:B:9:SER:HB3	1.93	0.69
2:E:131:THR:HG22	2:E:133:LYS:H	1.56	0.69
1:G:8:PRO:O	1:G:9:SER:HB3	1.92	0.69
2:L:237:TRP:CE3	2:L:237:TRP:HA	2.27	0.69
2:D:200:LEU:HD21	2:D:296:SER:OG	1.92	0.69
2:J:200:LEU:HD21	2:J:296:SER:OG	1.92	0.69
2:D:237:TRP:HE3	2:D:237:TRP:HA	1.57	0.69
1:H:8:PRO:O	1:H:9:SER:HB3	1.93	0.69
2:J:237:TRP:HE3	2:J:237:TRP:HA	1.58	0.69
1:A:125:GLN:NE2	1:C:8:PRO:HA	2.07	0.69
2:D:131:THR:HG22	2:D:133:LYS:H	1.58	0.69
2:K:208:TYR:O	2:K:209:PRO:C	2.31	0.69
2:D:237:TRP:CE3	2:D:237:TRP:HA	2.27	0.69
2:D:73:MET:HG2	2:D:140:MET:CE	2.23	0.69
2:F:237:TRP:HA	2:F:237:TRP:HE3	1.58	0.69
2:K:184:PRO:HB3	2:K:207:PHE:HB3	1.73	0.69
1:B:50:VAL:HG21	1:B:126:LEU:HD23	1.72	0.69
2:E:237:TRP:CE3	2:E:237:TRP:HA	2.28	0.68
1:I:100:PRO:HG2	1:I:101:CYS:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:19:ASN:CA	1:I:29:LEU:HD11	2.22	0.68
2:K:237:TRP:HA	2:K:237:TRP:HE3	1.59	0.68
1:C:8:PRO:O	1:C:9:SER:HB3	1.92	0.68
2:F:237:TRP:CE3	2:F:237:TRP:HA	2.28	0.68
3:F:326:NAG:H83	3:F:326:NAG:H3	1.76	0.68
1:G:112:LYS:HE3	1:I:103:ARG:HD3	1.74	0.68
1:I:8:PRO:O	1:I:9:SER:HB3	1.92	0.68
1:C:19:ASN:CA	1:C:29:LEU:HD11	2.23	0.68
1:G:86:SER:O	2:K:157:GLY:HA2	1.92	0.68
1:C:50:VAL:HG21	1:C:126:LEU:HD23	1.75	0.68
2:D:191:ASN:O	2:D:192:GLU:HG3	1.94	0.68
2:D:73:MET:HG2	2:D:140:MET:HE2	1.74	0.68
1:G:50:VAL:HG21	1:G:126:LEU:HD23	1.76	0.68
2:L:209:PRO:HG2	2:L:285:HIS:CE1	2.28	0.68
2:L:31:THR:OG1	2:L:47:ARG:NH1	2.27	0.68
2:J:237:TRP:HA	2:J:237:TRP:CE3	2.27	0.68
1:A:100:PRO:HG2	1:A:101:CYS:H	1.58	0.68
2:J:257:ASP:OD1	2:J:262:THR:HG23	1.94	0.68
1:A:8:PRO:O	1:A:9:SER:HB3	1.93	0.67
2:F:280:VAL:HG23	2:F:294:THR:HG22	1.76	0.67
2:K:280:VAL:HG23	2:K:294:THR:HG22	1.76	0.67
2:F:218:GLU:HB3	2:F:277:SER:HB2	1.75	0.67
1:B:100:PRO:HG2	1:B:101:CYS:H	1.59	0.67
2:K:191:ASN:O	2:K:192:GLU:HG3	1.94	0.67
2:F:209:PRO:HG2	2:F:285:HIS:CE1	2.28	0.67
2:K:237:TRP:HA	2:K:237:TRP:CE3	2.28	0.67
1:C:100:PRO:HG2	1:C:101:CYS:H	1.58	0.67
1:B:109:ALA:O	1:B:110:GLU:HB2	1.95	0.66
2:D:31:THR:OG1	2:D:47:ARG:NH1	2.28	0.66
2:K:73:MET:HG2	2:K:140:MET:CE	2.25	0.66
2:E:218:GLU:HB3	2:E:277:SER:HB2	1.76	0.66
2:E:209:PRO:HG2	2:E:285:HIS:CE1	2.30	0.66
2:J:94:ILE:CD1	3:J:325:NAG:H82	2.26	0.66
2:L:237:TRP:HE3	2:L:237:TRP:HA	1.57	0.66
2:E:237:TRP:HE3	2:E:237:TRP:HA	1.59	0.66
1:A:50:VAL:HG21	1:A:126:LEU:HD23	1.76	0.66
2:J:218:GLU:HB3	2:J:277:SER:HB2	1.77	0.66
2:L:191:ASN:O	2:L:192:GLU:HG3	1.95	0.66
2:J:31:THR:OG1	2:J:47:ARG:NH1	2.28	0.66
2:D:208:TYR:O	2:D:209:PRO:C	2.34	0.66
1:I:109:ALA:O	1:I:110:GLU:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ALA:O	1:A:110:GLU:HB2	1.96	0.66
1:C:109:ALA:O	1:C:110:GLU:HB2	1.96	0.66
1:I:9:SER:O	1:I:10:ASP:CB	2.44	0.66
2:L:218:GLU:HB3	2:L:277:SER:HB2	1.77	0.66
1:H:9:SER:O	1:H:10:ASP:CB	2.43	0.66
1:H:17:VAL:O	1:H:29:LEU:HD12	1.96	0.66
2:D:209:PRO:HG2	2:D:285:HIS:CE1	2.31	0.65
2:J:206:SER:HA	2:J:263:TYR:O	1.96	0.65
2:K:209:PRO:HG2	2:K:285:HIS:CE1	2.30	0.65
2:F:208:TYR:O	2:F:209:PRO:C	2.32	0.65
1:G:109:ALA:O	1:G:110:GLU:HB2	1.96	0.65
2:E:280:VAL:HG23	2:E:294:THR:HG22	1.77	0.65
1:H:109:ALA:O	1:H:110:GLU:HB2	1.96	0.65
1:C:9:SER:O	1:C:10:ASP:CB	2.44	0.65
2:K:218:GLU:HB3	2:K:277:SER:HB2	1.78	0.65
2:L:73:MET:HG2	2:L:140:MET:HE2	1.78	0.65
1:A:103:ARG:HH21	1:C:112:LYS:HE2	1.60	0.65
2:D:218:GLU:HB3	2:D:277:SER:HB2	1.78	0.65
1:A:9:SER:O	1:A:10:ASP:CB	2.44	0.65
1:G:9:SER:O	1:G:10:ASP:CB	2.44	0.65
2:F:31:THR:OG1	2:F:47:ARG:NH1	2.30	0.64
2:J:191:ASN:O	2:J:192:GLU:HG3	1.96	0.64
2:K:287:THR:O	2:K:288:LEU:HD13	1.98	0.64
2:E:31:THR:OG1	2:E:47:ARG:NH1	2.30	0.64
1:H:50:VAL:HG21	1:H:126:LEU:HD23	1.77	0.64
1:H:100:PRO:HG2	1:H:101:CYS:H	1.60	0.64
2:L:206:SER:HA	2:L:263:TYR:O	1.97	0.64
1:B:9:SER:O	1:B:10:ASP:CB	2.44	0.64
2:E:208:TYR:O	2:E:209:PRO:C	2.32	0.64
2:F:206:SER:HA	2:F:263:TYR:O	1.98	0.64
3:L:327:NAG:O3	3:L:327:NAG:H83	1.98	0.64
1:A:17:VAL:O	1:A:29:LEU:HD12	1.98	0.64
1:B:98:LYS:HD3	1:B:116:GLU:HG3	1.79	0.64
2:J:209:PRO:HG2	2:J:285:HIS:CE1	2.33	0.64
2:L:208:TYR:O	2:L:209:PRO:C	2.33	0.64
1:B:17:VAL:O	1:B:29:LEU:HD12	1.98	0.63
2:E:55:ARG:HD3	3:E:326:NAG:H82	1.79	0.63
2:L:280:VAL:HG23	2:L:294:THR:HG22	1.80	0.63
1:G:12:PRO:HG2	1:G:156:ALA:HB2	1.79	0.63
1:C:17:VAL:O	1:C:29:LEU:HD12	1.98	0.63
1:A:19:ASN:ND2	1:A:21:GLN:H	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:191:ASN:O	2:E:192:GLU:HG3	1.98	0.63
1:A:98:LYS:HD3	1:A:116:GLU:HG3	1.80	0.63
1:B:12:PRO:HG2	1:B:156:ALA:HB2	1.79	0.63
1:G:98:LYS:HD3	1:G:116:GLU:HG3	1.81	0.63
1:H:9:SER:O	1:H:10:ASP:HB3	1.99	0.63
2:J:73:MET:HG2	2:J:140:MET:HE2	1.80	0.63
2:K:206:SER:HA	2:K:263:TYR:O	1.98	0.63
2:D:280:VAL:HG23	2:D:294:THR:HG22	1.79	0.63
2:J:208:TYR:O	2:J:209:PRO:C	2.31	0.62
1:C:98:LYS:HD3	1:C:116:GLU:HG3	1.80	0.62
1:H:83:ILE:HG13	1:H:83:ILE:O	1.98	0.62
1:B:8:PRO:HA	1:C:125:GLN:NE2	2.14	0.62
2:K:31:THR:OG1	2:K:47:ARG:NH1	2.33	0.62
2:D:206:SER:HA	2:D:263:TYR:O	2.00	0.62
1:H:98:LYS:HD3	1:H:116:GLU:HG3	1.81	0.62
1:H:12:PRO:HG2	1:H:156:ALA:HB2	1.81	0.62
1:G:8:PRO:HA	1:I:125:GLN:NE2	2.15	0.62
1:I:9:SER:O	1:I:10:ASP:HB3	2.00	0.62
1:A:112:LYS:HE2	1:B:103:ARG:HH21	1.65	0.61
1:G:83:ILE:O	1:G:83:ILE:HG13	2.00	0.61
1:B:143:LEU:HD11	1:B:145:ALA:HB3	1.83	0.61
1:G:17:VAL:O	1:G:29:LEU:HD12	1.99	0.61
1:A:83:ILE:O	1:A:83:ILE:HG13	1.99	0.61
2:F:73:MET:HG2	2:F:140:MET:HE1	1.83	0.61
1:I:17:VAL:O	1:I:29:LEU:HD12	2.00	0.61
1:G:19:ASN:ND2	1:G:21:GLN:H	1.99	0.60
1:I:143:LEU:HD11	1:I:145:ALA:HB3	1.83	0.60
2:D:217:ILE:O	2:D:280:VAL:HG12	2.01	0.60
1:I:98:LYS:HD3	1:I:116:GLU:HG3	1.84	0.60
2:K:73:MET:HG2	2:K:140:MET:HE1	1.84	0.60
1:A:9:SER:O	1:A:10:ASP:HB3	2.00	0.60
2:E:206:SER:HA	2:E:263:TYR:O	2.00	0.60
1:C:143:LEU:HD11	1:C:145:ALA:HB3	1.84	0.60
1:B:19:ASN:ND2	1:B:21:GLN:H	1.98	0.60
1:C:9:SER:O	1:C:10:ASP:HB3	2.01	0.60
1:B:9:SER:O	1:B:10:ASP:HB3	2.00	0.60
1:C:83:ILE:HG13	1:C:83:ILE:O	2.02	0.60
1:C:31:ARG:HD2	2:F:99:GLU:HG2	1.83	0.60
1:H:19:ASN:ND2	1:H:21:GLN:H	1.99	0.60
2:D:88:THR:CG2	2:D:112:THR:HG23	2.31	0.60
2:E:217:ILE:O	2:E:280:VAL:HG12	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:73:MET:HG2	2:J:140:MET:HE1	1.82	0.60
2:D:287:THR:O	2:D:288:LEU:HD13	2.01	0.60
1:B:83:ILE:HG13	1:B:83:ILE:O	2.02	0.59
1:C:19:ASN:ND2	1:C:21:GLN:H	1.99	0.59
2:L:287:THR:O	2:L:288:LEU:HD13	2.01	0.59
2:F:73:MET:HG2	2:F:140:MET:HE2	1.83	0.59
2:J:272:THR:HG21	2:J:274:LYS:HE3	1.85	0.59
2:L:275:MET:SD	2:L:279:PRO:HD3	2.42	0.59
2:D:275:MET:SD	2:D:279:PRO:HD3	2.42	0.59
2:D:55:ARG:HD3	3:D:326:NAG:H82	1.85	0.59
2:L:55:ARG:CG	3:L:326:NAG:H82	2.33	0.59
1:H:55:LEU:HD21	1:I:13:VAL:HG11	1.84	0.59
2:J:208:TYR:O	2:J:210:PRO:N	2.36	0.59
2:D:192:GLU:HG2	2:D:197:ASN:O	2.03	0.59
2:K:55:ARG:CD	3:K:326:NAG:H82	2.33	0.59
2:F:88:THR:CG2	2:F:112:THR:HG23	2.31	0.59
2:F:275:MET:SD	2:F:279:PRO:HD3	2.43	0.59
2:K:217:ILE:O	2:K:280:VAL:HG12	2.02	0.59
2:L:88:THR:CG2	2:L:112:THR:HG23	2.33	0.59
1:G:9:SER:O	1:G:10:ASP:HB3	2.01	0.59
2:J:287:THR:O	2:J:288:LEU:HD13	2.03	0.59
1:G:143:LEU:HD11	1:G:145:ALA:HB3	1.83	0.58
2:F:208:TYR:O	2:F:210:PRO:N	2.36	0.58
2:F:287:THR:O	2:F:288:LEU:HD13	2.03	0.58
2:L:217:ILE:O	2:L:280:VAL:HG12	2.02	0.58
1:I:12:PRO:HG2	1:I:156:ALA:HB2	1.85	0.58
1:B:112:LYS:HE3	1:C:103:ARG:HD3	1.84	0.58
2:E:208:TYR:O	2:E:210:PRO:N	2.37	0.58
1:H:143:LEU:HD11	1:H:145:ALA:HB3	1.85	0.58
1:B:112:LYS:HE2	1:C:103:ARG:NH2	2.15	0.58
2:D:272:THR:HG21	2:D:274:LYS:HE3	1.85	0.58
2:J:257:ASP:HB2	2:J:258:LYS:HD3	1.86	0.58
2:K:192:GLU:HG2	2:K:197:ASN:O	2.03	0.58
1:B:102:GLN:HB2	1:B:104:GLU:OE1	2.04	0.58
2:E:192:GLU:HG2	2:E:197:ASN:O	2.03	0.58
2:E:272:THR:HG21	2:E:274:LYS:HE3	1.86	0.58
1:A:143:LEU:HD11	1:A:145:ALA:HB3	1.84	0.58
2:J:192:GLU:HG2	2:J:197:ASN:O	2.03	0.58
2:L:192:GLU:HG2	2:L:197:ASN:O	2.03	0.58
1:A:19:ASN:HA	1:A:29:LEU:HD11	1.86	0.58
1:A:110:GLU:O	1:A:111:ALA:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:19:ASN:HA	1:H:29:LEU:HD11	1.85	0.57
2:J:275:MET:SD	2:J:279:PRO:HD3	2.44	0.57
2:K:272:THR:HG21	2:K:274:LYS:HE3	1.85	0.57
2:E:275:MET:SD	2:E:279:PRO:HD3	2.44	0.57
2:F:272:THR:HG21	2:F:274:LYS:HE3	1.86	0.57
1:I:102:GLN:HB2	1:I:104:GLU:OE1	2.04	0.57
1:I:110:GLU:O	1:I:111:ALA:HB3	2.05	0.57
1:B:19:ASN:HA	1:B:29:LEU:HD11	1.85	0.57
2:K:88:THR:CG2	2:K:112:THR:HG23	2.33	0.57
2:L:257:ASP:HB2	2:L:258:LYS:HD3	1.86	0.57
2:L:272:THR:HG21	2:L:274:LYS:HE3	1.86	0.57
1:C:110:GLU:O	1:C:111:ALA:HB3	2.05	0.57
2:K:214:THR:HG21	2:K:267:ASP:OD2	2.05	0.57
1:A:12:PRO:HG2	1:A:156:ALA:HB2	1.86	0.57
2:E:88:THR:CG2	2:E:112:THR:HG23	2.33	0.57
1:G:110:GLU:O	1:G:111:ALA:HB3	2.03	0.57
1:B:110:GLU:O	1:B:111:ALA:HB3	2.05	0.57
2:F:192:GLU:HG2	2:F:197:ASN:O	2.04	0.57
2:L:208:TYR:O	2:L:210:PRO:N	2.38	0.57
1:A:102:GLN:HB2	1:A:104:GLU:OE1	2.04	0.57
1:G:125:GLN:NE2	1:H:8:PRO:HA	2.19	0.57
1:H:110:GLU:O	1:H:111:ALA:HB3	2.04	0.57
2:K:275:MET:SD	2:K:279:PRO:HD3	2.44	0.57
1:C:19:ASN:HA	1:C:29:LEU:HD11	1.87	0.57
1:I:19:ASN:ND2	1:I:21:GLN:H	2.02	0.57
1:G:19:ASN:HA	1:G:29:LEU:HD11	1.86	0.57
2:K:208:TYR:O	2:K:210:PRO:N	2.38	0.57
2:F:9:VAL:HA	2:F:18:ASP:O	2.05	0.57
1:I:82:ARG:HH11	2:J:161:MET:HE1	1.70	0.57
2:F:288:LEU:HD22	2:F:288:LEU:O	2.05	0.56
1:H:102:GLN:HB2	1:H:104:GLU:OE1	2.05	0.56
1:I:26:LEU:HD13	1:I:142:LEU:HD11	1.86	0.56
1:I:83:ILE:O	1:I:83:ILE:HG13	2.05	0.56
2:J:88:THR:CG2	2:J:112:THR:HG23	2.34	0.56
1:C:102:GLN:HB2	1:C:104:GLU:OE1	2.05	0.56
2:F:217:ILE:O	2:F:280:VAL:HG12	2.06	0.56
1:B:26:LEU:HD13	1:B:142:LEU:HD11	1.87	0.56
2:F:257:ASP:HB2	2:F:258:LYS:HD3	1.86	0.56
1:B:146:GLU:HB3	1:B:149:GLN:CD	2.26	0.56
1:G:102:GLN:HB2	1:G:104:GLU:OE1	2.05	0.56
1:C:26:LEU:HD13	1:C:142:LEU:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:55:ARG:CG	3:F:326:NAG:H82	2.34	0.56
2:E:287:THR:O	2:E:288:LEU:HD13	2.04	0.56
2:J:39:THR:HG21	2:J:41:HIS:NE2	2.20	0.56
2:D:39:THR:O	2:D:40:ARG:HB2	2.04	0.56
2:E:39:THR:HG21	2:E:41:HIS:CE1	2.41	0.56
1:G:82:ARG:NH2	1:G:130:ASP:OD2	2.39	0.56
2:K:257:ASP:HB2	2:K:258:LYS:HD3	1.88	0.56
2:E:257:ASP:HB2	2:E:258:LYS:HD3	1.88	0.56
2:D:186:VAL:O	2:D:187:LYS:HG3	2.06	0.56
2:D:209:PRO:O	2:D:285:HIS:HE1	1.89	0.56
1:G:120:LEU:HD12	1:H:61:GLN:HE22	1.71	0.56
2:J:214:THR:HG21	2:J:267:ASP:OD2	2.04	0.56
1:C:146:GLU:HB3	1:C:149:GLN:CD	2.26	0.56
2:K:296:SER:O	2:K:297:GLU:HB2	2.05	0.56
2:D:39:THR:HG21	2:D:41:HIS:NE2	2.21	0.55
2:D:9:VAL:HA	2:D:18:ASP:O	2.06	0.55
2:E:239:ARG:HB3	2:E:239:ARG:NH1	2.20	0.55
2:F:239:ARG:NH1	2:F:239:ARG:HB3	2.18	0.55
2:F:296:SER:O	2:F:297:GLU:HB2	2.06	0.55
1:H:103:ARG:HH21	1:I:112:LYS:HE2	1.70	0.55
2:J:209:PRO:O	2:J:285:HIS:HE1	1.90	0.55
2:F:209:PRO:O	2:F:285:HIS:HE1	1.89	0.55
2:F:296:SER:C	2:F:298:GLY:N	2.60	0.55
2:L:9:VAL:HA	2:L:18:ASP:O	2.06	0.55
2:L:239:ARG:NH1	2:L:239:ARG:HB3	2.21	0.55
2:E:186:VAL:O	2:E:187:LYS:HG3	2.05	0.55
1:I:69:CYS:CB	1:I:106:PRO:HD3	2.36	0.55
2:J:280:VAL:CG2	2:J:294:THR:HG22	2.36	0.55
2:L:73:MET:HG2	2:L:140:MET:HE1	1.86	0.55
1:C:86:SER:O	2:E:157:GLY:HA2	2.06	0.55
1:I:146:GLU:HB3	1:I:149:GLN:CD	2.27	0.55
2:J:217:ILE:O	2:J:280:VAL:HG12	2.06	0.55
2:K:209:PRO:O	2:K:285:HIS:HE1	1.89	0.55
2:K:183:THR:HG23	2:K:288:LEU:HD12	1.88	0.55
2:L:186:VAL:O	2:L:187:LYS:HG3	2.07	0.55
2:L:39:THR:O	2:L:40:ARG:HB2	2.07	0.55
1:G:26:LEU:HD13	1:G:142:LEU:HD11	1.88	0.55
2:J:94:ILE:HD12	3:J:325:NAG:H82	1.89	0.55
1:A:146:GLU:HB3	1:A:149:GLN:CD	2.27	0.55
2:E:288:LEU:O	2:E:288:LEU:HD22	2.07	0.55
2:E:296:SER:O	2:E:297:GLU:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:296:SER:O	2:J:297:GLU:HB2	2.07	0.55
2:E:214:THR:HG21	2:E:267:ASP:OD2	2.07	0.55
1:A:82:ARG:NH2	1:A:130:ASP:OD2	2.40	0.54
1:C:12:PRO:HG2	1:C:156:ALA:HB2	1.88	0.54
2:D:60:PRO:HB2	2:D:64:TYR:HA	1.90	0.54
1:G:146:GLU:HB3	1:G:149:GLN:CD	2.27	0.54
2:L:39:THR:HG21	2:L:41:HIS:NE2	2.22	0.54
2:F:183:THR:HG23	2:F:288:LEU:HD12	1.90	0.54
2:J:239:ARG:NH1	2:J:239:ARG:HB3	2.19	0.54
1:I:44:ARG:NH1	2:L:232:ARG:HH22	2.04	0.54
2:L:288:LEU:HD22	2:L:288:LEU:O	2.06	0.54
1:B:103:ARG:HG2	1:B:103:ARG:HH21	1.73	0.54
1:H:103:ARG:HH21	1:H:103:ARG:HG2	1.72	0.54
2:L:183:THR:HG23	2:L:288:LEU:HD12	1.88	0.54
2:L:296:SER:O	2:L:297:GLU:HB2	2.07	0.54
2:D:257:ASP:HB2	2:D:258:LYS:HD3	1.87	0.54
2:F:288:LEU:CD2	2:F:288:LEU:O	2.55	0.54
2:J:288:LEU:O	2:J:288:LEU:CD2	2.56	0.54
2:K:9:VAL:HA	2:K:18:ASP:O	2.07	0.54
1:B:69:CYS:CB	1:B:106:PRO:HD3	2.37	0.54
1:B:146:GLU:O	1:B:147:SER:HB2	2.06	0.54
2:J:288:LEU:O	2:J:288:LEU:HD22	2.07	0.54
2:F:208:TYR:C	2:F:208:TYR:CD1	2.80	0.54
2:J:50:TRP:CB	2:J:177:LYS:HD2	2.22	0.54
2:F:39:THR:HG21	2:F:41:HIS:CE1	2.43	0.54
1:I:146:GLU:OE2	1:I:147:SER:N	2.41	0.54
2:J:39:THR:HG21	2:J:41:HIS:CE1	2.42	0.54
2:E:39:THR:HG21	2:E:41:HIS:NE2	2.23	0.54
2:K:36:ASN:HB2	2:K:43:ASN:ND2	2.22	0.54
2:E:208:TYR:CD1	2:E:208:TYR:C	2.79	0.54
2:F:214:THR:HG21	2:F:267:ASP:OD2	2.08	0.54
2:F:36:ASN:HB2	2:F:43:ASN:ND2	2.22	0.54
2:K:60:PRO:HB2	2:K:64:TYR:HA	1.90	0.54
2:F:39:THR:O	2:F:40:ARG:HB2	2.07	0.54
2:F:39:THR:HG21	2:F:41:HIS:NE2	2.23	0.54
2:D:296:SER:C	2:D:298:GLY:N	2.61	0.53
2:E:285:HIS:CD2	2:E:287:THR:H	2.26	0.53
2:E:183:THR:HG23	2:E:288:LEU:HD12	1.90	0.53
2:K:73:MET:HG2	2:K:140:MET:HE2	1.90	0.53
1:A:103:ARG:HG2	1:A:103:ARG:HH21	1.73	0.53
2:D:296:SER:O	2:D:297:GLU:HB2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:88:THR:HG22	2:D:89:THR:N	2.24	0.53
1:G:146:GLU:O	1:G:147:SER:HB2	2.08	0.53
2:L:285:HIS:CD2	2:L:287:THR:H	2.26	0.53
2:L:39:THR:HG21	2:L:41:HIS:CE1	2.43	0.53
2:L:36:ASN:HB2	2:L:43:ASN:ND2	2.23	0.53
1:C:146:GLU:OE2	1:C:147:SER:N	2.42	0.53
2:J:36:ASN:HB2	2:J:43:ASN:ND2	2.23	0.53
1:A:120:LEU:HD12	1:C:61:GLN:HE22	1.73	0.53
