



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:13 PM UTC

PDB ID : 3IT8 / pdb_00003it8
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

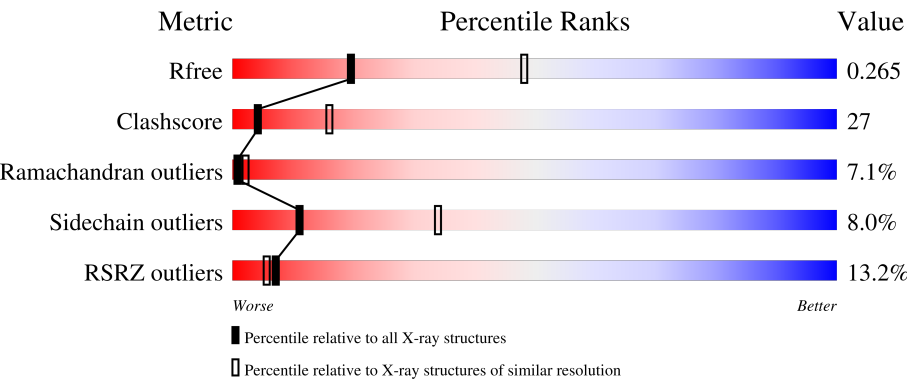
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 of 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	
1	B	161	
1	C	161	
1	G	161	
1	H	161	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	I	161	11% 48% 34% 11% 6%
2	D	324	15% 53% 31% 7% 8%
2	E	324	11% 51% 32% 7% 8%
2	F	324	10% 52% 32% 7% 8%
2	J	324	13% 51% 32% 7% 8%
2	K	324	14% 53% 31% 7% 8%
2	L	324	14% 52% 33% 6% 8%

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:

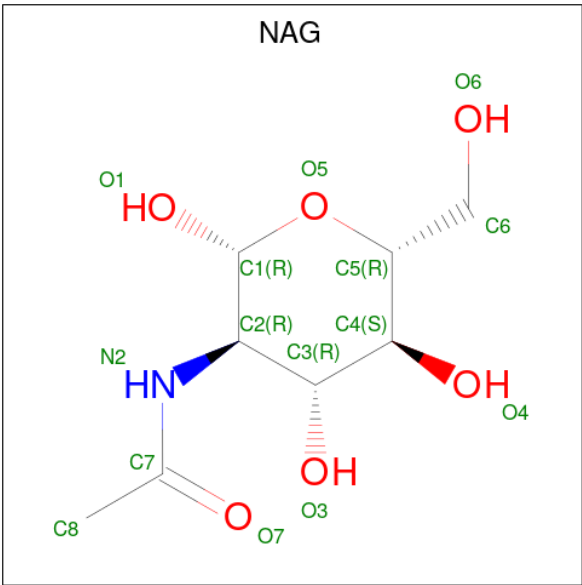
Chain	Residue	Modelled	Actual	Comment	Reference
D	317	GLY	-	expression tag	UNP Q9DHW0
D	318	SER	-	expression tag	UNP Q9DHW0
D	319	HIS	-	expression tag	UNP Q9DHW0
D	320	HIS	-	expression tag	UNP Q9DHW0
D	321	HIS	-	expression tag	UNP Q9DHW0
D	322	HIS	-	expression tag	UNP Q9DHW0
D	323	HIS	-	expression tag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

Continued on next page...

Continued from previous page...

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 (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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		

Continued on next page...

Continued from previous page...

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		

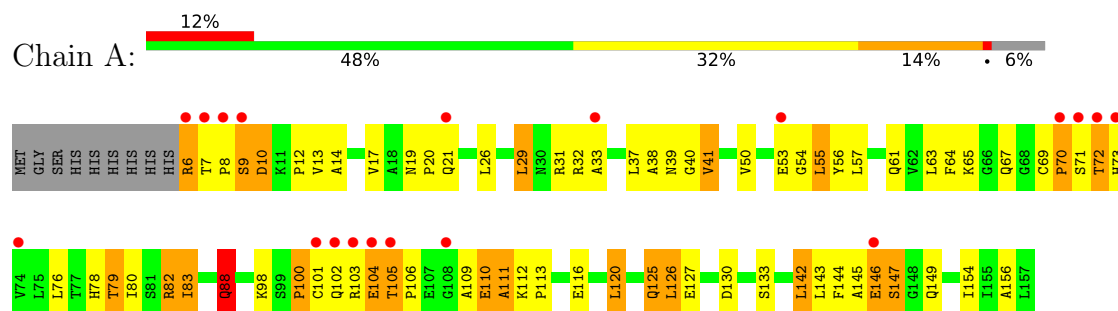
- Molecule 4 is water.

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		

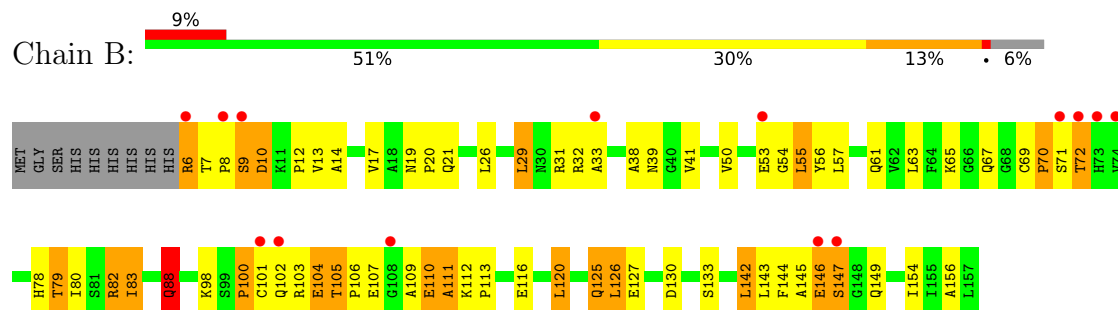
3 Residue-property plots

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.

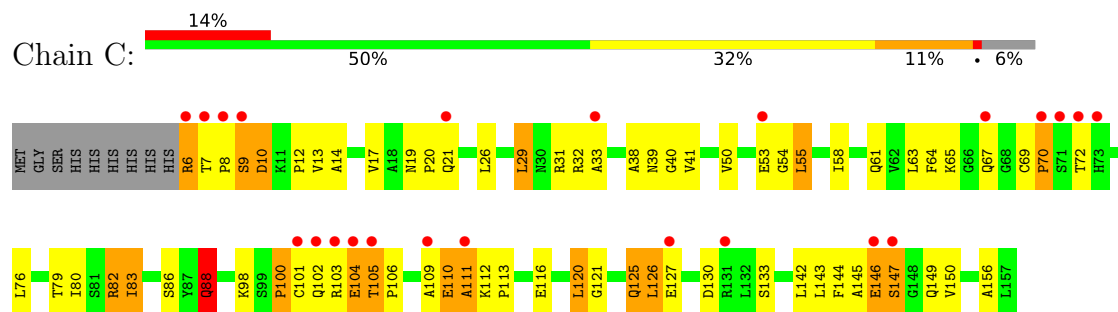
- Molecule 1: Tumor necrosis factor



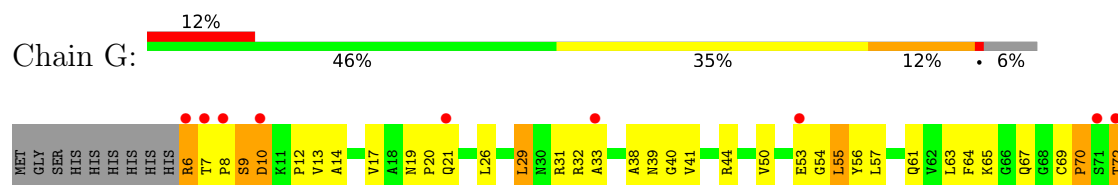
- Molecule 1: Tumor necrosis factor

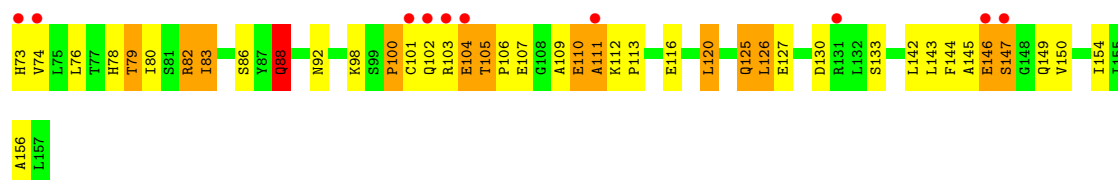


- Molecule 1: Tumor necrosis factor

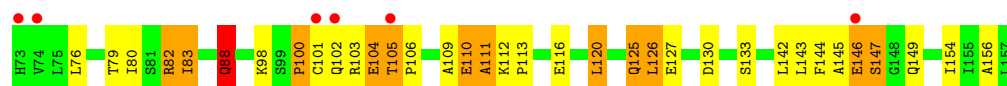


- Molecule 1: Tumor necrosis factor

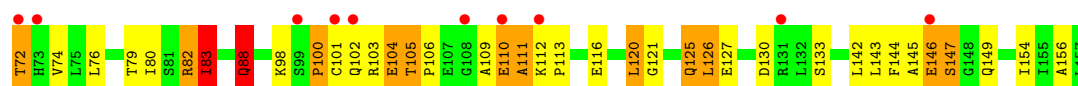
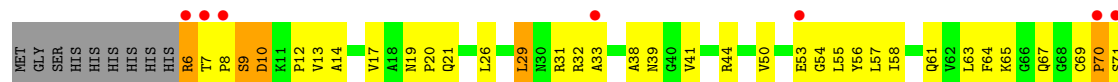