2:E:50:TRP:CB	2:E:177:LYS:HD2	2.23	0.53
1:H:146:GLU:HB3	1:H:149:GLN:CD	2.28	0.53
2:L:296:SER:C	2:L:298:GLY:N	2.60	0.53
1:H:146:GLU:OE2	1:H:147:SER:N	2.42	0.53
1:I:13:VAL:HG22	1:I:14:ALA:N	2.23	0.53
2:F:55:ARG:HD3	3:F:326:NAG:H82	1.90	0.53
1:I:103:ARG:HG2	1:I:103:ARG:HH21	1.73	0.53
2:L:50:TRP:CB	2:L:177:LYS:HD2	2.21	0.53
2:L:208:TYR:CD1	2:L:208:TYR:C	2.82	0.53
1:C:103:ARG:HH21	1:C:103:ARG:HG2	1.73	0.53
2:D:239:ARG:HB3	2:D:239:ARG:NH1	2.22	0.53
2:E:296:SER:C	2:E:298:GLY:N	2.60	0.53
2:J:9:VAL:HA	2:J:18:ASP:O	2.08	0.53
2:J:285:HIS:CD2	2:J:287:THR:H	2.27	0.53
2:J:39:THR:O	2:J:40:ARG:HB2	2.08	0.53
2:K:285:HIS:CD2	2:K:287:THR:H	2.26	0.53
2:L:288:LEU:CD2	2:L:288:LEU:O	2.57	0.53
1:A:146:GLU:O	1:A:147:SER:HB2	2.09	0.53
1:A:146:GLU:OE2	1:A:147:SER:N	2.42	0.53
2:D:214:THR:HG21	2:D:267:ASP:OD2	2.07	0.53
2:E:209:PRO:O	2:E:285:HIS:HE1	1.91	0.53
3:E:326:NAG:H3	3:E:326:NAG:C8	2.35	0.53
1:G:146:GLU:OE2	1:G:147:SER:N	2.42	0.53
2:D:12:LYS:O	2:D:13:ASP:O	2.27	0.53
2:E:9:VAL:HA	2:E:18:ASP:O	2.08	0.52
1:H:26:LEU:HD13	1:H:142:LEU:HD11	1.89	0.52
1:I:19:ASN:HA	1:I:29:LEU:HD11	1.88	0.52
2:L:178:ILE:HB	2:L:179:PRO:HD2	1.91	0.52
2:L:214:THR:HG21	2:L:267:ASP:OD2	2.09	0.52
1:A:26:LEU:HD13	1:A:142:LEU:HD11	1.91	0.52
2:J:178:ILE:HB	2:J:179:PRO:HD2	1.91	0.52
2:J:60:PRO:HB2	2:J:64:TYR:HA	1.90	0.52
2:L:88:THR:HG22	2:L:89:THR:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:GLU:OE2	1:B:147:SER:N	2.42	0.52
2:D:183:THR:HG23	2:D:288:LEU:HD12	1.90	0.52
2:L:209:PRO:O	2:L:285:HIS:HE1	1.92	0.52
2:D:208:TYR:O	2:D:210:PRO:N	2.41	0.52
2:J:183:THR:HG23	2:J:288:LEU:HD12	1.91	0.52
2:E:288:LEU:CD2	2:E:288:LEU:O	2.57	0.52
2:K:178:ILE:HB	2:K:179:PRO:HD2	1.91	0.52
2:D:39:THR:HG21	2:D:41:HIS:CE1	2.45	0.52
1:G:103:ARG:HH21	1:G:103:ARG:HG2	1.73	0.52
2:E:272:THR:CG2	2:E:274:LYS:HG3	2.40	0.52
2:J:296:SER:O	2:J:298:GLY:N	2.42	0.52
2:J:36:ASN:HD22	2:J:43:ASN:ND2	2.08	0.52
2:K:39:THR:HG21	2:K:41:HIS:NE2	2.25	0.52
1:C:146:GLU:O	1:C:147:SER:HB2	2.10	0.52
2:F:285:HIS:CD2	2:F:287:THR:H	2.27	0.52
1:I:82:ARG:NH2	1:I:130:ASP:OD2	2.42	0.52
2:D:272:THR:CG2	2:D:274:LYS:HG3	2.40	0.52
2:F:60:PRO:HB2	2:F:64:TYR:HA	1.91	0.52
2:K:288:LEU:O	2:K:288:LEU:CD2	2.58	0.52
2:K:296:SER:C	2:K:298:GLY:N	2.60	0.52
1:A:80:ILE:HA	1:A:133:SER:O	2.10	0.51
2:D:288:LEU:O	2:D:288:LEU:CD2	2.58	0.51
2:D:288:LEU:HD22	2:D:288:LEU:O	2.10	0.51
1:G:109:ALA:O	1:G:110:GLU:CB	2.58	0.51
2:J:272:THR:CG2	2:J:274:LYS:HG3	2.40	0.51
2:L:60:PRO:HB2	2:L:64:TYR:HA	1.92	0.51
1:B:61:GLN:HE22	1:C:120:LEU:HD12	1.75	0.51
1:C:53:GLU:OE1	1:C:127:GLU:HA	2.10	0.51
2:E:60:PRO:HB2	2:E:64:TYR:HA	1.92	0.51
2:F:50:TRP:CB	2:F:177:LYS:HD2	2.22	0.51
2:F:88:THR:HG22	2:F:89:THR:N	2.26	0.51
1:A:8:PRO:HA	1:B:125:GLN:NE2	2.25	0.51
2:D:285:HIS:CD2	2:D:287:THR:H	2.28	0.51
2:E:296:SER:O	2:E:298:GLY:N	2.43	0.51
1:H:109:ALA:O	1:H:110:GLU:CB	2.59	0.51
1:H:13:VAL:HG22	1:H:14:ALA:N	2.26	0.51
2:J:271:THR:O	2:J:271:THR:HG22	2.10	0.51
2:K:288:LEU:HD22	2:K:288:LEU:O	2.09	0.51
1:B:80:ILE:HA	1:B:133:SER:O	2.11	0.51
1:G:53:GLU:OE1	1:G:127:GLU:HA	2.11	0.51
2:F:280:VAL:CG2	2:F:294:THR:HG22	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:36:ASN:HD22	2:J:43:ASN:HD21	1.57	0.51
2:K:39:THR:O	2:K:40:ARG:HB2	2.10	0.51
1:B:109:ALA:O	1:B:110:GLU:CB	2.58	0.51
2:D:208:TYR:CG	2:D:209:PRO:N	2.77	0.51
2:E:41:HIS:CD2	2:E:41:HIS:C	2.84	0.51
2:F:178:ILE:HB	2:F:179:PRO:HD2	1.93	0.51
2:F:296:SER:O	2:F:298:GLY:N	2.43	0.51
1:I:109:ALA:O	1:I:110:GLU:CB	2.58	0.51
2:K:272:THR:CG2	2:K:274:LYS:HG3	2.40	0.51
2:K:287:THR:C	2:K:288:LEU:HD13	2.30	0.51
1:C:69:CYS:CB	1:C:106:PRO:HD3	2.38	0.51
2:F:186:VAL:O	2:F:187:LYS:HG3	2.10	0.51
2:F:272:THR:CG2	2:F:274:LYS:HG3	2.40	0.51
2:J:62:ASN:OD1	2:J:62:ASN:N	2.44	0.51
2:L:294:THR:O	2:L:295:CYS:SG	2.68	0.51
2:F:202:CYS:HB2	2:F:216:TRP:CZ2	2.45	0.51
1:B:82:ARG:NH2	1:B:130:ASP:OD2	2.41	0.51
1:C:109:ALA:O	1:C:110:GLU:CB	2.59	0.51
2:D:202:CYS:HB2	2:D:216:TRP:CZ2	2.46	0.51
2:D:294:THR:O	2:D:295:CYS:SG	2.69	0.51
1:H:69:CYS:CB	1:H:106:PRO:HD3	2.36	0.51
1:H:19:ASN:N	1:H:29:LEU:HD11	2.24	0.51
2:J:202:CYS:HB2	2:J:216:TRP:CZ2	2.46	0.51
2:K:208:TYR:CD1	2:K:208:TYR:C	2.79	0.51
1:A:109:ALA:O	1:A:110:GLU:CB	2.58	0.50
1:H:53:GLU:OE1	1:H:127:GLU:HA	2.11	0.50
1:I:146:GLU:O	1:I:147:SER:HB2	2.10	0.50
2:J:208:TYR:CD1	2:J:208:TYR:C	2.81	0.50
1:B:12:PRO:HA	1:B:39:ASN:HB2	1.93	0.50
2:D:36:ASN:HB2	2:D:43:ASN:ND2	2.26	0.50
1:I:53:GLU:OE1	1:I:127:GLU:HA	2.11	0.50
2:L:272:THR:CG2	2:L:274:LYS:HG3	2.41	0.50
2:L:287:THR:C	2:L:288:LEU:HD13	2.31	0.50
2:D:287:THR:C	2:D:288:LEU:HD13	2.32	0.50
2:J:50:TRP:HB3	2:J:177:LYS:CD	2.24	0.50
2:K:208:TYR:CG	2:K:209:PRO:N	2.76	0.50
1:A:61:GLN:HE22	1:B:120:LEU:HD12	1.75	0.50
2:E:36:ASN:HB2	2:E:43:ASN:ND2	2.27	0.50
2:K:271:THR:HG22	2:K:271:THR:O	2.11	0.50
3:L:326:NAG:H3	3:L:326:NAG:H83	1.94	0.50
1:A:69:CYS:CB	1:A:106:PRO:HD3	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ASN:N	1:A:29:LEU:HD11	2.27	0.50
2:E:271:THR:HG22	2:E:271:THR:O	2.12	0.50
2:E:39:THR:O	2:E:40:ARG:HB2	2.10	0.50
1:G:69:CYS:CB	1:G:106:PRO:HD3	2.38	0.50
1:G:110:GLU:HG3	1:I:103:ARG:HH22	1.77	0.50
2:K:186:VAL:O	2:K:187:LYS:HG3	2.12	0.50
1:A:13:VAL:HG22	1:A:14:ALA:N	2.26	0.50
1:H:146:GLU:O	1:H:147:SER:HB2	2.11	0.50
2:L:296:SER:O	2:L:298:GLY:N	2.44	0.50
1:A:103:ARG:NH2	1:C:112:LYS:HE2	2.25	0.50
2:D:208:TYR:C	2:D:208:TYR:CD1	2.78	0.50
2:E:73:MET:HG2	2:E:140:MET:HE1	1.92	0.50
2:E:88:THR:HG22	2:E:89:THR:N	2.27	0.50
1:B:13:VAL:HG22	1:B:14:ALA:N	2.27	0.50
2:D:178:ILE:HB	2:D:179:PRO:HD2	1.93	0.50
2:J:41:HIS:CD2	2:J:41:HIS:C	2.85	0.50
2:E:208:TYR:CG	2:E:209:PRO:N	2.77	0.49
1:G:19:ASN:N	1:G:29:LEU:HD11	2.27	0.49
1:G:61:GLN:HE22	1:I:120:LEU:HD12	1.76	0.49
1:G:82:ARG:HH11	2:K:161:MET:HE1	1.77	0.49
2:F:287:THR:C	2:F:288:LEU:HD13	2.32	0.49
2:J:186:VAL:O	2:J:187:LYS:HG3	2.12	0.49
2:K:142:THR:HG22	2:K:144:LYS:H	1.77	0.49
2:K:239:ARG:HB3	2:K:239:ARG:NH1	2.22	0.49
1:B:102:GLN:O	1:B:103:ARG:HB3	2.13	0.49
2:E:12:LYS:O	2:E:13:ASP:O	2.30	0.49
1:A:55:LEU:HD21	1:C:13:VAL:HG11	1.93	0.49
2:F:109:TYR:HB2	2:F:130:MET:HE2	1.94	0.49
2:D:271:THR:O	2:D:271:THR:HG22	2.13	0.49
2:F:86:THR:O	2:F:87:LYS:C	2.51	0.49
2:L:202:CYS:HB2	2:L:216:TRP:CZ2	2.47	0.49
1:A:12:PRO:HA	1:A:39:ASN:HB2	1.95	0.49
1:C:80:ILE:HA	1:C:133:SER:O	2.12	0.49
1:H:80:ILE:HA	1:H:133:SER:O	2.12	0.49
2:J:88:THR:HG22	2:J:89:THR:N	2.27	0.49
1:A:102:GLN:O	1:A:103:ARG:HB3	2.13	0.49
1:A:53:GLU:OE1	1:A:127:GLU:HA	2.11	0.49
1:G:67:GLN:OE1	1:G:113:PRO:HB3	2.13	0.49
2:J:12:LYS:O	2:J:13:ASP:O	2.30	0.49
2:J:52:ASN:OD1	2:J:54:SER:HB2	2.12	0.49
2:E:178:ILE:HB	2:E:179:PRO:HD2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:12:PRO:HA	1:H:39:ASN:HB2	1.94	0.49
1:I:102:GLN:O	1:I:103:ARG:HB3	2.12	0.49
2:L:12:LYS:O	2:L:13:ASP:O	2.30	0.49
2:L:208:TYR:CG	2:L:209:PRO:N	2.80	0.49
1:A:50:VAL:HG13	1:A:56:TYR:OH	2.13	0.49
1:B:53:GLU:OE1	1:B:127:GLU:HA	2.12	0.49
1:B:110:GLU:HG3	1:C:103:ARG:HH22	1.78	0.49
2:E:202:CYS:HB2	2:E:216:TRP:CZ2	2.48	0.49
1:C:12:PRO:HA	1:C:39:ASN:HB2	1.95	0.48
1:G:102:GLN:O	1:G:103:ARG:HB3	2.13	0.48
2:K:12:LYS:O	2:K:13:ASP:O	2.31	0.48
1:A:104:GLU:O	1:A:105:THR:O	2.30	0.48
1:A:19:ASN:HD22	1:A:20:PRO:CD	2.26	0.48
2:F:12:LYS:O	2:F:13:ASP:O	2.31	0.48
2:F:142:THR:HG22	2:F:144:LYS:H	1.78	0.48
2:F:294:THR:O	2:F:295:CYS:SG	2.70	0.48
2:F:41:HIS:C	2:F:41:HIS:CD2	2.86	0.48
1:I:12:PRO:HA	1:I:39:ASN:HB2	1.95	0.48
2:K:202:CYS:HB2	2:K:216:TRP:CZ2	2.48	0.48
2:K:294:THR:O	2:K:295:CYS:SG	2.70	0.48
2:L:131:THR:HG22	2:L:132:HIS:N	2.28	0.48
1:C:82:ARG:NH2	1:C:130:ASP:OD2	2.44	0.48
1:G:7:THR:O	1:G:8:PRO:C	2.51	0.48
1:H:102:GLN:O	1:H:103:ARG:HB3	2.14	0.48
1:I:19:ASN:N	1:I:29:LEU:HD11	2.27	0.48
2:L:271:THR:O	2:L:271:THR:HG22	2.12	0.48
1:B:106:PRO:HB3	1:B:111:ALA:HB2	1.95	0.48
1:I:104:GLU:O	1:I:105:THR:O	2.31	0.48
2:K:280:VAL:CG2	2:K:294:THR:HG22	2.43	0.48
1:C:13:VAL:HG22	1:C:14:ALA:N	2.28	0.48
1:I:7:THR:O	1:I:8:PRO:C	2.52	0.48
2:D:197:ASN:ND2	2:D:271:THR:O	2.47	0.48
2:J:178:ILE:HB	2:J:179:PRO:CD	2.44	0.48
2:L:41:HIS:CD2	2:L:41:HIS:C	2.86	0.48
1:G:104:GLU:O	1:G:105:THR:O	2.32	0.48
2:K:178:ILE:HB	2:K:179:PRO:CD	2.43	0.48
2:D:142:THR:HG22	2:D:144:LYS:H	1.77	0.48
2:E:86:THR:O	2:E:87:LYS:C	2.52	0.48
2:F:131:THR:HG22	2:F:132:HIS:N	2.29	0.48
1:G:55:LEU:HD21	1:H:13:VAL:HG11	1.94	0.48
1:H:67:GLN:OE1	1:H:113:PRO:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:131:THR:HG22	2:J:132:HIS:N	2.29	0.48
2:J:237:TRP:HE1	2:J:275:MET:CE	2.27	0.48
2:J:287:THR:C	2:J:288:LEU:HD13	2.34	0.48
1:C:104:GLU:O	1:C:105:THR:O	2.31	0.48
2:F:271:THR:O	2:F:271:THR:HG22	2.13	0.48
2:L:197:ASN:ND2	2:L:271:THR:O	2.47	0.48
1:B:19:ASN:HD22	1:B:20:PRO:CD	2.27	0.48
2:E:287:THR:C	2:E:288:LEU:HD13	2.35	0.48
2:E:294:THR:O	2:E:295:CYS:SG	2.72	0.48
1:I:67:GLN:OE1	1:I:113:PRO:HB3	2.13	0.48
2:K:216:TRP:CE2	2:K:269:VAL:HG21	2.49	0.48
2:K:41:HIS:C	2:K:41:HIS:CD2	2.86	0.48
2:L:36:ASN:HD22	2:L:43:ASN:ND2	2.12	0.48
1:A:83:ILE:C	1:A:83:ILE:HD12	2.35	0.47
1:B:19:ASN:N	1:B:29:LEU:HD11	2.29	0.47
1:H:104:GLU:O	1:H:105:THR:O	2.32	0.47
1:H:106:PRO:HB3	1:H:111:ALA:HB2	1.96	0.47
1:H:19:ASN:HD22	1:H:20:PRO:CD	2.27	0.47
1:I:80:ILE:HA	1:I:133:SER:O	2.13	0.47
2:L:86:THR:O	2:L:87:LYS:C	2.52	0.47
1:A:7:THR:O	1:A:8:PRO:C	2.51	0.47
1:B:98:LYS:CD	1:B:116:GLU:HG3	2.44	0.47
1:C:7:THR:O	1:C:8:PRO:C	2.52	0.47
2:D:178:ILE:HB	2:D:179:PRO:CD	2.43	0.47
2:D:280:VAL:CG2	2:D:294:THR:HG22	2.44	0.47
2:F:197:ASN:ND2	2:F:271:THR:O	2.47	0.47
1:G:31:ARG:HD2	2:J:99:GLU:HG2	1.95	0.47
2:L:142:THR:HG22	2:L:144:LYS:H	1.78	0.47
1:A:112:LYS:HE2	1:B:103:ARG:NH2	2.29	0.47
1:C:102:GLN:O	1:C:103:ARG:HB3	2.13	0.47
1:C:103:ARG:O	1:C:103:ARG:HG3	2.15	0.47
2:D:86:THR:O	2:D:87:LYS:C	2.53	0.47
2:E:112:THR:CG2	2:E:113:ALA:N	2.77	0.47
1:I:106:PRO:HB3	1:I:111:ALA:HB2	1.96	0.47
2:J:206:SER:HB2	2:J:262:THR:HG21	1.97	0.47
2:K:39:THR:HG21	2:K:41:HIS:CE1	2.49	0.47
1:C:19:ASN:N	1:C:29:LEU:HD11	2.29	0.47
2:E:237:TRP:HE1	2:E:275:MET:CE	2.27	0.47
2:J:142:THR:HG22	2:J:144:LYS:H	1.78	0.47
2:K:131:THR:HG22	2:K:132:HIS:N	2.29	0.47
1:B:67:GLN:OE1	1:B:113:PRO:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:106:PRO:HB3	1:G:111:ALA:HB2	1.96	0.47
2:L:237:TRP:HE1	2:L:275:MET:CE	2.27	0.47
1:A:67:GLN:OE1	1:A:113:PRO:HB3	2.14	0.47
1:B:103:ARG:O	1:B:103:ARG:HG3	2.15	0.47
1:B:83:ILE:HD12	1:B:83:ILE:C	2.35	0.47
1:C:106:PRO:HB3	1:C:111:ALA:HB2	1.96	0.47
1:C:19:ASN:HD22	1:C:20:PRO:CD	2.28	0.47
2:D:237:TRP:HE1	2:D:275:MET:CE	2.26	0.47
2:E:131:THR:HG22	2:E:132:HIS:N	2.29	0.47
1:G:12:PRO:HG2	1:G:156:ALA:CB	2.44	0.47
2:L:178:ILE:HB	2:L:179:PRO:CD	2.45	0.47
1:B:104:GLU:O	1:B:105:THR:O	2.31	0.47
1:C:82:ARG:HH11	2:E:161:MET:HE1	1.80	0.47
2:J:272:THR:HG22	2:J:274:LYS:HG3	1.97	0.47
2:K:272:THR:HG22	2:K:274:LYS:HG3	1.96	0.47
1:G:80:ILE:HA	1:G:133:SER:O	2.14	0.47
1:H:83:ILE:C	1:H:83:ILE:HD12	2.35	0.47
1:H:7:THR:O	1:H:8:PRO:C	2.51	0.47
2:K:296:SER:O	2:K:298:GLY:N	2.44	0.47
2:L:112:THR:CG2	2:L:113:ALA:N	2.78	0.47
2:L:280:VAL:CG2	2:L:294:THR:HG22	2.45	0.47
1:B:12:PRO:HG2	1:B:156:ALA:CB	2.44	0.47
2:F:52:ASN:OD1	2:F:54:SER:HB2	2.15	0.47
2:K:88:THR:HG22	2:K:89:THR:N	2.29	0.47
1:C:67:GLN:OE1	1:C:113:PRO:HB3	2.15	0.47
2:F:178:ILE:HB	2:F:179:PRO:CD	2.45	0.47
1:G:103:ARG:HH21	1:H:112:LYS:HE2	1.79	0.47
1:G:98:LYS:CD	1:G:116:GLU:HG3	2.45	0.47
2:K:237:TRP:HE1	2:K:275:MET:CE	2.27	0.47
2:D:88:THR:HG22	2:D:90:SER:H	1.80	0.47
2:E:216:TRP:CE2	2:E:269:VAL:HG21	2.50	0.47
1:G:12:PRO:HA	1:G:39:ASN:HB2	1.96	0.47
2:E:142:THR:HG22	2:E:144:LYS:H	1.80	0.46
2:F:112:THR:CG2	2:F:113:ALA:N	2.77	0.46
1:H:103:ARG:O	1:H:103:ARG:HG3	2.15	0.46
2:J:294:THR:O	2:J:295:CYS:SG	2.73	0.46
2:D:220:GLU:HG3	2:D:221:HIS:N	2.31	0.46
2:E:294:THR:HB	2:E:295:CYS:H	1.56	0.46
2:E:50:TRP:HB3	2:E:177:LYS:CD	2.23	0.46
1:H:82:ARG:NH2	1:H:130:ASP:OD2	2.46	0.46
2:J:112:THR:CG2	2:J:113:ALA:N	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:197:ASN:ND2	2:K:271:THR:O	2.48	0.46
1:A:103:ARG:HG3	1:A:103:ARG:O	2.15	0.46
1:B:7:THR:O	1:B:8:PRO:C	2.52	0.46
2:F:237:TRP:HE1	2:F:275:MET:CE	2.27	0.46
1:I:103:ARG:HG3	1:I:103:ARG:O	2.14	0.46
1:I:69:CYS:HA	1:I:70:PRO:HD3	1.80	0.46
2:K:36:ASN:HD22	2:K:43:ASN:ND2	2.13	0.46
1:A:31:ARG:O	1:A:32:ARG:HD3	2.16	0.46
1:C:143:LEU:HD12	1:C:145:ALA:H	1.81	0.46
2:D:41:HIS:CD2	2:D:41:HIS:C	2.88	0.46
1:H:83:ILE:CG1	1:H:83:ILE:O	2.63	0.46
2:J:88:THR:HG22	2:J:90:SER:H	1.79	0.46
2:K:52:ASN:OD1	2:K:54:SER:HB2	2.15	0.46
1:C:98:LYS:CD	1:C:116:GLU:HG3	2.45	0.46
1:I:31:ARG:O	1:I:32:ARG:HD3	2.16	0.46
2:E:197:ASN:ND2	2:E:271:THR:O	2.49	0.46
2:E:88:THR:HG22	2:E:90:SER:H	1.81	0.46
1:H:7:THR:HG22	1:H:9:SER:H	1.81	0.46
1:B:31:ARG:O	1:B:32:ARG:HD3	2.16	0.46
2:F:272:THR:HG22	2:F:274:LYS:HG3	1.97	0.46
1:I:19:ASN:HD22	1:I:20:PRO:CD	2.29	0.46
2:J:208:TYR:CG	2:J:209:PRO:N	2.80	0.46
2:J:86:THR:O	2:J:87:LYS:C	2.54	0.46
2:K:285:HIS:HD2	2:K:287:THR:OG1	1.99	0.46
2:L:52:ASN:OD1	2:L:54:SER:HB2	2.16	0.46
1:A:106:PRO:HB3	1:A:111:ALA:HB2	1.96	0.46
2:D:36:ASN:HD22	2:D:43:ASN:ND2	2.13	0.46
2:D:52:ASN:OD1	2:D:54:SER:HB2	2.16	0.46
2:E:13:ASP:OD1	2:E:14:ASP:N	2.49	0.46
1:G:103:ARG:O	1:G:103:ARG:HG3	2.15	0.46
2:K:220:GLU:HG3	2:K:221:HIS:N	2.31	0.46
1:A:7:THR:HG22	1:A:9:SER:H	1.80	0.46
1:A:7:THR:HG22	1:A:9:SER:N	2.31	0.46
2:D:272:THR:HG22	2:D:274:LYS:HG3	1.96	0.46
2:E:178:ILE:HB	2:E:179:PRO:CD	2.46	0.46
2:F:258:LYS:N	2:F:258:LYS:HD3	2.31	0.46
2:F:294:THR:HB	2:F:295:CYS:H	1.55	0.46
1:G:19:ASN:HD22	1:G:20:PRO:CD	2.29	0.46
1:I:50:VAL:HG13	1:I:56:TYR:OH	2.16	0.46
1:I:83:ILE:HD12	1:I:83:ILE:C	2.36	0.46