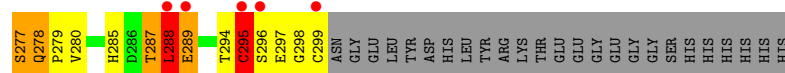
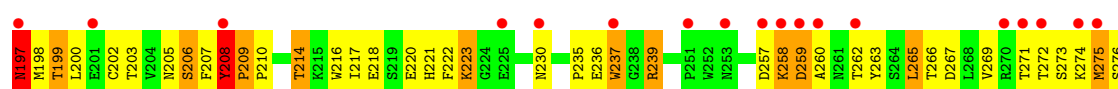
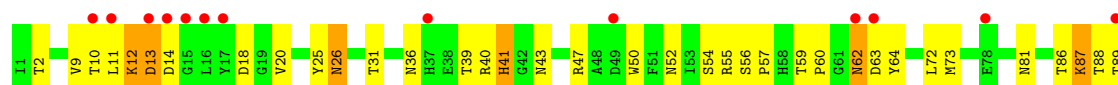
- Molecule 1: Tumor necrosis factor



- Molecule 1: Tumor necrosis factor

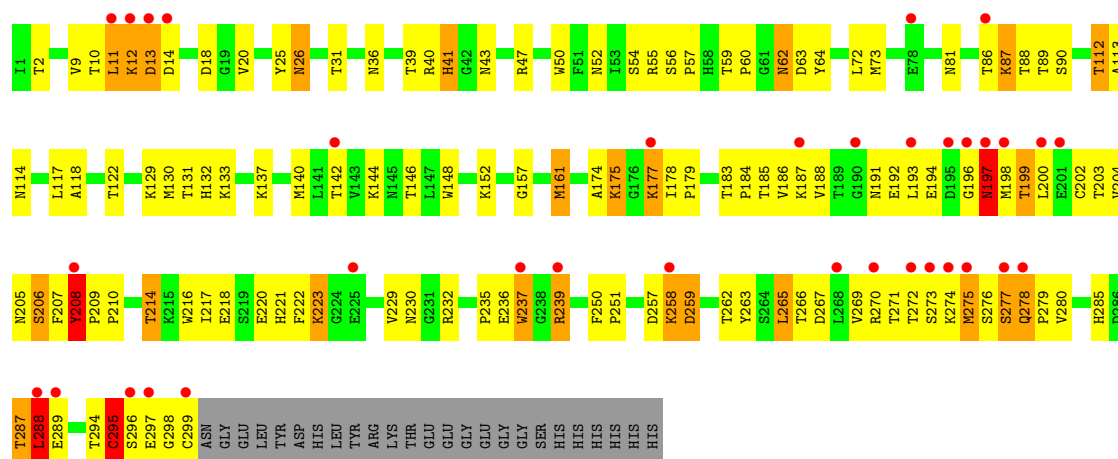


- Molecule 2: 2L protein

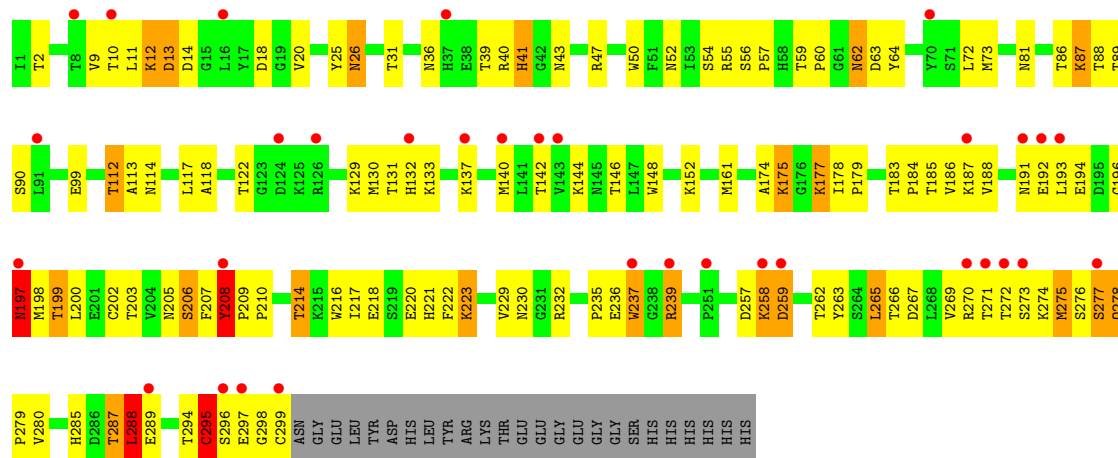


- Molecule 2: 2L protein

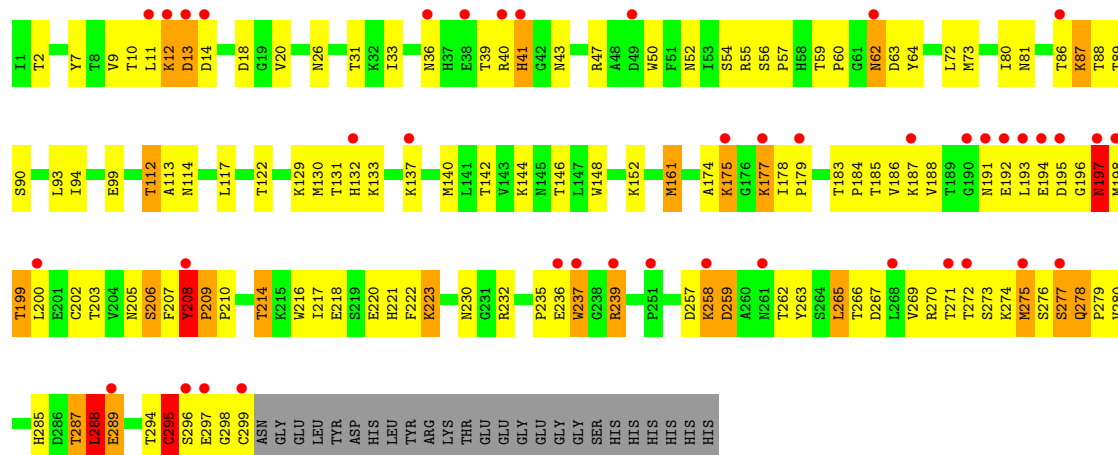




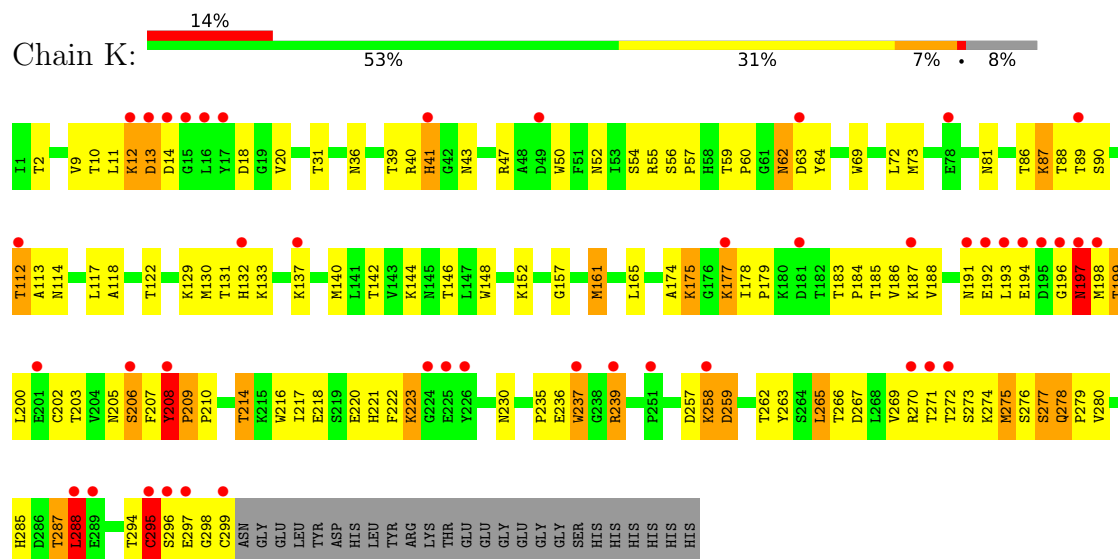
• Molecule 2: 2L protein



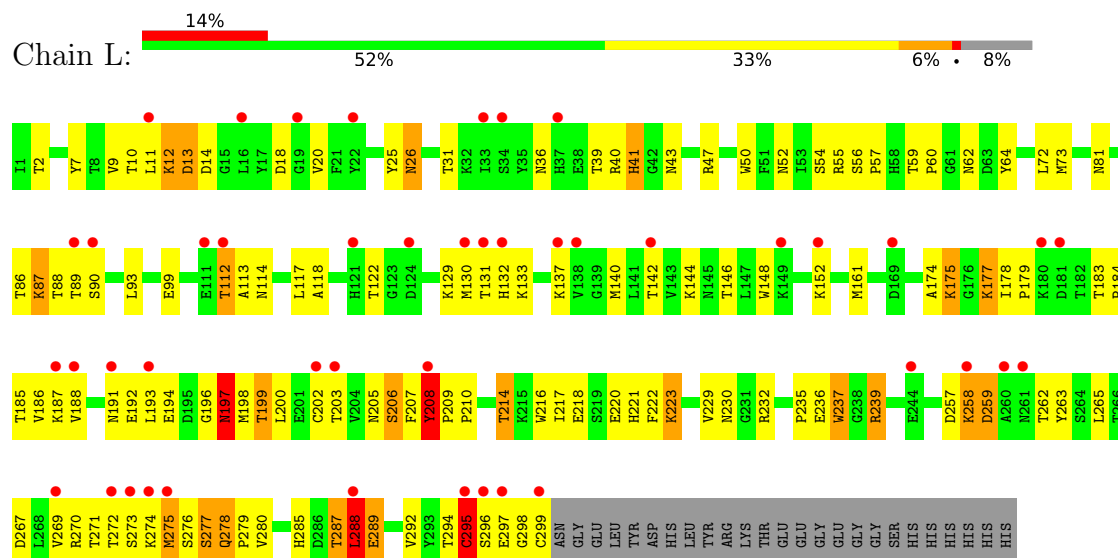
• Molecule 2: 2L protein



- Molecule 2: 2L protein



- 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 38.77 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (38.77-2.80) 96.8 (38.77-2.80)	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 , 66.7	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	0.49	0/1217	0.95	3/1656 (0.2%)
1	B	0.50	0/1217	0.93	2/1656 (0.1%)
1	C	0.50	0/1217	0.95	3/1656 (0.2%)
1	G	0.49	0/1217	0.95	3/1656 (0.2%)
1	H	0.46	0/1217	0.93	2/1656 (0.1%)
1	I	0.49	1/1217 (0.1%)	0.95	2/1656 (0.1%)
2	D	0.49	0/2487	1.01	15/3374 (0.4%)
2	E	0.47	0/2487	1.01	13/3374 (0.4%)
2	F	0.42	0/2487	1.00	13/3374 (0.4%)
2	J	0.48	0/2487	1.02	15/3374 (0.4%)
2	K	0.47	0/2487	1.00	14/3374 (0.4%)
2	L	0.39	0/2487	0.99	13/3374 (0.4%)
All	All	0.47	1/22224 (0.0%)	0.98	98/30180 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	83	ILE	CA-CB	5.04	1.60	1.53

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	236	GLU	N-CA-C	10.68	126.82	112.30
2	J	236	GLU	N-CA-C	10.67	126.82	112.30
2	D	236	GLU	N-CA-C	10.61	126.73	112.30
2	F	236	GLU	N-CA-C	10.61	126.72	112.30
2	K	236	GLU	N-CA-C	10.58	126.69	112.30
2	E	236	GLU	N-CA-C	10.49	126.56	112.30
2	D	177	LYS	N-CA-C	8.07	121.97	112.93
2	F	177	LYS	N-CA-C	7.96	121.85	112.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	177	LYS	N-CA-C	7.78	121.64	112.93
2	E	287	THR	N-CA-C	-7.74	99.02	110.48
2	L	287	THR	N-CA-C	-7.61	99.22	110.48
2	J	208	TYR	CA-C-N	-7.59	112.56	120.38
2	J	208	TYR	C-N-CA	-7.59	112.56	120.38
2	D	59	THR	N-CA-C	-7.46	100.39	109.72
2	F	208	TYR	CA-C-N	-7.44	112.71	120.38
2	F	208	TYR	C-N-CA	-7.44	112.71	120.38
2	E	208	TYR	CA-C-N	-7.43	112.72	120.38
2	E	208	TYR	C-N-CA	-7.43	112.72	120.38
2	K	208	TYR	CA-C-N	-7.41	112.75	120.38
2	K	208	TYR	C-N-CA	-7.41	112.75	120.38
2	D	287	THR	N-CA-C	-7.38	99.56	110.48
2	E	177	LYS	N-CA-C	7.34	121.16	112.93
2	F	287	THR	N-CA-C	-7.34	99.62	110.48
2	J	177	LYS	N-CA-C	7.30	121.78	113.02
2	J	59	THR	N-CA-C	-7.28	100.61	109.72
2	K	287	THR	N-CA-C	-7.23	99.77	110.48
2	J	287	THR	N-CA-C	-7.20	99.82	110.48
2	L	59	THR	N-CA-C	-7.11	100.83	109.72
2	K	59	THR	N-CA-C	-7.10	100.85	109.72
2	L	208	TYR	CA-C-N	-7.05	113.11	120.38
2	L	208	TYR	C-N-CA	-7.05	113.11	120.38