2:J:296:SER:C	2:J:298:GLY:N	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:258:LYS:HD3	2:K:258:LYS:N	2.30	0.46
2:K:36:ASN:HD22	2:K:43:ASN:HD21	1.64	0.46
2:D:216:TRP:CE2	2:D:269:VAL:HG21	2.51	0.45
2:E:272:THR:HG22	2:E:273:SER:N	2.31	0.45
2:F:192:GLU:CG	2:F:198:MET:HA	2.44	0.45
1:H:7:THR:HG22	1:H:9:SER:N	2.31	0.45
1:I:7:THR:HG22	1:I:9:SER:H	1.81	0.45
1:B:50:VAL:HG13	1:B:56:TYR:OH	2.16	0.45
1:C:31:ARG:O	1:C:32:ARG:HD3	2.16	0.45
2:D:13:ASP:OD1	2:D:14:ASP:N	2.50	0.45
2:D:272:THR:HG22	2:D:273:SER:N	2.32	0.45
2:D:36:ASN:HD22	2:D:43:ASN:HD21	1.64	0.45
1:H:12:PRO:HG2	1:H:156:ALA:CB	2.47	0.45
1:I:31:ARG:HD2	2:L:99:GLU:HG2	1.97	0.45
2:J:258:LYS:O	2:J:259:ASP:C	2.55	0.45
2:L:220:GLU:HG3	2:L:221:HIS:N	2.31	0.45
1:A:98:LYS:CD	1:A:116:GLU:HG3	2.46	0.45
2:J:13:ASP:OD1	2:J:14:ASP:N	2.50	0.45
2:K:55:ARG:CG	3:K:326:NAG:H82	2.47	0.45
2:L:216:TRP:CE2	2:L:269:VAL:HG21	2.51	0.45
2:L:88:THR:HG22	2:L:90:SER:H	1.81	0.45
2:D:73:MET:HG2	2:D:140:MET:HE1	1.97	0.45
2:F:220:GLU:HG3	2:F:221:HIS:N	2.32	0.45
2:F:25:TYR:O	2:F:26:ASN:HB2	2.17	0.45
1:C:7:THR:HG22	1:C:9:SER:H	1.81	0.45
2:D:112:THR:CG2	2:D:113:ALA:N	2.78	0.45
2:D:296:SER:O	2:D:298:GLY:N	2.45	0.45
1:G:143:LEU:HD12	1:G:145:ALA:H	1.82	0.45
1:G:7:THR:HG22	1:G:9:SER:H	1.81	0.45
1:C:83:ILE:C	1:C:83:ILE:HD12	2.37	0.45
2:E:280:VAL:CG2	2:E:294:THR:HG22	2.43	0.45
2:K:183:THR:CG2	2:K:288:LEU:HD12	2.47	0.45
2:L:272:THR:HG22	2:L:273:SER:N	2.32	0.45
2:L:272:THR:HG22	2:L:274:LYS:HG3	1.98	0.45
3:D:327:NAG:C7	3:D:327:NAG:O3	2.65	0.45
2:E:250:PHE:HA	2:E:251:PRO:HD3	1.81	0.45
2:K:183:THR:HG23	2:K:288:LEU:CD1	2.47	0.45
2:K:86:THR:O	2:K:87:LYS:C	2.54	0.45
2:L:258:LYS:HD3	2:L:258:LYS:N	2.32	0.45
2:L:36:ASN:HD22	2:L:43:ASN:HD21	1.65	0.45
2:E:272:THR:HG22	2:E:274:LYS:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:272:THR:HG22	2:F:273:SER:N	2.32	0.45
1:G:50:VAL:HG13	1:G:56:TYR:OH	2.17	0.45
1:G:7:THR:HG22	1:G:9:SER:N	2.32	0.45
1:I:98:LYS:CD	1:I:116:GLU:HG3	2.47	0.45
2:J:197:ASN:ND2	2:J:271:THR:O	2.50	0.45
2:K:72:LEU:HG	2:K:140:MET:HB3	1.99	0.45
2:L:206:SER:HB2	2:L:262:THR:HG21	1.99	0.45
1:B:7:THR:HG22	1:B:9:SER:H	1.81	0.44
2:J:88:THR:HG21	2:J:113:ALA:H	1.81	0.44
2:L:55:ARG:HD3	3:L:326:NAG:H82	1.98	0.44
1:B:13:VAL:HG11	1:C:55:LEU:HD21	1.99	0.44
2:E:206:SER:HB2	2:E:262:THR:HG21	1.99	0.44
1:G:13:VAL:HG22	1:G:14:ALA:N	2.32	0.44
1:I:7:THR:HG22	1:I:9:SER:N	2.32	0.44
2:L:285:HIS:HD2	2:L:287:THR:OG1	2.00	0.44
1:C:7:THR:HG22	1:C:9:SER:N	2.32	0.44
2:E:220:GLU:HG3	2:E:221:HIS:N	2.32	0.44
2:E:52:ASN:OD1	2:E:54:SER:HB2	2.17	0.44
2:F:55:ARG:CD	3:F:326:NAG:H82	2.47	0.44
2:E:285:HIS:HD2	2:E:287:THR:OG1	2.01	0.44
2:J:72:LEU:HG	2:J:140:MET:HB3	1.99	0.44
2:L:185:THR:CG2	2:L:187:LYS:HE3	2.48	0.44
1:A:13:VAL:HG11	1:B:55:LEU:HD21	2.00	0.44
1:B:7:THR:HG22	1:B:9:SER:N	2.32	0.44
3:D:327:NAG:H83	3:D:327:NAG:O3	2.18	0.44
2:F:174:ALA:O	2:F:175:LYS:C	2.56	0.44
1:H:98:LYS:CD	1:H:116:GLU:HG3	2.46	0.44
2:J:220:GLU:HG3	2:J:221:HIS:N	2.32	0.44
1:A:83:ILE:O	1:A:83:ILE:CG1	2.64	0.44
2:D:72:LEU:HG	2:D:140:MET:HB3	1.99	0.44
2:E:257:ASP:O	2:E:258:LYS:O	2.36	0.44
1:B:6:ARG:O	1:B:6:ARG:CZ	2.66	0.44
2:D:131:THR:HG22	2:D:132:HIS:N	2.32	0.44
2:F:36:ASN:HD22	2:F:43:ASN:ND2	2.15	0.44
1:G:83:ILE:HD12	1:G:83:ILE:C	2.38	0.44
2:J:258:LYS:HD3	2:J:258:LYS:N	2.33	0.44
2:K:112:THR:CG2	2:K:113:ALA:N	2.79	0.44
1:H:31:ARG:O	1:H:32:ARG:HD3	2.17	0.44
2:E:81:ASN:OD1	2:E:87:LYS:HA	2.18	0.43
2:L:258:LYS:O	2:L:259:ASP:C	2.56	0.43
2:L:72:LEU:HG	2:L:140:MET:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:PRO:HG2	1:C:156:ALA:CB	2.48	0.43
2:D:206:SER:HB2	2:D:262:THR:HG21	2.00	0.43
1:H:50:VAL:HG13	1:H:56:TYR:OH	2.17	0.43
1:H:125:GLN:HE21	1:I:8:PRO:HA	1.79	0.43
2:K:174:ALA:O	2:K:175:LYS:C	2.57	0.43
2:F:72:LEU:HG	2:F:140:MET:HB3	2.00	0.43
2:F:13:ASP:OD1	2:F:14:ASP:N	2.50	0.43
2:F:206:SER:HB2	2:F:262:THR:HG21	2.00	0.43
1:G:73:HIS:HB2	1:H:112:LYS:HG2	2.00	0.43
2:J:216:TRP:CE2	2:J:269:VAL:HG21	2.53	0.43
2:K:272:THR:HG22	2:K:273:SER:N	2.33	0.43
1:A:6:ARG:O	1:A:6:ARG:CZ	2.67	0.43
2:D:258:LYS:N	2:D:258:LYS:HD3	2.33	0.43
2:F:196:GLY:HA3	2:F:270:ARG:CZ	2.49	0.43
2:F:285:HIS:HD2	2:F:287:THR:OG1	2.01	0.43
1:H:64:PHE:CG	1:H:76:LEU:HD13	2.53	0.43
1:H:120:LEU:HD12	1:I:61:GLN:HE22	1.83	0.43
2:J:257:ASP:O	2:J:258:LYS:O	2.37	0.43
2:K:185:THR:CG2	2:K:187:LYS:HE3	2.48	0.43
2:E:185:THR:CG2	2:E:187:LYS:HE3	2.48	0.43
2:L:13:ASP:OD1	2:L:14:ASP:N	2.51	0.43
2:L:174:ALA:O	2:L:175:LYS:C	2.57	0.43
2:L:257:ASP:O	2:L:258:LYS:O	2.36	0.43
2:J:112:THR:HG23	2:J:113:ALA:N	2.33	0.43
2:J:272:THR:HG22	2:J:273:SER:N	2.33	0.43
2:D:143:VAL:HG13	2:D:148:TRP:CD1	2.54	0.43
2:D:25:TYR:O	2:D:26:ASN:HB2	2.18	0.43
2:E:112:THR:HG23	2:E:113:ALA:N	2.34	0.43
2:E:72:LEU:HG	2:E:140:MET:HB3	1.99	0.43
2:E:285:HIS:HD2	2:E:287:THR:H	1.67	0.43
1:H:6:ARG:CZ	1:H:6:ARG:O	2.67	0.43
2:J:285:HIS:HD2	2:J:287:THR:OG1	2.02	0.43
2:K:50:TRP:CB	2:K:177:LYS:HD2	2.23	0.43
1:A:57:LEU:O	1:A:154:ILE:HA	2.19	0.43
2:D:277:SER:O	2:D:278:GLN:HB3	2.19	0.43
3:E:327:NAG:O3	3:E:327:NAG:C7	2.66	0.43
1:I:110:GLU:O	1:I:111:ALA:CB	2.67	0.43
2:J:81:ASN:OD1	2:J:87:LYS:HA	2.19	0.43
2:K:109:TYR:HB2	2:K:130:MET:HE2	2.00	0.43
3:K:327:NAG:C7	3:K:327:NAG:O3	2.67	0.43
2:K:88:THR:HG22	2:K:90:SER:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:HD12	1:A:145:ALA:H	1.83	0.43
1:C:6:ARG:CZ	1:C:6:ARG:O	2.67	0.43
1:C:64:PHE:CG	1:C:76:LEU:HD13	2.54	0.43
2:E:258:LYS:HD3	2:E:258:LYS:N	2.34	0.43
2:F:208:TYR:CG	2:F:209:PRO:N	2.79	0.43
2:F:265:LEU:HD12	2:F:266:THR:H	1.84	0.43
2:F:81:ASN:OD1	2:F:87:LYS:HA	2.19	0.43
2:F:88:THR:HG22	2:F:90:SER:H	1.83	0.43
2:K:258:LYS:O	2:K:259:ASP:C	2.56	0.43
2:E:97:CYS:CB	2:E:163:CYS:HG	2.32	0.43
2:F:216:TRP:CD1	2:F:269:VAL:HG21	2.54	0.43
1:I:74:VAL:O	1:I:100:PRO:HD2	2.19	0.43
2:J:109:TYR:HB2	2:J:130:MET:HE2	2.00	0.43
2:K:188:VAL:HB	2:K:294:THR:O	2.19	0.43
1:A:110:GLU:O	1:A:111:ALA:CB	2.66	0.42
1:A:69:CYS:HA	1:A:70:PRO:HD3	1.79	0.42
1:C:112:LYS:HB3	1:C:113:PRO:HD2	2.01	0.42
2:F:258:LYS:O	2:F:259:ASP:C	2.57	0.42
1:H:143:LEU:HD12	1:H:145:ALA:H	1.84	0.42
2:J:185:THR:CG2	2:J:187:LYS:HE3	2.49	0.42
2:J:33:ILE:HD13	2:J:63:ASP:HB3	2.00	0.42
2:K:277:SER:O	2:K:278:GLN:HB3	2.19	0.42
2:D:294:THR:HB	2:D:295:CYS:H	1.54	0.42
2:E:88:THR:HG21	2:E:113:ALA:H	1.82	0.42
2:F:216:TRP:CE2	2:F:269:VAL:HG21	2.54	0.42
3:F:326:NAG:C8	3:F:326:NAG:H3	2.41	0.42
1:H:110:GLU:O	1:H:111:ALA:CB	2.66	0.42
2:J:196:GLY:HA3	2:J:270:ARG:CZ	2.49	0.42
2:K:81:ASN:OD1	2:K:87:LYS:HA	2.18	0.42
1:B:143:LEU:HD12	1:B:145:ALA:H	1.83	0.42
1:A:125:GLN:HE21	1:C:8:PRO:HA	1.81	0.42
2:D:258:LYS:O	2:D:259:ASP:C	2.57	0.42
2:E:196:GLY:HA3	2:E:270:ARG:CZ	2.49	0.42
1:G:50:VAL:HG13	1:G:56:TYR:CZ	2.54	0.42
1:G:83:ILE:O	1:G:83:ILE:CG1	2.66	0.42
1:I:57:LEU:O	1:I:154:ILE:HA	2.19	0.42
2:J:265:LEU:HD12	2:J:266:THR:H	1.84	0.42
2:L:109:TYR:HB2	2:L:130:MET:HE2	2.00	0.42
2:L:294:THR:HB	2:L:295:CYS:H	1.56	0.42
2:E:36:ASN:HD22	2:E:43:ASN:ND2	2.18	0.42
1:G:61:GLN:O	1:G:150:VAL:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:6:ARG:CZ	1:I:6:ARG:O	2.67	0.42
2:K:209:PRO:HA	2:K:210:PRO:HD2	1.84	0.42
1:A:19:ASN:HD22	1:A:20:PRO:N	2.18	0.42
1:B:110:GLU:O	1:B:111:ALA:CB	2.67	0.42
1:B:19:ASN:HD22	1:B:20:PRO:N	2.18	0.42
2:F:88:THR:HG21	2:F:113:ALA:H	1.85	0.42
2:F:196:GLY:HA3	2:F:270:ARG:NH2	2.35	0.42
1:H:19:ASN:HD22	1:H:20:PRO:N	2.18	0.42
1:I:143:LEU:HD12	1:I:145:ALA:H	1.84	0.42
2:J:88:THR:HG23	2:J:113:ALA:HB3	2.01	0.42
2:K:196:GLY:HA3	2:K:270:ARG:CZ	2.50	0.42
2:L:112:THR:HG23	2:L:113:ALA:N	2.35	0.42
2:L:12:LYS:HG3	2:L:18:ASP:OD2	2.20	0.42
1:A:100:PRO:CG	1:A:101:CYS:H	2.31	0.42
1:A:37:LEU:HD12	1:A:41:VAL:HG22	2.02	0.42
1:B:57:LEU:O	1:B:154:ILE:HA	2.19	0.42
1:B:83:ILE:CG1	1:B:83:ILE:O	2.67	0.42
2:D:185:THR:CG2	2:D:187:LYS:HE3	2.49	0.42
2:E:186:VAL:C	2:E:187:LYS:HG3	2.40	0.42
2:F:257:ASP:O	2:F:258:LYS:O	2.37	0.42
1:G:74:VAL:O	1:G:100:PRO:HD2	2.20	0.42
2:K:64:TYR:N	2:K:64:TYR:CD1	2.88	0.42
2:D:258:LYS:O	2:D:260:ALA:N	2.53	0.42
2:D:81:ASN:OD1	2:D:87:LYS:HA	2.19	0.42
2:J:55:ARG:CG	3:J:326:NAG:H82	2.49	0.42
2:L:88:THR:HG23	2:L:113:ALA:HB3	2.02	0.42
1:C:110:GLU:O	1:C:111:ALA:CB	2.67	0.42
1:C:83:ILE:O	1:C:83:ILE:CG1	2.67	0.42
2:D:109:TYR:HB2	2:D:130:MET:HE2	2.02	0.42
2:D:216:TRP:CD1	2:D:269:VAL:HG21	2.55	0.42
2:E:216:TRP:CD1	2:E:269:VAL:HG21	2.54	0.42
1:G:31:ARG:O	1:G:32:ARG:HD3	2.19	0.42
1:G:6:ARG:CZ	1:G:6:ARG:O	2.68	0.42
1:I:13:VAL:CG2	1:I:14:ALA:N	2.83	0.42
2:L:97:CYS:HG	2:L:163:CYS:HG	1.64	0.42
1:A:64:PHE:CG	1:A:76:LEU:HD13	2.55	0.42
1:H:19:ASN:HB2	1:H:29:LEU:HD11	2.01	0.42
2:K:69:TRP:O	2:K:73:MET:HG3	2.20	0.42
2:L:179:PRO:HB2	2:L:208:TYR:CZ	2.55	0.42
3:L:326:NAG:H3	3:L:326:NAG:C8	2.50	0.42
1:C:58:ILE:O	1:C:121:GLY:HA2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:25:TYR:O	2:E:26:ASN:HB2	2.20	0.41
1:H:69:CYS:HA	1:H:70:PRO:HD3	1.80	0.41
2:L:88:THR:HG21	2:L:113:ALA:H	1.85	0.41
1:A:31:ARG:HD2	2:D:99:GLU:HG2	2.01	0.41
1:A:72:THR:HG22	1:A:73:HIS:N	2.35	0.41
1:B:69:CYS:H	1:B:106:PRO:CG	2.33	0.41
2:F:88:THR:HG23	2:F:113:ALA:HB3	2.02	0.41
2:F:12:LYS:HG3	2:F:18:ASP:OD2	2.20	0.41
2:F:209:PRO:HA	2:F:210:PRO:HD2	1.83	0.41
2:F:280:VAL:HG23	2:F:294:THR:CG2	2.49	0.41
1:G:110:GLU:O	1:G:111:ALA:CB	2.66	0.41
2:K:88:THR:HG21	2:K:113:ALA:H	1.86	0.41
2:L:229:VAL:HG21	2:L:232:ARG:CZ	2.51	0.41
1:A:50:VAL:HG13	1:A:56:TYR:CZ	2.54	0.41
2:E:174:ALA:O	2:E:175:LYS:C	2.57	0.41
2:F:50:TRP:HB3	2:F:177:LYS:CD	2.23	0.41
1:G:64:PHE:CG	1:G:76:LEU:HD13	2.54	0.41
2:J:277:SER:O	2:J:278:GLN:HB3	2.20	0.41
1:H:33:ALA:HB2	2:K:165:LEU:HD21	2.02	0.41
2:E:265:LEU:HD12	2:E:266:THR:H	1.85	0.41
2:E:88:THR:HG23	2:E:113:ALA:HB3	2.03	0.41
2:F:64:TYR:N	2:F:64:TYR:CD1	2.88	0.41
1:I:50:VAL:HG13	1:I:56:TYR:CZ	2.55	0.41
2:K:206:SER:HB2	2:K:262:THR:HG21	2.01	0.41
2:L:81:ASN:OD1	2:L:87:LYS:HA	2.18	0.41
1:A:19:ASN:HB2	1:A:29:LEU:HD11	2.02	0.41
1:B:100:PRO:CG	1:B:101:CYS:H	2.32	0.41
1:G:69:CYS:HA	1:G:70:PRO:HD3	1.79	0.41
2:J:179:PRO:HB2	2:J:208:TYR:CZ	2.56	0.41
2:K:216:TRP:CD1	2:K:269:VAL:HG21	2.55	0.41
2:L:196:GLY:HA3	2:L:270:ARG:CZ	2.50	0.41
2:L:25:TYR:O	2:L:26:ASN:HB2	2.20	0.41
2:L:216:TRP:CD1	2:L:269:VAL:HG21	2.55	0.41
2:L:277:SER:O	2:L:278:GLN:HB3	2.20	0.41
2:L:7:TYR:HB2	2:L:93:LEU:HB3	2.02	0.41
2:D:88:THR:HG21	2:D:113:ALA:H	1.85	0.41
2:D:55:ARG:C	2:D:57:PRO:HD3	2.41	0.41
2:E:258:LYS:O	2:E:259:ASP:C	2.58	0.41
1:H:19:ASN:CB	1:H:29:LEU:HD11	2.49	0.41
2:K:112:THR:HG23	2:K:113:ALA:N	2.36	0.41
1:G:112:LYS:HB3	1:G:113:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:32:ARG:HD3	1:G:32:ARG:HA	1.84	0.41
1:H:57:LEU:O	1:H:154:ILE:HA	2.20	0.41
1:I:64:PHE:CG	1:I:76:LEU:HD13	2.56	0.41
1:I:69:CYS:H	1:I:106:PRO:CG	2.33	0.41
2:K:196:GLY:HA3	2:K:270:ARG:NH2	2.36	0.41
1:A:112:LYS:HE3	1:B:103:ARG:HD3	2.03	0.41
1:B:69:CYS:HA	1:B:70:PRO:HD3	1.80	0.41
2:E:179:PRO:HB2	2:E:208:TYR:CZ	2.56	0.41
2:F:112:THR:HG23	2:F:113:ALA:N	2.35	0.41
2:J:209:PRO:HA	2:J:210:PRO:HD2	1.83	0.41
2:J:222:PHE:O	2:J:223:LYS:C	2.59	0.41
2:K:13:ASP:OD1	2:K:14:ASP:N	2.54	0.41
1:A:112:LYS:HB3	1:A:113:PRO:HD2	2.03	0.41
2:D:265:LEU:HD12	2:D:266:THR:H	1.86	0.41
2:E:277:SER:O	2:E:278:GLN:HB3	2.20	0.41
2:F:97:CYS:CB	2:F:163:CYS:HG	2.34	0.41
1:G:83:ILE:CD1	1:G:88:GLN:HA	2.51	0.41
1:I:29:LEU:N	1:I:29:LEU:HD12	2.36	0.41
2:L:50:TRP:HB3	2:L:177:LYS:CD	2.22	0.41
2:L:64:TYR:N	2:L:64:TYR:CD1	2.89	0.41
2:L:97:CYS:CB	2:L:163:CYS:HG	2.34	0.41
1:C:61:GLN:O	1:C:150:VAL:HA	2.21	0.41
1:C:69:CYS:HA	1:C:70:PRO:HD3	1.79	0.41
2:E:12:LYS:HG3	2:E:18:ASP:OD2	2.20	0.41
2:F:185:THR:CG2	2:F:187:LYS:HE3	2.50	0.41
2:F:277:SER:O	2:F:278:GLN:HB3	2.21	0.41
1:G:57:LEU:O	1:G:154:ILE:HA	2.21	0.41
1:H:103:ARG:NH2	1:H:103:ARG:HG2	2.35	0.41
1:H:69:CYS:H	1:H:106:PRO:CG	2.34	0.41
2:K:265:LEU:HD12	2:K:266:THR:H	1.86	0.41
2:J:216:TRP:CD1	2:J:269:VAL:HG21	2.56	0.41
2:D:285:HIS:HD2	2:D:287:THR:OG1	2.04	0.40
2:E:229:VAL:HG21	2:E:232:ARG:CZ	2.51	0.40
1:G:103:ARG:NH2	1:G:103:ARG:HG2	2.36	0.40
1:G:29:LEU:N	1:G:29:LEU:HD12	2.36	0.40
1:H:32:ARG:HD3	1:H:32:ARG:HA	1.83	0.40
1:I:112:LYS:HB3	1:I:113:PRO:HD2	2.02	0.40
1:I:83:ILE:O	1:I:83:ILE:CG1	2.69	0.40
2:J:80:ILE:HG23	2:J:86:THR:CG2	2.51	0.40
2:K:257:ASP:O	2:K:258:LYS:O	2.39	0.40
2:K:285:HIS:HD2	2:K:287:THR:H	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:55:ARG:CD	3:L:326:NAG:H82	2.51	0.40
2:E:188:VAL:HB	2:E:294:THR:O	2.21	0.40
2:F:229:VAL:HG21	2:F:232:ARG:CZ	2.51	0.40
2:J:174:ALA:O	2:J:175:LYS:C	2.60	0.40
2:L:237:TRP:HE1	2:L:275:MET:HE1	1.86	0.40
1:A:12:PRO:HG2	1:A:156:ALA:CB	2.50	0.40
1:B:83:ILE:CD1	1:B:88:GLN:HA	2.52	0.40
2:E:191:ASN:C	2:E:199:THR:HG22	2.42	0.40
1:G:55:LEU:HA	1:G:55:LEU:HD12	1.93	0.40
1:G:72:THR:HG22	1:G:73:HIS:N	2.36	0.40
1:I:100:PRO:CG	1:I:101:CYS:H	2.31	0.40
1:I:58:ILE:O	1:I:121:GLY:HA2	2.22	0.40
1:I:12:PRO:HG2	1:I:156:ALA:CB	2.49	0.40
1:I:19:ASN:HB2	1:I:29:LEU:HD11	2.04	0.40
2:J:196:GLY:HA3	2:J:270:ARG:NH2	2.36	0.40
2:L:280:VAL:CG2	2:L:292:VAL:HG12	2.51	0.40
2:L:55:ARG:C	2:L:57:PRO:HD3	2.42	0.40
1:A:103:ARG:HD3	1:C:112:LYS:HE3	2.04	0.40
2:D:186:VAL:C	2:D:187:LYS:HG3	2.42	0.40
2:E:55:ARG:C	2:E:57:PRO:HD3	2.42	0.40
1:G:32:ARG:HH21	1:G:32:ARG:HG3	1.87	0.40
2:J:64:TYR:CD1	2:J:64:TYR:N	2.89	0.40
2:D:174:ALA:O	2:D:175:LYS:C	2.59	0.40
2:D:206:SER:C	2:D:262:THR:OG1	2.60	0.40
2:E:184:PRO:HB2	2:E:204:VAL:HG12	2.04	0.40
2:E:196:GLY:HA3	2:E:270:ARG:NH2	2.36	0.40
1:G:92:ASN:ND2	1:H:146:GLU:OE1	2.45	0.40
1:H:19:ASN:HD22	1:H:19:ASN:C	2.25	0.40
2:J:280:VAL:HG23	2:J:294:THR:CG2	2.47	0.40
2:J:7:TYR:HB2	2:J:93:LEU:HB3	2.04	0.40
2:K:88:THR:HG23	2:K:113:ALA:HB3	2.03	0.40