2	K	177	LYS	N-CA-C	6.98	121.40	113.02
2	F	59	THR	N-CA-C	-6.97	101.01	109.72
2	E	59	THR	N-CA-C	-6.77	101.26	109.72
2	D	208	TYR	CA-C-N	-6.70	113.48	120.38
2	D	208	TYR	C-N-CA	-6.70	113.48	120.38
2	F	56	SER	CA-C-N	6.59	127.11	119.47
2	F	56	SER	C-N-CA	6.59	127.11	119.47
1	C	38	ALA	N-CA-C	6.58	118.94	109.14
2	L	235	PRO	N-CA-C	-6.53	101.00	111.38
2	J	56	SER	CA-C-N	6.48	126.99	119.47
2	J	56	SER	C-N-CA	6.48	126.99	119.47
1	G	38	ALA	N-CA-C	6.42	118.70	109.14
2	E	235	PRO	N-CA-C	-6.42	101.18	111.38
2	E	56	SER	CA-C-N	6.41	126.91	119.47
2	E	56	SER	C-N-CA	6.41	126.91	119.47
2	J	235	PRO	N-CA-C	-6.41	101.19	111.38
1	G	54	GLY	N-CA-C	6.39	118.56	110.96
1	I	54	GLY	N-CA-C	6.38	118.56	110.96
2	D	56	SER	CA-C-N	6.37	126.86	119.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	56	SER	C-N-CA	6.37	126.86	119.47
2	L	56	SER	CA-C-N	6.34	126.82	119.47
2	L	56	SER	C-N-CA	6.34	126.82	119.47
1	I	38	ALA	N-CA-C	6.33	118.57	109.14
2	F	235	PRO	N-CA-C	-6.32	101.33	111.38
2	D	235	PRO	N-CA-C	-6.26	101.43	111.38
1	H	38	ALA	N-CA-C	6.20	118.38	109.14
1	A	38	ALA	N-CA-C	6.20	118.37	109.14
2	D	209	PRO	CA-C-N	6.20	125.88	119.56
2	D	209	PRO	C-N-CA	6.20	125.88	119.56
1	A	54	GLY	N-CA-C	6.18	118.31	110.96
1	B	54	GLY	N-CA-C	6.15	118.28	110.96
1	H	54	GLY	N-CA-C	6.09	118.21	110.96
2	E	205	ASN	N-CA-C	6.09	119.16	109.24
2	K	209	PRO	CA-C-N	6.05	125.73	119.56
2	K	209	PRO	C-N-CA	6.05	125.73	119.56
2	L	205	ASN	N-CA-C	6.04	119.09	109.24
2	F	205	ASN	N-CA-C	6.02	119.06	109.24
2	L	26	ASN	CB-CA-C	-6.01	109.65	116.63
2	K	235	PRO	N-CA-C	-6.01	101.82	111.38
2	F	26	ASN	CB-CA-C	-5.98	109.69	116.63
2	J	205	ASN	N-CA-C	5.98	118.98	109.24
1	B	38	ALA	N-CA-C	5.95	118.00	109.14
2	K	205	ASN	N-CA-C	5.91	118.86	109.24
2	D	26	ASN	CB-CA-C	-5.88	109.81	116.63
1	C	54	GLY	N-CA-C	5.88	117.95	110.96
2	K	56	SER	CA-C-N	5.87	127.18	119.84
2	K	56	SER	C-N-CA	5.87	127.18	119.84
2	J	209	PRO	CA-C-N	5.84	125.51	119.56
2	J	209	PRO	C-N-CA	5.84	125.51	119.56
2	D	205	ASN	N-CA-C	5.79	118.68	109.24
2	K	288	LEU	CA-CB-CG	5.63	136.00	116.30
2	J	288	LEU	CA-CB-CG	5.62	135.97	116.30
2	E	288	LEU	CA-CB-CG	5.59	135.88	116.30
2	D	288	LEU	CA-CB-CG	5.57	135.80	116.30
1	C	40	GLY	N-CA-C	5.51	120.24	113.79
2	L	288	LEU	CA-CB-CG	5.46	135.43	116.30
2	F	288	LEU	CA-CB-CG	5.34	134.98	116.30
1	G	40	GLY	N-CA-C	5.17	119.84	113.79
2	F	295	CYS	N-CA-C	5.09	121.64	110.80
2	L	295	CYS	N-CA-C	5.08	121.63	110.80
2	E	26	ASN	CB-CA-C	-5.08	109.23	116.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	295	CYS	N-CA-C	5.06	121.58	110.80
2	J	26	ASN	CB-CA-C	-5.06	109.26	116.34
2	J	295	CYS	N-CA-C	5.05	121.56	110.80
1	A	40	GLY	N-CA-C	5.03	119.67	113.79
2	D	295	CYS	N-CA-C	5.02	121.50	110.80
2	E	295	CYS	N-CA-C	5.01	121.48	110.80