All (1) 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)
2:D:14:ASP:O	2:J:62:ASN:OD1[2_545]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	150/161 (93%)	127 (85%)	11 (7%)	12 (8%)	1	2
1	B	150/161 (93%)	127 (85%)	11 (7%)	12 (8%)	1	2
1	C	150/161 (93%)	128 (85%)	10 (7%)	12 (8%)	1	2
1	G	150/161 (93%)	127 (85%)	11 (7%)	12 (8%)	1	2
1	H	150/161 (93%)	127 (85%)	11 (7%)	12 (8%)	1	2
1	I	150/161 (93%)	128 (85%)	10 (7%)	12 (8%)	1	2
2	D	297/324 (92%)	256 (86%)	21 (7%)	20 (7%)	1	3
2	E	297/324 (92%)	256 (86%)	22 (7%)	19 (6%)	1	3
2	F	297/324 (92%)	257 (86%)	20 (7%)	20 (7%)	1	3
2	J	297/324 (92%)	256 (86%)	21 (7%)	20 (7%)	1	3
2	K	297/324 (92%)	255 (86%)	23 (8%)	19 (6%)	1	3
2	L	297/324 (92%)	256 (86%)	21 (7%)	20 (7%)	1	3
All	All	2682/2910 (92%)	2300 (86%)	192 (7%)	190 (7%)	1	2