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	82	0
1	B	1190	0	1192	78	0
1	C	1190	0	1192	78	0
1	G	1190	0	1192	91	0
1	H	1190	0	1192	78	0
1	I	1190	0	1192	84	0
2	D	2419	0	2309	111	1
2	E	2419	0	2309	124	0
2	F	2419	0	2308	121	0
2	J	2419	0	2308	128	1
2	K	2419	0	2309	122	0
2	L	2419	0	2308	121	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1177	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 27.

All (1177) 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:F:50:TRP:HB3	2:F:177:LYS:HD2	1.31	1.07
2:K:50:TRP:HB3	2:K:177:LYS:HD2	1.32	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:237:TRP:HE1	2:E:275:MET:HE2	1.41	0.85
2:L:148:TRP:NE1	2:L:152:LYS:HE3	1.91	0.85
2:D:237:TRP:HE1	2:D:275:MET:HE2	1.42	0.84
2:F:237:TRP:HE1	2:F:275:MET:HE2	1.42	0.84
2:K:237:TRP:HE1	2:K:275:MET:HE2	1.43	0.84
2:L:237:TRP:HE1	2:L:275:MET:HE2	1.43	0.83
2:J:237:TRP:HE1	2:J:275:MET:HE2	1.42	0.83
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
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:H	1:G:88:GLN:HE21	1.29	0.80
2:J:296:SER:C	2:J:298:GLY:H	1.89	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:HH11	2:F:239:ARG:HB3	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:H	1:C:88:GLN:HE21	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:H	1:A:88:GLN:HE21	1.32	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:GLN:H	1:B:88:GLN:HE21	1.32	0.77
2:D:296:SER:C	2:D:298:GLY:H	1.92	0.77
2:E:112:THR:HG22	2:E:114:ASN:N	1.96	0.77
2:E:239:ARG:HH11	2:E:239:ARG:HB3	1.49	0.77
2:E:296:SER:C	2:E:298:GLY:H	1.91	0.77
2:F:296:SER:C	2:F:298:GLY:H	1.91	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:N	1:I:88:GLN:HE21	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
2:K:296:SER:C	2:K:298:GLY:H	1.91	0.76
2:L:296:SER:C	2:L:298:GLY:H	1.91	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:HH11	2:D:239:ARG:HB3	1.51	0.76
1:H:70:PRO:O	1:H:105:THR:HG22	1.86	0.76
2:K:239:ARG:HH11	2:K:239:ARG:HB3	1.51	0.76
1:I:88:GLN:HE21	1:I:88:GLN:H	1.32	0.75
2:L:239:ARG:HH11	2:L:239:ARG:HB3	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
1:H:88:GLN:HE21	1:H:88:GLN:N	1.84	0.75
1:H:65:LYS:HD2	1:H:143:LEU:HD22	1.68	0.74
1:A:88:GLN:HE21	1:A:88:GLN:N	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:208:TYR:O	2:K:209:PRO:C	2.31	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
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: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: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
2:E:73:MET:HG2	2:E:140:MET:CE	2.20	0.71
2:E:188:VAL:O	2:E:299:CYS:SG	2.48	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:73:MET:HG2	2:F:140:MET:CE	2.21	0.71
2:F:257:ASP:OD1	2:F:262:THR:HG23	1.91	0.71
2:J:131:THR:HG22	2:J:133:LYS:H	1.56	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:D:208:TYR:O	2:D:209:PRO:C	2.34	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:F:208:TYR:O	2:F:209:PRO:C	2.32	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	2:L:237:TRP:CE3	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:HA	2:D:237:TRP:HE3	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:D:237:TRP:HA	2:D:237:TRP:CE3	2.27	0.69
2:D:73:MET:HG2	2:D:140:MET:CE	2.23	0.69
2:F:237:TRP:HE3	2:F:237:TRP:HA	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:208:TYR:O	2:E:209:PRO:C	2.32	0.69
2:E:237:TRP:HA	2:E:237:TRP:CE3	2.28	0.68
1:I:19:ASN:CA	1:I:29:LEU:HD11	2.22	0.68
1:I:100:PRO:HG2	1:I:101:CYS:H	1.58	0.68
2:K:237:TRP:HE3	2:K:237:TRP:HA	1.59	0.68
1:C:8:PRO:O	1:C:9:SER:HB3	1.92	0.68
2:F:237:TRP:HA	2:F:237:TRP:CE3	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
2:L:208:TYR:O	2:L:209:PRO:C	2.33	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
1:G:50:VAL:HG21	1:G:126:LEU:HD23	1.76	0.68
2:L:31:THR:OG1	2:L:47:ARG:NH1	2.27	0.68
2:L:209:PRO:HG2	2:L:285:HIS:CE1	2.28	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:218:GLU:HB3	2:F:277:SER:HB2	1.75	0.67
2:J:208:TYR:O	2:J:209:PRO:C	2.31	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:209:PRO:HG2	2:E:285:HIS:CE1	2.30	0.66
2:E:218:GLU:HB3	2:E:277:SER:HB2	1.76	0.66
2:J:94:ILE:CD1	3:J:325:NAG:H82	2.26	0.66
2:L:237:TRP:HA	2:L:237:TRP:HE3	1.57	0.66
2:E:237:TRP:HA	2:E:237:TRP:HE3	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
1:I:109:ALA:O	1:I:110:GLU:HB2	1.96	0.66
1:A:109:ALA:O	1:A: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
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
1:A:103:ARG:HH21	1:C:112:LYS:HE2	1.60	0.65
1:C:109:ALA:O	1:C:110:GLU:HB2	1.96	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:206:SER:HA	2:F:263:TYR:O	1.98	0.64
3:L:327:NAG:H83	3:L:327:NAG:O3	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
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
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: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:L:73:MET:HG2	2:L:140:MET:HE2	1.81	0.63
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:F:73:MET:HG2	2:F:140:MET:HE1	1.82	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:G:8:PRO:HA	1:I:125:GLN:NE2	2.15	0.62
1:H:12:PRO:HG2	1:H:156:ALA:HB2	1.81	0.62
1:H:98:LYS:HD3	1:H:116:GLU:HG3	1.81	0.62
1:I:9:SER:O	1:I:10:ASP:HB3	2.00	0.62
2:J:73:MET:HG2	2:J:140:MET:HE2	1.81	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:HG13	1:A:83:ILE:O	1.99	0.61
2:J:73:MET:HG2	2:J:140:MET:HE1	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:GLU:HB3	1:B:149:GLN:CD	2.26	0.61
2:E:73:MET:HG2	2:E:140:MET:HE2	1.82	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
2:D:237:TRP:NE1	2:D:275:MET:HE2	2.15	0.60
1:I:98:LYS:HD3	1:I:116:GLU:HG3	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:C:146:GLU:HB3	1:C:149:GLN:CD	2.26	0.60
2:L:237:TRP:NE1	2:L:275:MET:HE2	2.16	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:G:146:GLU:HB3	1:G:149:GLN:CD	2.27	0.60
2:E:296:SER:C	2:E:298:GLY:N	2.60	0.60
1:B:9:SER:O	1:B:10:ASP:HB3	2.00	0.60
1:C:31:ARG:HD2	2:F:99:GLU:HG2	1.83	0.60
1:C:83:ILE:O	1:C:83:ILE:HG13	2.02	0.60
2:E:73:MET:HG2	2:E:140:MET:HE1	1.82	0.60
2:F:296:SER:C	2:F:298:GLY:N	2.60	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
2:K:296:SER:C	2:K:298:GLY:N	2.60	0.60
2:D:287:THR:O	2:D:288:LEU:HD13	2.01	0.60
1:I:146:GLU:HB3	1:I:149:GLN:CD	2.27	0.59
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
1:A:146:GLU:HB3	1:A:149:GLN:CD	2.27	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
1:I:82:ARG:HH11	2:J:161:MET:HE1	1.67	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:208:TYR:CD1	2:F:208:TYR:C	2.80	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:J:237:TRP:NE1	2:J:275:MET:HE2	2.15	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
2:E:208:TYR:CD1	2:E:208:TYR:C	2.79	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:73:MET:HG2	2:D:140:MET:HE2	1.84	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
2:F:237:TRP:NE1	2:F:275:MET:HE2	2.15	0.58
1:A:143:LEU:HD11	1:A:145:ALA:HB3	1.84	0.58
2:F:73:MET:HG2	2:F:140:MET:HE2	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:H:146:GLU:HB3	1:H:149:GLN:CD	2.28	0.58
1:A:19:ASN:HA	1:A:29:LEU:HD11	1.86	0.58
2:L:73:MET:HG2	2:L:140:MET:HE1	1.84	0.58
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:L:208:TYR:CD1	2:L:208:TYR:C	2.82	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:110:GLU:O	1:I:111:ALA:HB3	2.05	0.57
2:K:73:MET:HG2	2:K:140:MET:HE2	1.86	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
1:A:110:GLU:O	1:A:111:ALA:HB3	2.04	0.57
2:E:88:THR:CG2	2:E:112:THR:HG23	2.33	0.57
2:E:237:TRP:NE1	2:E:275:MET:HE2	2.15	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
2:K:237:TRP:NE1	2:K:275:MET:HE2	2.16	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
2:J:88:THR:CG2	2:J:112:THR:HG23	2.34	0.56
2:K:73:MET:HG2	2:K:140:MET:HE1	1.87	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: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
2:F:55:ARG:CG	3:F:326:NAG:H82	2.34	0.56
2:J:296:SER:C	2:J:298:GLY:N	2.58	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:39:THR:O	2:D:40:ARG:HB2	2.04	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
2:L:287:THR:C	2:L:288:LEU:HD13	2.31	0.56
2:E:41:HIS:C	2:E:41:HIS:CD2	2.84	0.56
2:K:287:THR:C	2:K:288:LEU:HD13	2.30	0.56
2:D:73:MET:HG2	2:D:140:MET:HE1	1.86	0.56
2:K:296:SER:O	2:K:297:GLU:HB2	2.05	0.56
2:D:9:VAL:HA	2:D:18:ASP:O	2.06	0.55
2:D:39:THR:HG21	2:D:41:HIS:NE2	2.21	0.55
2:D:117:LEU:N	2:D:130:MET:HE3	2.21	0.55
2:E:239:ARG:HB3	2:E:239:ARG:NH1	2.20	0.55
2:F:239:ARG:HB3	2:F:239:ARG:NH1	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:K:208:TYR:CD1	2:K:208:TYR:C	2.79	0.55
2:L:9:VAL:HA	2:L:18:ASP:O	2.06	0.55
2:L:239:ARG:HB3	2:L:239:ARG:NH1	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
1:I:83:ILE:HG13	1:I:83:ILE:O	2.05	0.55
2:J:208:TYR:CD1	2:J:208:TYR:C	2.81	0.55
2:J:280:VAL:CG2	2:J:294:THR:HG22	2.36	0.55
1:C:86:SER:O	2:E:157:GLY:HA2	2.06	0.55
2:D:287:THR:C	2:D:288:LEU:HD13	2.32	0.55
2:J:217:ILE:O	2:J:280:VAL:HG12	2.06	0.55
2:K:183:THR:HG23	2:K:288:LEU:HD12	1.88	0.55
2:K:209:PRO:O	2:K:285:HIS:HE1	1.89	0.55
2:L:39:THR:O	2:L:40:ARG:HB2	2.07	0.55
2:L:186:VAL:O	2:L:187:LYS:HG3	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
2:E:288:LEU:O	2:E:288:LEU:HD22	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:296:SER:O	2:E:297:GLU:HB2	2.06	0.55
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
2:D:208:TYR:CD1	2:D:208:TYR:C	2.78	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
1:I:44:ARG:NH1	2:L:232:ARG:HH22	2.04	0.54
2:J:41:HIS:C	2:J:41:HIS:CD2	2.85	0.54
2:J:239:ARG:HB3	2:J:239:ARG:NH1	2.19	0.54
2:L:288:LEU:O	2:L:288:LEU:HD22	2.06	0.54
1:B:103:ARG:HH21	1:B:103:ARG:HG2	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:D:257:ASP:HB2	2:D:258:LYS:HD3	1.87	0.54
2:E:117:LEU:N	2:E:130:MET:HE3	2.23	0.54
2:F:288:LEU:O	2:F:288:LEU:CD2	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:F:287:THR:C	2:F:288:LEU:HD13	2.32	0.54
2:J:288:LEU:O	2:J:288:LEU:HD22	2.07	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
2:F:86:THR:O	2:F:87:LYS:C	2.51	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:F:36:ASN:HB2	2:F:43:ASN:ND2	2.22	0.54
2:F:214:THR:HG21	2:F:267:ASP:OD2	2.08	0.54
2:K:60:PRO:HB2	2:K:64:TYR:HA	1.90	0.54
2:F:39:THR:HG21	2:F:41:HIS:NE2	2.23	0.54
2:E:183:THR:HG23	2:E:288:LEU:HD12	1.90	0.53
2:E:285:HIS:CD2	2:E:287:THR:H	2.26	0.53
1:A:103:ARG:HH21	1:A:103:ARG:HG2	1.73	0.53
2:D:88:THR:HG22	2:D:89:THR:N	2.24	0.53
2:D:296:SER:O	2:D:297:GLU:HB2	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:146:GLU:O	1:G:147:SER:HB2	2.08	0.53
2:L:36:ASN:HB2	2:L:43:ASN:ND2	2.23	0.53
2:L:39:THR:HG21	2:L:41:HIS:CE1	2.43	0.53
2:L:285:HIS:CD2	2:L:287:THR:H	2.26	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:F:41:HIS:C	2:F:41:HIS:CD2	2.86	0.53
2:E:50:TRP:CB	2:E:177:LYS:HD2	2.23	0.53
1:G:7:THR:O	1:G:8:PRO:C	2.51	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:J:117:LEU:N	2:J:130:MET:HE3	2.22	0.53
2:L:296:SER:O	2:L:297:GLU:HB2	2.07	0.53
2:F:55:ARG:HD3	3:F:326:NAG:H82	1.90	0.53
1:I:7:THR:O	1:I:8:PRO:C	2.52	0.53
1:I:103:ARG:HH21	1:I:103:ARG:HG2	1.73	0.53
2:L:41:HIS:C	2:L:41:HIS:CD2	2.86	0.53
2:L:50:TRP:CB	2:L:177:LYS:HD2	2.21	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:F:39:THR:O	2:F:40:ARG:HB2	2.07	0.53
2:J:9:VAL:HA	2:J:18:ASP:O	2.08	0.53
2:J:39:THR:O	2:J:40:ARG:HB2	2.08	0.53
2:J:285:HIS:CD2	2:J:287:THR:H	2.27	0.53
2:K:285:HIS:CD2	2:K:287:THR:H	2.26	0.53
2:L:288:LEU:O	2:L:288:LEU:CD2	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:86:THR:O	2:E:87:LYS:C	2.52	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:J:287:THR:C	2:J:288:LEU:HD13	2.34	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:K:41:HIS:C	2:K:41:HIS:CD2	2.86	0.52
2:L:178:ILE:HB	2:L:179:PRO:HD2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:287:THR:C	2:E:288:LEU:HD13	2.35	0.52
2:J:60:PRO:HB2	2:J:64:TYR:HA	1.90	0.52
2:J:178:ILE:HB	2:J:179:PRO:HD2	1.91	0.52
2:L:88:THR:HG22	2:L:89:THR:N	2.24	0.52
1:A:83:ILE:HD12	1:A:83:ILE:C	2.35	0.52
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:86:THR:O	2:L:87:LYS:C	2.52	0.52
2:L:209:PRO:O	2:L:285:HIS:HE1	1.92	0.52
1:A:7:THR:O	1:A:8:PRO:C	2.51	0.52
1:C:7:THR:O	1:C:8:PRO:C	2.52	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:D:86:THR:O	2:D:87:LYS:C	2.53	0.52
2:E:288:LEU:O	2:E:288:LEU:CD2	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:HG2	1:G:103:ARG:HH21	1.73	0.52
1:B:83:ILE:C	1:B:83:ILE:HD12	2.35	0.52
2:E:272:THR:CG2	2:E:274:LYS:HG3	2.40	0.52
2:F:117:LEU:N	2:F:130:MET:HE3	2.24	0.52
2:J:36:ASN:HD22	2:J:43:ASN:ND2	2.08	0.52
2:J:296:SER:O	2:J:298:GLY:N	2.42	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
1:H:7:THR:O	1:H:8:PRO:C	2.51	0.52
1:H:83:ILE:C	1:H:83:ILE:HD12	2.35	0.52
2:K:288:LEU:O	2:K:288:LEU:CD2	2.58	0.52
1:A:80:ILE:HA	1:A:133:SER:O	2.10	0.51
2:D:288:LEU:CD2	2:D:288:LEU:O	2.58	0.51
2:D:288:LEU:O	2:D:288:LEU:HD22	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:13:VAL:HG22	1:H:14:ALA:N	2.26	0.51
1:H:109:ALA:O	1:H:110:GLU:CB	2.59	0.51
2:J:271:THR:HG22	2:J:271:THR:O	2.10	0.51
2:K:288:LEU:O	2:K:288:LEU:HD22	2.09	0.51
2:L:117:LEU:N	2:L:130:MET:HE3	2.25	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
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: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
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:D:41:HIS:CD2	2:D:41:HIS:C	2.88	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:19:ASN:N	1:H:29:LEU:HD11	2.24	0.51
1:H:69:CYS:CB	1:H:106:PRO:HD3	2.36	0.51
2:J:202:CYS:HB2	2:J:216:TRP:CZ2	2.46	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:86:THR:O	2:J:87:LYS:C	2.54	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:I:83:ILE:HD12	1:I:83:ILE:C	2.36	0.50
2:K:117:LEU:N	2:K:130:MET:HE3	2.26	0.50
2:L:272:THR:CG2	2:L:274:LYS:HG3	2.41	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:J:258:LYS:O	2:J:259:ASP:C	2.55	0.50
3:L:326:NAG:H83	3:L:326:NAG:H3	1.94	0.50
1:A:19:ASN:N	1:A:29:LEU:HD11	2.27	0.50
1:A:69:CYS:CB	1:A:106:PRO:HD3	2.36	0.50
2:D:296:SER:C	2:D:298:GLY:N	2.61	0.50
2:E:39:THR:O	2:E:40:ARG:HB2	2.10	0.50
2:E:271:THR:HG22	2:E:271:THR:O	2.12	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: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:K:271:THR:O	2:K:271:THR:HG22	2.11	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:C:83:ILE:C	1:C:83:ILE:HD12	2.37	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
2:E:12:LYS:O	2:E:13:ASP:O	2.30	0.49
2:K:86:THR:O	2:K:87:LYS:C	2.54	0.49
1:A:55:LEU:HD21	1:C:13:VAL:HG11	1.93	0.49
2:D:271:THR:O	2:D:271:THR:HG22	2.13	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:53:GLU:OE1	1:A:127:GLU:HA	2.11	0.49
1:A:102:GLN:O	1:A:103:ARG:HB3	2.13	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
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
1:I:82:ARG:NH1	2:J:161:MET:HE1	2.28	0.49
2:E:202:CYS:HB2	2:E:216:TRP:CZ2	2.48	0.49
2:F:174:ALA:O	2:F:175:LYS:C	2.56	0.49
2:L:296:SER:C	2:L:298:GLY:N	2.60	0.49
1:B:102:GLN:O	1:B:103:ARG:HB3	2.13	0.48
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:19:ASN:HD22	1:A:20:PRO:CD	2.26	0.48
1:A:104:GLU:O	1:A:105:THR:O	2.30	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
1:G:83:ILE:C	1:G:83:ILE:HD12	2.38	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
1:C:82:ARG:NH2	1:C:130:ASP:OD2	2.44	0.48
1:I:19:ASN:N	1:I:29:LEU:HD11	2.27	0.48
2:L:271:THR:HG22	2:L:271:THR:O	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
2:K:174:ALA:O	2:K:175:LYS:C	2.57	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:197:ASN:ND2	2:D:271:THR:O	2.47	0.48
1:H:102:GLN:O	1:H:103:ARG:HB3	2.14	0.48
2:J:178:ILE:HB	2:J:179:PRO:CD	2.44	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:L:258:LYS:O	2:L:259:ASP:C	2.56	0.48
2:D:142:THR:HG22	2:D:144:LYS:H	1.77	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
2:J:131:THR:HG22	2:J:132:HIS:N	2.29	0.48
1:B:7:THR:O	1:B:8:PRO:C	2.52	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: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:L:36:ASN:HD22	2:L:43:ASN:ND2	2.12	0.48
1:B:19:ASN:N	1:B:29:LEU:HD11	2.29	0.47
1:H:19:ASN:HD22	1:H:20:PRO:CD	2.27	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:I:80:ILE:HA	1:I:133:SER:O	2.13	0.47
1:B:98:LYS:CD	1:B:116:GLU:HG3	2.44	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:K:258:LYS:O	2:K:259:ASP:C	2.56	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: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:F:258:LYS:O	2:F:259:ASP:C	2.57	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:106:PRO:HB3	1:G:111:ALA:HB2	1.96	0.47
2:L:131:THR:HG22	2:L:132:HIS:N	2.28	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:C:19:ASN:HD22	1:C:20:PRO:CD	2.28	0.47
1:C:106:PRO:HB3	1:C:111:ALA:HB2	1.96	0.47
2:D:258:LYS:O	2:D:259:ASP:C	2.57	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:G:80:ILE:HA	1:G:133:SER:O	2.14	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
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:174:ALA:O	2:L:175:LYS:C	2.57	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:E:186:VAL:C	2:E:187:LYS:HG3	2.40	0.47
2:F:178:ILE:HB	2:F:179:PRO:CD	2.45	0.47
1:G:98:LYS:CD	1:G:116:GLU:HG3	2.45	0.47
1:G:103:ARG:HH21	1:H:112:LYS:HE2	1.79	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:50:TRP:HB3	2:E:177:LYS:CD	2.23	0.46
2:E:294:THR:HB	2:E:295:CYS:H	1.56	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