All (190) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	33	ALA
1	A	88	GLN
1	A	105	THR
1	A	110	GLU
1	B	9	SER
1	B	33	ALA
1	B	88	GLN
1	B	105	THR
1	B	110	GLU
1	C	9	SER
1	C	33	ALA

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Mol	Chain	Res	Type
1	C	88	GLN
1	C	105	THR
1	C	110	GLU
2	D	13	ASP
2	D	258	LYS
2	D	259	ASP
2	E	13	ASP
2	E	258	LYS
2	E	259	ASP
2	F	13	ASP
2	F	258	LYS
2	F	259	ASP
1	G	9	SER
1	G	33	ALA
1	G	88	GLN
1	G	105	THR
1	G	110	GLU
1	H	9	SER
1	H	33	ALA
1	H	88	GLN
1	H	105	THR
1	H	110	GLU
1	I	9	SER
1	I	33	ALA
1	I	88	GLN
1	I	105	THR
1	I	110	GLU
2	J	13	ASP
2	J	258	LYS
2	J	259	ASP
2	K	13	ASP
2	K	258	LYS
2	K	259	ASP
2	L	13	ASP
2	L	258	LYS
2	L	259	ASP
1	A	10	ASP
1	A	111	ALA
1	A	147	SER
1	B	10	ASP
1	B	111	ALA
1	B	147	SER