Continued on next page...

Continued from previous page...

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:I:69:CYS:HA	1:I:70:PRO:HD3	1.80	0.46
1:I:103:ARG:O	1:I:103:ARG:HG3	2.14	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:E:174:ALA:O	2:E:175:LYS:C	2.57	0.46
1:H:83:ILE:O	1:H:83:ILE:CG1	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:88:THR:HG22	2:E:90:SER:H	1.81	0.46
2:E:197:ASN:ND2	2:E:271:THR:O	2.49	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:D:55:ARG:C	2:D:57:PRO:HD3	2.41	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: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:HD3	2:F:258:LYS:N	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
2:K:36:ASN:HD22	2:K:43:ASN:HD21	1.64	0.46
2:K:258:LYS:HD3	2:K:258:LYS:N	2.30	0.46
2:D:216:TRP:CE2	2:D:269:VAL:HG21	2.51	0.45
2:F:192:GLU:CG	2:F:198:MET:HA	2.44	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:36:ASN:HD22	2:D:43:ASN:HD21	1.64	0.45
2:D:272:THR:HG22	2:D:273:SER:N	2.32	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: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:88:THR:HG22	2:L:90:SER:H	1.81	0.45
2:L:216:TRP:CE2	2:L:269:VAL:HG21	2.51	0.45
2:F:220:GLU:HG3	2:F:221:HIS:N	2.32	0.45
2:E:258:LYS:O	2:E:259:ASP:C	2.58	0.45
2:F:25:TYR:O	2:F:26:ASN:HB2	2.17	0.45
1:H:19:ASN:HD22	1:H:19:ASN:C	2.25	0.45
1:C:7:THR:HG22	1:C:9:SER:H	1.81	0.45
2:D:296:SER:O	2:D:298:GLY:N	2.45	0.45
2:E:191:ASN:C	2:E:199:THR:HG22	2.42	0.45
2:D:112:THR:CG2	2:D:113:ALA:N	2.78	0.45
2:D:186:VAL:C	2:D:187:LYS:HG3	2.42	0.45
2:E:55:ARG:C	2:E:57:PRO:HD3	2.42	0.45
1:G:7:THR:HG22	1:G:9:SER:H	1.81	0.45
1:G:143:LEU:HD12	1:G:145:ALA:H	1.82	0.45
2:D:174:ALA:O	2:D:175:LYS:C	2.59	0.45
2:D:206:SER:C	2:D:262:THR:OG1	2.60	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:55:ARG:C	2:L:57:PRO:HD3	2.42	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:L:36:ASN:HD22	2:L:43:ASN:HD21	1.65	0.45
2:L:258:LYS:HD3	2:L:258:LYS:N	2.32	0.45
2:E:272:THR:HG22	2:E:274:LYS:HG3	1.97	0.45
2:E:272:THR:HG22	2:E:273:SER:N	2.31	0.45

Continued on next page...