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Mol	Chain	Res	Type
1	C	10	ASP
1	C	72	THR
1	C	111	ALA
1	C	147	SER
2	D	206	SER
2	D	230	ASN
2	E	206	SER
2	E	230	ASN
2	F	206	SER
2	F	230	ASN
1	G	10	ASP
1	G	111	ALA
1	G	147	SER
1	H	10	ASP
1	H	100	PRO
1	H	111	ALA
1	H	147	SER
1	I	10	ASP
1	I	111	ALA
1	I	147	SER
2	J	206	SER
2	J	230	ASN
2	K	206	SER
2	K	230	ASN
2	L	206	SER
2	L	230	ASN
1	A	72	THR
1	A	100	PRO
1	B	72	THR
1	B	100	PRO
1	C	100	PRO
2	D	12	LYS
2	D	175	LYS
2	D	275	MET
2	D	276	SER
2	D	295	CYS
2	E	12	LYS
2	E	175	LYS
2	E	275	MET
2	E	276	SER
2	E	295	CYS
2	F	12	LYS

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Mol	Chain	Res	Type
2	F	175	LYS
2	F	275	MET
2	F	276	SER
2	F	295	CYS
1	G	72	THR
1	G	100	PRO
1	H	72	THR
1	I	72	THR
1	I	100	PRO
2	J	12	LYS
2	J	175	LYS
2	J	275	MET
2	J	276	SER
2	J	295	CYS
2	K	12	LYS
2	K	175	LYS
2	K	275	MET
2	K	276	SER
2	K	295	CYS
2	L	12	LYS
2	L	175	LYS
2	L	223	LYS
2	L	275	MET
2	L	276	SER
2	L	295	CYS
1	A	70	PRO
1	B	70	PRO
1	C	70	PRO
2	D	87	LYS
2	D	197	ASN
2	D	208	TYR
2	D	278	GLN
2	E	87	LYS
2	E	161	MET
2	E	197	ASN
2	E	223	LYS
2	E	278	GLN
2	F	87	LYS
2	F	194	GLU
2	F	223	LYS
2	F	278	GLN
1	G	70	PRO

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Mol	Chain	Res	Type
1	H	70	PRO
1	I	70	PRO
2	J	87	LYS
2	J	194	GLU
2	J	197	ASN
2	J	223	LYS
2	J	278	GLN
2	K	87	LYS
2	K	161	MET
2	K	193	LEU
2	K	194	GLU
2	K	197	ASN
2	K	278	GLN
2	L	87	LYS
2	L	197	ASN
2	L	278	GLN
1	C	146	GLU
2	D	161	MET
2	D	193	LEU
2	D	194	GLU
2	D	277	SER
2	D	289	GLU
2	E	193	LEU
2	E	194	GLU
2	E	208	TYR
2	E	277	SER
2	F	161	MET
2	F	193	LEU
2	F	197	ASN
2	F	208	TYR
2	F	277	SER
2	F	289	GLU
1	H	146	GLU
1	I	146	GLU
2	J	161	MET
2	J	193	LEU
2	J	208	TYR
2	J	277	SER
2	K	208	TYR
2	K	223	LYS
2	K	277	SER
2	L	161	MET

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Mol	Chain	Res	Type
2	L	193	LEU
2	L	194	GLU
2	L	208	TYR
2	L	277	SER
1	A	146	GLU
1	B	146	GLU
2	D	223	LYS
1	G	146	GLU
2	J	289	GLU
2	L	289	GLU

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	128/136 (94%)	111 (87%)	17 (13%)	4	12
1	B	128/136 (94%)	110 (86%)	18 (14%)	3	10
1	C	128/136 (94%)	110 (86%)	18 (14%)	3	10
1	G	128/136 (94%)	111 (87%)	17 (13%)	4	12
1	H	128/136 (94%)	110 (86%)	18 (14%)	3	10
1	I	128/136 (94%)	110 (86%)	18 (14%)	3	10
2	D	267/288 (93%)	249 (93%)	18 (7%)	16	43
2	E	267/288 (93%)	249 (93%)	18 (7%)	16	43
2	F	267/288 (93%)	249 (93%)	18 (7%)	16	43
2	J	267/288 (93%)	249 (93%)	18 (7%)	16	43
2	K	267/288 (93%)	249 (93%)	18 (7%)	16	43
2	L	267/288 (93%)	249 (93%)	18 (7%)	16	43
All	All	2370/2544 (93%)	2156 (91%)	214 (9%)	9	28

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	19	ASN
1	A	29	LEU
1	A	41	VAL
1	A	55	LEU
1	A	63	LEU
1	A	79	THR
1	A	82	ARG
1	A	83	ILE
1	A	88	GLN
1	A	104	GLU
1	A	120	LEU
1	A	125	GLN
1	A	126	LEU
1	A	140	ASP
1	A	142	LEU
1	A	144	PHE
1	B	6	ARG
1	B	19	ASN
1	B	29	LEU
1	B	30	ASN
1	B	41	VAL
1	B	55	LEU
1	B	63	LEU
1	B	79	THR
1	B	82	ARG
1	B	83	ILE
1	B	88	GLN
1	B	104	GLU
1	B	120	LEU
1	B	125	GLN
1	B	126	LEU
1	B	140	ASP
1	B	142	LEU
1	B	144	PHE
1	C	6	ARG
1	C	19	ASN
1	C	29	LEU
1	C	30	ASN
1	C	41	VAL
1	C	55	LEU
1	C	63	LEU
1	C	79	THR

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Mol	Chain	Res	Type
1	C	82	ARG
1	C	83	ILE
1	C	88	GLN
1	C	104	GLU
1	C	120	LEU
1	C	125	GLN
1	C	126	LEU
1	C	140	ASP
1	C	142	LEU
1	C	144	PHE
2	D	2	THR
2	D	11	LEU
2	D	20	VAL
2	D	41	HIS
2	D	62	ASN
2	D	112	THR
2	D	122	THR
2	D	146	THR
2	D	195	ASP
2	D	197	ASN
2	D	199	THR
2	D	203	THR
2	D	214	THR
2	D	237	TRP
2	D	239	ARG
2	D	258	LYS
2	D	270	ARG
2	D	288	LEU
2	E	2	THR
2	E	11	LEU
2	E	20	VAL
2	E	41	HIS
2	E	62	ASN
2	E	112	THR
2	E	122	THR
2	E	146	THR
2	E	195	ASP
2	E	197	ASN
2	E	199	THR
2	E	203	THR
2	E	214	THR
2	E	237	TRP

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Mol	Chain	Res	Type
2	E	239	ARG
2	E	258	LYS
2	E	270	ARG
2	E	288	LEU
2	F	2	THR
2	F	11	LEU
2	F	20	VAL
2	F	41	HIS
2	F	62	ASN
2	F	112	THR
2	F	122	THR
2	F	146	THR
2	F	195	ASP
2	F	197	ASN
2	F	199	THR
2	F	203	THR
2	F	214	THR
2	F	237	TRP
2	F	239	ARG
2	F	258	LYS
2	F	270	ARG
2	F	288	LEU
1	G	6	ARG
1	G	19	ASN
1	G	29	LEU
1	G	41	VAL
1	G	55	LEU
1	G	63	LEU
1	G	79	THR
1	G	82	ARG
1	G	83	ILE
1	G	88	GLN
1	G	104	GLU
1	G	120	LEU
1	G	125	GLN
1	G	126	LEU
1	G	140	ASP
1	G	142	LEU
1	G	144	PHE
1	H	6	ARG
1	H	19	ASN
1	H	29	LEU

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Mol	Chain	Res	Type
1	H	30	ASN
1	H	41	VAL
1	H	55	LEU
1	H	63	LEU
1	H	79	THR
1	H	82	ARG
1	H	83	ILE
1	H	88	GLN
1	H	104	GLU
1	H	120	LEU
1	H	125	GLN
1	H	126	LEU
1	H	140	ASP
1	H	142	LEU
1	H	144	PHE
1	I	6	ARG
1	I	19	ASN
1	I	29	LEU
1	I	30	ASN
1	I	41	VAL
1	I	55	LEU
1	I	63	LEU
1	I	79	THR
1	I	82	ARG
1	I	83	ILE
1	I	88	GLN
1	I	104	GLU
1	I	120	LEU
1	I	125	GLN
1	I	126	LEU
1	I	140	ASP
1	I	142	LEU
1	I	144	PHE
2	J	2	THR
2	J	11	LEU
2	J	20	VAL
2	J	41	HIS
2	J	62	ASN
2	J	112	THR
2	J	122	THR
2	J	146	THR
2	J	195	ASP

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Mol	Chain	Res	Type
2	J	197	ASN
2	J	199	THR
2	J	203	THR
2	J	214	THR
2	J	237	TRP
2	J	239	ARG
2	J	258	LYS
2	J	270	ARG
2	J	288	LEU
2	K	2	THR
2	K	11	LEU
2	K	20	VAL
2	K	41	HIS
2	K	62	ASN
2	K	112	THR
2	K	122	THR
2	K	146	THR
2	K	195	ASP
2	K	197	ASN
2	K	199	THR
2	K	203	THR
2	K	214	THR
2	K	237	TRP
2	K	239	ARG
2	K	258	LYS
2	K	270	ARG
2	K	288	LEU
2	L	2	THR
2	L	11	LEU
2	L	20	VAL
2	L	41	HIS
2	L	62	ASN
2	L	112	THR
2	L	122	THR
2	L	146	THR
2	L	195	ASP
2	L	197	ASN
2	L	199	THR
2	L	203	THR
2	L	214	THR
2	L	237	TRP
2	L	239	ARG

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Mol	Chain	Res	Type
2	L	258	LYS
2	L	270	ARG
2	L	288	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	27	GLN
1	A	30	ASN
1	A	61	GLN
1	A	88	GLN
1	A	102	GLN
1	A	125	GLN
1	B	19	ASN
1	B	27	GLN
1	B	30	ASN
1	B	61	GLN
1	B	88	GLN
1	B	102	GLN
1	B	125	GLN
1	C	19	ASN
1	C	27	GLN
1	C	30	ASN
1	C	61	GLN
1	C	88	GLN
1	C	102	GLN
1	C	125	GLN
2	D	28	GLN
2	D	41	HIS
2	D	43	ASN
2	D	45	ASN
2	D	114	ASN
2	D	121	HIS
2	D	278	GLN
2	D	285	HIS
2	E	28	GLN
2	E	41	HIS
2	E	43	ASN
2	E	45	ASN
2	E	114	ASN
2	E	121	HIS

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Mol	Chain	Res	Type
2	E	278	GLN
2	E	285	HIS
2	F	28	GLN
2	F	41	HIS
2	F	43	ASN
2	F	45	ASN
2	F	114	ASN
2	F	121	HIS
2	F	278	GLN
2	F	285	HIS
1	G	19	ASN
1	G	27	GLN
1	G	30	ASN
1	G	61	GLN
1	G	88	GLN
1	G	102	GLN
1	G	125	GLN
1	H	19	ASN
1	H	27	GLN
1	H	30	ASN
1	H	61	GLN
1	H	88	GLN
1	H	102	GLN
1	H	125	GLN
1	I	19	ASN
1	I	27	GLN
1	I	30	ASN
1	I	61	GLN
1	I	88	GLN
1	I	102	GLN
1	I	125	GLN
2	J	28	GLN
2	J	41	HIS
2	J	43	ASN
2	J	45	ASN
2	J	114	ASN
2	J	121	HIS
2	J	278	GLN
2	J	285	HIS
2	K	28	GLN
2	K	41	HIS
2	K	43	ASN

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Mol	Chain	Res	Type
2	K	45	ASN
2	K	114	ASN
2	K	121	HIS
2	K	278	GLN
2	K	285	HIS
2	L	28	GLN
2	L	41	HIS
2	L	43	ASN
2	L	45	ASN
2	L	114	ASN
2	L	121	HIS
2	L	278	GLN
2	L	285	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

18 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	E	327	2	14,14,15	0.75	1 (7%)	17,19,21	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	326	2	14,14,15	1.08	1 (7%)	17,19,21	0.93	1 (5%)
3	NAG	K	326	2	14,14,15	0.85	1 (7%)	17,19,21	0.90	0
3	NAG	F	326	2	14,14,15	0.82	1 (7%)	17,19,21	0.66	0
3	NAG	E	326	2	14,14,15	1.01	1 (7%)	17,19,21	1.16	1 (5%)
3	NAG	F	327	2	14,14,15	0.79	1 (7%)	17,19,21	0.65	0
3	NAG	J	327	2	14,14,15	0.70	0	17,19,21	0.59	0
3	NAG	E	325	2	14,14,15	0.55	0	17,19,21	0.82	0
3	NAG	D	327	2	14,14,15	0.85	1 (7%)	17,19,21	0.86	0
3	NAG	L	325	2	14,14,15	0.57	0	17,19,21	0.76	1 (5%)
3	NAG	K	327	2	14,14,15	0.89	1 (7%)	17,19,21	0.63	0
3	NAG	J	325	2	14,14,15	0.54	0	17,19,21	0.93	1 (5%)
3	NAG	D	325	2	14,14,15	0.61	0	17,19,21	0.87	0
3	NAG	J	326	2	14,14,15	0.86	1 (7%)	17,19,21	0.95	2 (11%)
3	NAG	L	326	2	14,14,15	0.87	1 (7%)	17,19,21	0.80	0
3	NAG	F	325	2	14,14,15	0.74	0	17,19,21	0.72	1 (5%)
3	NAG	K	325	2	14,14,15	0.58	0	17,19,21	0.73	0
3	NAG	L	327	2	14,14,15	0.65	0	17,19,21	0.73	1 (5%)

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	E	327	2	-	5/6/23/26	0/1/1/1
3	NAG	D	326	2	-	3/6/23/26	0/1/1/1
3	NAG	K	326	2	-	5/6/23/26	0/1/1/1
3	NAG	F	326	2	-	3/6/23/26	0/1/1/1
3	NAG	E	326	2	-	5/6/23/26	0/1/1/1
3	NAG	F	327	2	-	5/6/23/26	0/1/1/1
3	NAG	J	327	2	-	4/6/23/26	0/1/1/1
3	NAG	E	325	2	-	0/6/23/26	0/1/1/1
3	NAG	D	327	2	-	6/6/23/26	0/1/1/1
3	NAG	L	325	2	-	4/6/23/26	0/1/1/1
3	NAG	K	327	2	-	4/6/23/26	0/1/1/1
3	NAG	J	325	2	-	2/6/23/26	0/1/1/1
3	NAG	D	325	2	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	J	326	2	-	5/6/23/26	0/1/1/1
3	NAG	L	326	2	-	5/6/23/26	0/1/1/1
3	NAG	F	325	2	-	4/6/23/26	0/1/1/1
3	NAG	K	325	2	-	0/6/23/26	0/1/1/1
3	NAG	L	327	2	-	3/6/23/26	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	326	NAG	C1-C2	3.41	1.57	1.52
3	E	326	NAG	C1-C2	3.21	1.57	1.52
3	K	327	NAG	C1-C2	2.81	1.56	1.52
3	J	326	NAG	C1-C2	2.74	1.56	1.52
3	D	327	NAG	C1-C2	2.58	1.56	1.52
3	K	326	NAG	C1-C2	2.57	1.56	1.52
3	L	326	NAG	C1-C2	2.52	1.56	1.52
3	F	326	NAG	C1-C2	2.40	1.55	1.52
3	E	327	NAG	C1-C2	2.33	1.55	1.52
3	F	327	NAG	C1-C2	2.30	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	326	NAG	C3-C4-C5	-3.12	104.68	110.24
3	J	325	NAG	C3-C4-C5	-2.55	105.68	110.24
3	L	325	NAG	C2-N2-C7	-2.30	119.63	122.90
3	F	325	NAG	C2-N2-C7	-2.21	119.75	122.90
3	D	326	NAG	C3-C4-C5	-2.18	106.36	110.24
3	J	326	NAG	C2-N2-C7	-2.10	119.91	122.90
3	J	326	NAG	C4-C3-C2	2.09	114.09	111.02
3	L	327	NAG	C2-N2-C7	-2.07	119.96	122.90