Continued from previous page...

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:7:THR:HG22	1:G:9:SER:N	2.32	0.45
1:G:50:VAL:HG13	1:G:56:TYR:OH	2.17	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
1:G:82:ARG:HH11	2:K:161:MET:HE1	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:I:7:THR:HG22	1:I:9:SER:N	2.32	0.44
2:L:186:VAL:C	2:L:187:LYS:HG3	2.42	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:J:174:ALA:O	2:J:175:LYS:C	2.60	0.44
2:K:55:ARG:C	2:K:57:PRO:HD3	2.42	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:O3	3:D:327:NAG:H83	2.18	0.44
1:H:98:LYS:CD	1:H:116:GLU:HG3	2.46	0.44
1:I:19:ASN:HD22	1:I:19:ASN:C	2.26	0.44
2:J:206:SER:C	2:J:262:THR:OG1	2.61	0.44
2:J:220:GLU:HG3	2:J:221:HIS:N	2.32	0.44
2:L:191:ASN:C	2:L:199:THR:HG22	2.42	0.44
1:A:19:ASN:ND2	1:A:19:ASN:C	2.76	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:CZ	1:B:6:ARG:O	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
2:F:55:ARG:C	2:F:57:PRO:HD3	2.42	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:L:206:SER:C	2:L:262:THR:OG1	2.61	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:K:222:PHE:O	2:K:223:LYS:C	2.61	0.43
2:L:72:LEU:HG	2:L:140:MET:HB3	1.99	0.43
1:C:12:PRO:HG2	1:C:156:ALA:CB	2.48	0.43
1:C:19:ASN:HD22	1:C:19:ASN:C	2.26	0.43
2:D:206:SER:HB2	2:D:262:THR:HG21	2.00	0.43
2:D:222:PHE:O	2:D:223:LYS:C	2.61	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:E:137:LYS:C	2:E:142:THR:OG1	2.62	0.43
2:F:13:ASP:OD1	2:F:14:ASP:N	2.50	0.43
2:F:72:LEU:HG	2:F:140:MET:HB3	2.00	0.43
2:F:186:VAL:C	2:F:187:LYS:HG3	2.43	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:J:222:PHE:O	2:J:223:LYS:C	2.59	0.43
2:K:272:THR:HG22	2:K:273:SER:N	2.33	0.43
1:A:6:ARG:CZ	1:A:6:ARG:O	2.67	0.43
2:D:258:LYS:HD3	2:D:258:LYS:N	2.33	0.43
2:F:196:GLY:HA3	2:F:270:ARG:CZ	2.49	0.43
2:F:222:PHE:O	2:F:223:LYS:C	2.60	0.43
2:F:285:HIS:HD2	2:F:287:THR:OG1	2.01	0.43
1:G:13:VAL:HG22	1:G:14:ALA:N	2.32	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
1:A:19:ASN:HD22	1:A:19:ASN:C	2.25	0.43
2:E:185:THR:CG2	2:E:187:LYS:HE3	2.48	0.43
2:F:206:SER:C	2:F:262:THR:OG1	2.61	0.43
2:L:13:ASP:OD1	2:L:14:ASP:N	2.51	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:25:TYR:O	2:D:26:ASN:HB2	2.18	0.43
2:D:143:VAL:HG13	2:D:148:TRP:CD1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:72:LEU:HG	2:E:140:MET:HB3	1.99	0.43
2:E:112:THR:HG23	2:E:113:ALA:N	2.34	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
2:K:62:ASN:O	2:K:63:ASP:C	2.62	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
2:D:288:LEU:O	2:D:289:GLU:C	2.61	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:88:THR:HG22	2:K:90:SER:H	1.83	0.43
3:K:327:NAG:O3	3:K:327:NAG:C7	2.67	0.43
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: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: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
1:I:101:CYS:C	1:I:103:ARG:H	2.27	0.43
1:C:7:THR:C	1:C:9:SER:N	2.77	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:K:188:VAL:HB	2:K:294:THR:O	2.19	0.43
1:A:69:CYS:HA	1:A:70:PRO:HD3	1.79	0.42
1:A:110:GLU:O	1:A:111:ALA:CB	2.66	0.42
1:B:19:ASN:ND2	1:B:19:ASN:C	2.77	0.42
1:C:112:LYS:HB3	1:C:113:PRO:HD2	2.01	0.42
2:D:191:ASN:C	2:D:199:THR:HG22	2.44	0.42
1:H:143:LEU:HD12	1:H:145:ALA:H	1.84	0.42
2:J:33:ILE:HD13	2:J:63:ASP:HB3	2.00	0.42
2:J:185:THR:CG2	2:J:187:LYS:HE3	2.49	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:E:206:SER:C	2:E:262:THR:OG1	2.62	0.42
2:F:216:TRP:CE2	2:F:269:VAL:HG21	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:326:NAG:H3	3:F:326:NAG:C8	2.41	0.42
1:H:110:GLU:O	1:H:111:ALA:CB	2.66	0.42
2:J:191:ASN:C	2:J:199:THR:HG22	2.44	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:A:125:GLN:HE21	1:C:8:PRO:HA	1.81	0.42
1:B:78:HIS:C	1:B:79:THR:HG22	2.43	0.42
1:B:143:LEU:HD12	1:B:145:ALA:H	1.83	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:G:101:CYS:C	1:G:103:ARG:H	2.27	0.42
1:I:19:ASN:ND2	1:I:19:ASN:C	2.77	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:294:THR:HB	2:L:295:CYS:H	1.56	0.42
1:A:101:CYS:C	1:A:103:ARG:H	2.27	0.42
2:E:36:ASN:HD22	2:E:43:ASN:ND2	2.18	0.42
1:G:19:ASN:ND2	1:G:19:ASN:C	2.78	0.42
1:G:61:GLN:O	1:G:150:VAL:HA	2.20	0.42
1:I:6:ARG:O	1:I:6:ARG:CZ	2.67	0.42
2:J:55:ARG:C	2:J:57:PRO:HD3	2.43	0.42
2:K:209:PRO:HA	2:K:210:PRO:HD2	1.84	0.42
2:L:137:LYS:C	2:L:142:THR:OG1	2.62	0.42
1:A:19:ASN:HD22	1:A:20:PRO:N	2.18	0.42
1:B:19:ASN:HD22	1:B:19:ASN:C	2.26	0.42
1:B:19:ASN:HD22	1:B:20:PRO:N	2.18	0.42
1:B:101:CYS:C	1:B:103:ARG:H	2.27	0.42
1:B:110:GLU:O	1:B:111:ALA:CB	2.67	0.42
2:F:88:THR:HG21	2:F:113:ALA:H	1.85	0.42
2:F:191:ASN:C	2:F:199:THR:HG22	2.44	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:62:ASN:O	2:J:63:ASP:C	2.62	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:12:LYS:HG3	2:L:18:ASP:OD2	2.20	0.42
2:L:112:THR:HG23	2:L:113:ALA:N	2.35	0.42
1:A:100:PRO:CG	1:A:101:CYS:H	2.31	0.42
2:E:118:ALA:C	2:E:130:MET:HE2	2.44	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:B:83:ILE:CG1	2.67	0.42
2:D:185:THR:CG2	2:D:187:LYS:HE3	2.49	0.42
2:E:62:ASN:O	2:E:63:ASP:C	2.62	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:CD1	2:K:64:TYR:N	2.88	0.42
2:L:222:PHE:O	2:L:223:LYS:C	2.63	0.42
1:C:19:ASN:ND2	1:C:19:ASN:C	2.78	0.42
1:C:101:CYS:C	1:C:103:ARG:H	2.27	0.42
2:D:81:ASN:OD1	2:D:87:LYS:HA	2.19	0.42
2:D:118:ALA:C	2:D:130:MET:HE2	2.45	0.42
2:D:258:LYS:O	2:D:260:ALA:N	2.53	0.42
2:J:55:ARG:CG	3:J:326:NAG:H82	2.49	0.42
2:K:137:LYS:C	2:K:142:THR:OG1	2.63	0.42
2:L:88:THR:HG23	2:L:113:ALA:HB3	2.02	0.42
1:C:83:ILE:O	1:C:83:ILE:CG1	2.67	0.42
1:C:110:GLU:O	1:C:111:ALA:CB	2.67	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:6:ARG:CZ	1:G:6:ARG:O	2.68	0.42
1:G:31:ARG:O	1:G:32:ARG:HD3	2.19	0.42