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	326	NAG	C3-C2-N2-C7
3	D	326	NAG	C8-C7-N2-C2
3	D	326	NAG	O7-C7-N2-C2
3	K	326	NAG	C3-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
3	K	326	NAG	C8-C7-N2-C2
3	K	326	NAG	O7-C7-N2-C2
3	F	326	NAG	C3-C2-N2-C7
3	F	326	NAG	C8-C7-N2-C2
3	F	326	NAG	O7-C7-N2-C2
3	E	326	NAG	C3-C2-N2-C7
3	E	326	NAG	C8-C7-N2-C2
3	E	326	NAG	O7-C7-N2-C2
3	F	327	NAG	C8-C7-N2-C2
3	F	327	NAG	O7-C7-N2-C2
3	J	327	NAG	C8-C7-N2-C2
3	J	327	NAG	O7-C7-N2-C2
3	D	327	NAG	C8-C7-N2-C2
3	D	327	NAG	O7-C7-N2-C2
3	K	327	NAG	C8-C7-N2-C2
3	K	327	NAG	O7-C7-N2-C2
3	L	326	NAG	C3-C2-N2-C7
3	L	326	NAG	C8-C7-N2-C2
3	L	326	NAG	O7-C7-N2-C2
3	J	326	NAG	C3-C2-N2-C7
3	J	326	NAG	C8-C7-N2-C2
3	J	326	NAG	O7-C7-N2-C2
3	E	327	NAG	C3-C2-N2-C7
3	E	327	NAG	C8-C7-N2-C2
3	E	327	NAG	O7-C7-N2-C2
3	L	327	NAG	C8-C7-N2-C2
3	L	327	NAG	O7-C7-N2-C2
3	J	326	NAG	O5-C5-C6-O6
3	J	327	NAG	C1-C2-N2-C7
3	D	327	NAG	C1-C2-N2-C7
3	L	325	NAG	O5-C5-C6-O6
3	K	326	NAG	O5-C5-C6-O6
3	J	326	NAG	C4-C5-C6-O6
3	F	325	NAG	O5-C5-C6-O6
3	L	325	NAG	C4-C5-C6-O6
3	L	326	NAG	C4-C5-C6-O6
3	K	326	NAG	C4-C5-C6-O6
3	F	325	NAG	C4-C5-C6-O6
3	F	325	NAG	C8-C7-N2-C2
3	L	326	NAG	O5-C5-C6-O6
3	D	327	NAG	C4-C5-C6-O6
3	E	326	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	F	327	NAG	C1-C2-N2-C7
3	F	325	NAG	O7-C7-N2-C2
3	K	327	NAG	C1-C2-N2-C7
3	D	327	NAG	O5-C5-C6-O6
3	E	327	NAG	O5-C5-C6-O6
3	E	326	NAG	C4-C5-C6-O6
3	K	327	NAG	C3-C2-N2-C7
3	F	327	NAG	C4-C5-C6-O6
3	J	325	NAG	C4-C5-C6-O6
3	D	325	NAG	C4-C5-C6-O6
3	E	327	NAG	C1-C2-N2-C7
3	F	327	NAG	C3-C2-N2-C7
3	J	327	NAG	C3-C2-N2-C7
3	D	327	NAG	C3-C2-N2-C7
3	J	325	NAG	O5-C5-C6-O6
3	L	325	NAG	C8-C7-N2-C2
3	L	327	NAG	C1-C2-N2-C7
3	L	325	NAG	O7-C7-N2-C2
3	D	325	NAG	O5-C5-C6-O6

There are no ring outliers.

11 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	327	NAG	1	0
3	D	326	NAG	1	0
3	K	326	NAG	3	0
3	F	326	NAG	5	0
3	E	326	NAG	3	0
3	D	327	NAG	2	0
3	K	327	NAG	1	0
3	J	325	NAG	2	0
3	J	326	NAG	1	0
3	L	326	NAG	5	0
3	L	327	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	152/161 (94%)	0.64	17 (11%) 5 3	31, 56, 172, 191	0
1	B	152/161 (94%)	0.57	16 (10%) 6 3	28, 53, 170, 200	0
1	C	152/161 (94%)	0.48	14 (9%) 9 5	28, 56, 176, 195	0
1	G	152/161 (94%)	0.78	21 (13%) 2 1	27, 56, 176, 195	0
1	H	152/161 (94%)	0.57	19 (12%) 3 2	33, 65, 169, 194	0
1	I	152/161 (94%)	0.56	17 (11%) 5 3	31, 59, 172, 201	0
2	D	299/324 (92%)	0.45	21 (7%) 16 9	29, 58, 138, 201	0
2	E	299/324 (92%)	0.32	19 (6%) 19 12	32, 59, 134, 199	0
2	F	299/324 (92%)	0.52	28 (9%) 8 4	35, 74, 144, 201	0
2	J	299/324 (92%)	0.27	19 (6%) 19 12	31, 57, 130, 189	0
2	K	299/324 (92%)	0.36	21 (7%) 16 9	27, 59, 136, 201	0
2	L	299/324 (92%)	0.96	49 (16%) 1 1	39, 90, 153, 201	0
All	All	2706/2910 (92%)	0.52	261 (9%) 8 4	27, 63, 159, 201	0

All (261) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	196	GLY	18.1
2	L	193	LEU	16.3
2	E	197	ASN	14.9
2	K	193	LEU	14.8
2	D	193	LEU	14.5
2	K	195	ASP	12.2
2	F	193	LEU	11.6
1	G	102	GLN	11.3
1	G	6	ARG	11.2
2	L	296	SER	10.5
2	J	193	LEU	10.1

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Mol	Chain	Res	Type	RSRZ
1	A	6	ARG	10.0
1	I	110	GLU	8.8
2	L	272	THR	8.0
2	L	275	MET	7.9
1	I	103	ARG	7.9
1	A	103	ARG	7.8
2	J	197	ASN	7.7
2	E	198	MET	7.6
2	L	273	SER	7.6
1	C	103	ARG	7.6
1	I	6	ARG	7.4
2	D	296	SER	7.4
1	B	102	GLN	7.4
1	C	6	ARG	7.2
2	D	196	GLY	7.2
2	L	16	LEU	6.9
2	F	197	ASN	6.9
2	L	274	LYS	6.9
1	H	103	ARG	6.7
1	B	6	ARG	6.6
1	G	103	ARG	6.5
2	J	296	SER	6.5
1	G	104	GLU	6.5
1	I	72	THR	6.5
1	I	111	ALA	6.5
1	G	106	PRO	6.4
1	G	105	THR	6.4
2	L	197	ASN	6.3
1	A	8	PRO	6.0
1	C	105	THR	6.0
1	C	72	THR	6.0
2	K	12	LYS	5.9
2	F	296	SER	5.9
2	F	274	LYS	5.9
2	D	194	GLU	5.9
2	D	16	LEU	5.8
2	K	296	SER	5.8
2	L	195	ASP	5.8
2	E	193	LEU	5.8
2	K	271	THR	5.7
2	K	194	GLU	5.7
1	G	101	CYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	102	GLN	5.5
2	D	274	LYS	5.5
1	C	104	GLU	5.5
1	C	102	GLN	5.4
2	D	258	LYS	5.4
2	E	194	GLU	5.4
1	I	106	PRO	5.3
1	B	110	GLU	5.3
2	E	195	ASP	5.3
1	G	109	ALA	5.1
2	E	274	LYS	5.1
1	I	112	LYS	5.1
2	L	15	GLY	5.1
1	B	109	ALA	5.1
2	D	195	ASP	5.0
2	L	194	GLU	4.9
2	K	272	THR	4.9
2	E	296	SER	4.9
1	A	72	THR	4.8
2	K	273	SER	4.8
2	D	275	MET	4.7
2	J	13	ASP	4.7
1	B	101	CYS	4.7
2	F	12	LYS	4.7
1	B	107	GLU	4.6
1	B	108	GLY	4.6
2	K	274	LYS	4.6
1	B	103	ARG	4.6
1	H	112	LYS	4.6
2	F	275	MET	4.5
1	A	110	GLU	4.5
1	H	6	ARG	4.4
2	E	13	ASP	4.4
1	C	110	GLU	4.4
2	L	192	GLU	4.4
2	F	192	GLU	4.3
2	F	195	ASP	4.3
1	G	7	THR	4.3
1	C	109	ALA	4.2
1	H	72	THR	4.2
1	I	108	GLY	4.2
1	G	72	THR	4.2

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Mol	Chain	Res	Type	RSRZ
2	L	276	SER	4.2
1	A	101	CYS	4.1
1	C	111	ALA	4.1
2	L	44	VAL	4.1
2	J	14	ASP	4.1
1	I	71	SER	4.1
1	G	107	GLU	4.0
2	J	86	THR	4.0
2	F	299	CYS	4.0
2	D	15	GLY	4.0
1	I	102	GLN	4.0
1	A	106	PRO	3.9
2	D	271	THR	3.9
1	G	8	PRO	3.9
2	F	272	THR	3.8
2	K	197	ASN	3.8
1	I	109	ALA	3.8
2	L	191	ASN	3.7
2	L	12	LYS	3.7
2	K	14	ASP	3.7
1	G	110	GLU	3.7
1	I	7	THR	3.7
2	L	34	SER	3.7
2	L	295	CYS	3.7
1	A	111	ALA	3.7
2	L	196	GLY	3.7
1	H	73	HIS	3.6
2	L	270	ARG	3.6
1	H	102	GLN	3.6
1	H	107	GLU	3.6
1	H	101	CYS	3.6
1	B	112	LYS	3.5
1	I	101	CYS	3.5
1	G	111	ALA	3.5
1	H	106	PRO	3.5
1	A	107	GLU	3.5
2	F	198	MET	3.4
1	A	109	ALA	3.4
1	C	112	LYS	3.4
2	J	275	MET	3.4
2	J	274	LYS	3.3
2	L	38	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	106	PRO	3.3
1	C	73	HIS	3.3
1	C	101	CYS	3.2
2	F	196	GLY	3.2
2	L	198	MET	3.2
2	J	12	LYS	3.2
1	B	9	SER	3.2
1	G	112	LYS	3.2
2	L	299	CYS	3.1
2	K	13	ASP	3.1
2	F	70	TYR	3.1
2	F	194	GLU	3.1
2	L	43	ASN	3.1
1	B	8	PRO	3.0
2	J	272	THR	3.0
1	C	7	THR	3.0
1	H	111	ALA	3.0
1	G	69	CYS	3.0
2	K	270	ARG	3.0
1	H	9	SER	2.9
2	L	190	GLY	2.9
1	G	73	HIS	2.9
2	F	271	THR	2.9
1	B	105	THR	2.9
2	D	89	THR	2.9
2	E	278	GLN	2.9
2	E	226	TYR	2.8
1	G	108	GLY	2.8
1	H	109	ALA	2.8
1	H	69	CYS	2.8
2	L	50	TRP	2.8
2	E	196	GLY	2.8
2	F	13	ASP	2.8
1	H	108	GLY	2.8
2	L	90	SER	2.8
1	I	107	GLU	2.8
2	E	192	GLU	2.8
2	L	84	ASP	2.8
1	H	104	GLU	2.7
2	L	175	LYS	2.7
2	L	11	LEU	2.7
1	A	105	THR	2.7

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Mol	Chain	Res	Type	RSRZ
2	L	258	LYS	2.7
1	G	70	PRO	2.7
2	K	49	ASP	2.7
1	A	7	THR	2.7
2	L	17	TYR	2.7
1	H	105	THR	2.7
2	D	197	ASN	2.7
2	F	16	LEU	2.7
2	L	14	ASP	2.7
2	F	11	LEU	2.7
2	E	86	THR	2.7
2	L	260	ALA	2.7
2	F	10	THR	2.6
1	A	104	GLU	2.6
2	J	268	LEU	2.6
2	D	14	ASP	2.6
2	D	63	ASP	2.6
2	K	191	ASN	2.6
1	B	72	THR	2.6
2	E	270	ARG	2.6
2	J	41	HIS	2.6
2	J	194	GLU	2.6
2	L	259	ASP	2.6
2	L	33	ILE	2.5
2	D	11	LEU	2.5
2	L	19	GLY	2.5
1	I	8	PRO	2.5
1	G	74	VAL	2.5
1	B	7	THR	2.5
2	L	46	PHE	2.5
2	L	51	PHE	2.5
1	B	111	ALA	2.5
1	H	110	GLU	2.4
2	E	200	LEU	2.4
2	F	223	LYS	2.4
1	A	71	SER	2.4
2	F	84	ASP	2.4
1	G	146	GLU	2.4
1	I	73	HIS	2.4
2	L	271	THR	2.4
2	J	198	MET	2.3
2	E	83	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	E	258	LYS	2.3
2	F	14	ASP	2.3
2	F	44	VAL	2.3
2	J	237	TRP	2.3
2	E	12	LYS	2.3
2	L	70	TYR	2.3
2	E	14	ASP	2.3
1	A	112	LYS	2.3
2	L	277	SER	2.3
2	L	132	HIS	2.3
2	K	226	TYR	2.3
2	F	8	THR	2.2
2	L	268	LEU	2.2
2	D	259	ASP	2.2
1	I	69	CYS	2.2
2	K	15	GLY	2.2
2	F	277	SER	2.2
2	F	9	VAL	2.2
1	C	107	GLU	2.2
2	D	299	CYS	2.2
2	L	121	HIS	2.2
1	H	7	THR	2.1
2	K	288	LEU	2.1
2	F	87	LYS	2.1
2	J	195	ASP	2.1
2	D	270	ARG	2.1
2	J	85	SER	2.1
2	L	42	GLY	2.1
2	J	224	GLY	2.1
1	A	147	SER	2.1
2	L	113	ALA	2.1
2	L	41	HIS	2.1
2	D	295	CYS	2.1
2	L	53	ILE	2.1
2	K	192	GLU	2.1
2	D	13	ASP	2.0
2	J	200	LEU	2.0
2	F	273	SER	2.0
2	K	198	MET	2.0
1	H	70	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
3	NAG	F	326	14/15	0.56	0.23	141,141,141,141	0
3	NAG	D	326	14/15	0.66	0.26	112,112,112,112	0
3	NAG	F	327	14/15	0.67	0.47	140,140,140,140	0
3	NAG	J	327	14/15	0.67	0.54	140,140,140,140	0
3	NAG	E	327	14/15	0.70	0.35	140,140,140,140	0
3	NAG	K	327	14/15	0.72	0.32	140,140,140,140	0
3	NAG	E	326	14/15	0.72	0.21	81,81,81,81	0
3	NAG	D	327	14/15	0.73	0.23	140,140,140,140	0
3	NAG	L	327	14/15	0.73	0.30	140,140,140,140	0
3	NAG	K	326	14/15	0.76	0.16	122,122,122,122	0
3	NAG	L	326	14/15	0.76	0.21	128,128,128,128	0
3	NAG	J	326	14/15	0.80	0.20	96,96,96,96	0
3	NAG	L	325	14/15	0.86	0.19	90,90,90,90	0
3	NAG	F	325	14/15	0.87	0.20	79,79,79,79	0
3	NAG	D	325	14/15	0.89	0.21	57,57,57,57	0
3	NAG	J	325	14/15	0.93	0.18	49,49,49,49	0
3	NAG	K	325	14/15	0.94	0.13	54,54,54,54	0
3	NAG	E	325	14/15	0.95	0.16	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.