1:I:13:VAL:CG2	1:I:14:ALA:N	2.83	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:A:78:HIS:C	1:A:79:THR:HG22	2.45	0.41
1:C:58:ILE:O	1:C:121:GLY:HA2	2.20	0.41
2:D:137:LYS:C	2:D:142:THR:OG1	2.63	0.41
1:H:69:CYS:HA	1:H:70:PRO:HD3	1.80	0.41
1:H:101:CYS:C	1:H:103:ARG:H	2.27	0.41
2:J:198:MET:HE1	2:J:297:GLU:OE2	2.20	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:12:LYS:HG3	2:F:18:ASP:OD2	2.20	0.41
2:F:88:THR:HG23	2:F:113:ALA:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:118:ALA:C	2:F:130:MET:HE2	2.45	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
1:B:102:GLN:H	1:B:104:GLU:CD	2.28	0.41
2:E:222:PHE:O	2:E:223:LYS:C	2.63	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
1:H:33:ALA:HB2	2:K:165:LEU:HD21	2.02	0.41
2:J:186:VAL:C	2:J:187:LYS:HG3	2.45	0.41
2:J:277:SER:O	2:J:278:GLN:HB3	2.20	0.41
2:K:191:ASN:C	2:K:199:THR:HG22	2.45	0.41
2:E:88:THR:HG23	2:E:113:ALA:HB3	2.03	0.41
2:E:265:LEU:HD12	2:E:266:THR:H	1.85	0.41
2:F:64:TYR:CD1	2:F:64:TYR:N	2.88	0.41
1:I:50:VAL:HG13	1:I:56:TYR:CZ	2.55	0.41
2:J:137:LYS:C	2:J:142:THR:OG1	2.64	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
2:F:137:LYS:C	2:F:142:THR:OG1	2.63	0.41
1:G:7:THR:C	1:G:9:SER:N	2.77	0.41
1:G:69:CYS:HA	1:G:70:PRO:HD3	1.79	0.41
1:G:78:HIS:C	1:G:79:THR:HG22	2.46	0.41
1:I:102:GLN:H	1:I:104:GLU:CD	2.28	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:7:TYR:HB2	2:L:93:LEU:HB3	2.02	0.41
2:L:25:TYR:O	2:L:26:ASN:HB2	2.20	0.41
2:L:196:GLY:HA3	2:L:270:ARG:CZ	2.50	0.41
2:L:216:TRP:CD1	2:L:269:VAL:HG21	2.55	0.41
2:L:288:LEU:O	2:L:289:GLU:C	2.62	0.41
2:D:88:THR:HG21	2:D:113:ALA:H	1.85	0.41
1:G:19:ASN:HD22	1:G:19:ASN:C	2.27	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:C:82:ARG:HH11	2:E:161:MET:HE1	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:11:LEU:O	2:E:12:LYS:C	2.64	0.41
1:G:32:ARG:HD3	1:G:32:ARG:HA	1.84	0.41
1:G:112:LYS:HB3	1:G:113:PRO:HD2	2.03	0.41
1:H:57:LEU:O	1:H:154:ILE:HA	2.20	0.41
1:H:102:GLN:H	1:H:104:GLU:CD	2.28	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: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
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
1:C:102:GLN:H	1:C:104:GLU:CD	2.29	0.41
2:D:198:MET:HE1	2:D:297:GLU:OE2	2.21	0.41
2:D:265:LEU:HD12	2:D:266:THR:H	1.86	0.41
2:E:12:LYS:HG3	2:E:18:ASP:OD2	2.20	0.41
2:E:198:MET:HE1	2:E:297:GLU:OE2	2.20	0.41
2:E:277:SER:O	2:E:278:GLN:HB3	2.20	0.41
2:E:288:LEU:O	2:E:289:GLU:C	2.62	0.41
2:F:62:ASN:O	2:F:63:ASP:C	2.63	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:G:83:ILE:CD1	1:G:88:GLN:HA	2.51	0.41
1:H:19:ASN:ND2	1:H:19:ASN:C	2.77	0.41
1:H:69:CYS:H	1:H:106:PRO:CG	2.34	0.41
1:H:103:ARG:HG2	1:H:103:ARG:NH2	2.35	0.41
1:I:29:LEU:HD12	1:I:29:LEU:N	2.36	0.41
2:K:186:VAL:C	2:K:187:LYS:HG3	2.46	0.41
2:K:265:LEU:HD12	2:K:266:THR:H	1.86	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
1:B:71:SER:O	1:B:72:THR:C	2.64	0.41
2:E:25:TYR:O	2:E:26:ASN:HB2	2.20	0.41
1:I:71:SER:O	1:I:72:THR:C	2.64	0.41
2:J:216:TRP:CD1	2:J:269:VAL:HG21	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:277:SER:O	2:L:278:GLN:HB3	2.20	0.41
1:A:102:GLN:H	1:A:104:GLU:CD	2.29	0.40
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:29:LEU:HD12	1:G:29:LEU:N	2.36	0.40
1:G:103:ARG:HG2	1:G:103:ARG:NH2	2.36	0.40
1:H:32:ARG:HD3	1:H:32:ARG:HA	1.83	0.40
1:I:83:ILE:O	1:I:83:ILE:CG1	2.69	0.40
1:I:112:LYS:HB3	1:I:113:PRO:HD2	2.02	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
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:K:206:SER:C	2:K:262:THR:OG1	2.64	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
1:G:55:LEU:HD12	1:G:55:LEU:HA	1.93	0.40
1:G:72:THR:HG22	1:G:73:HIS:N	2.36	0.40
1:G:102:GLN:H	1:G:104:GLU:CD	2.28	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
1:I:58:ILE:O	1:I:121:GLY:HA2	2.22	0.40
1:I:100:PRO:CG	1:I:101:CYS:H	2.31	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
1:A:71:SER:O	1:A:72:THR:C	2.65	0.40
1:A:103:ARG:HD3	1:C:112:LYS:HE3	2.04	0.40
1:G:32:ARG:HG3	1:G:32:ARG:HH21	1.87	0.40
2:J:64:TYR:CD1	2:J:64:TYR:N	2.89	0.40
2:J:288:LEU:O	2:J:289:GLU:C	2.64	0.40
2:K:118:ALA:C	2:K:130:MET:HE2	2.47	0.40
1:B:107:GLU:CD	1:B:107:GLU:C	2.90	0.40
2:D:62:ASN:O	2:D:63:ASP:C	2.64	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:G:107:GLU:CD	1:G:107:GLU:C	2.89	0.40
1:H:7:THR:C	1:H:9:SER:N	2.77	0.40
2:J:7:TYR:HB2	2:J:93:LEU:HB3	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:280:VAL:HG23	2:J:294:THR:CG2	2.47	0.40
2:K:88:THR:HG23	2:K:113:ALA:HB3	2.03	0.40
2:L:118:ALA:C	2:L:130:MET:HE2	2.47	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	1
1	B	150/161 (93%)	127 (85%)	11 (7%)	12 (8%)	1	1
1	C	150/161 (93%)	128 (85%)	10 (7%)	12 (8%)	1	1
1	G	150/161 (93%)	127 (85%)	11 (7%)	12 (8%)	1	1
1	H	150/161 (93%)	127 (85%)	11 (7%)	12 (8%)	1	1
1	I	150/161 (93%)	128 (85%)	10 (7%)	12 (8%)	1	1
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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%)	113 (88%)	15 (12%)	5	18
1	B	128/136 (94%)	113 (88%)	15 (12%)	5	18
1	C	128/136 (94%)	114 (89%)	14 (11%)	6	21
1	G	128/136 (94%)	114 (89%)	14 (11%)	6	21
1	H	128/136 (94%)	114 (89%)	14 (11%)	6	21
1	I	128/136 (94%)	114 (89%)	14 (11%)	6	21
2	D	267/288 (93%)	250 (94%)	17 (6%)	16	44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	E	267/288 (93%)	250 (94%)	17 (6%)	16	44
2	F	267/288 (93%)	250 (94%)	17 (6%)	16	44
2	J	267/288 (93%)	249 (93%)	18 (7%)	15	42
2	K	267/288 (93%)	250 (94%)	17 (6%)	16	44
2	L	267/288 (93%)	250 (94%)	17 (6%)	16	44
All	All	2370/2544 (93%)	2181 (92%)	189 (8%)	11	34

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
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	142	LEU
1	A	144	PHE
1	B	6	ARG
1	B	29	LEU
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	142	LEU
1	B	144	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	6	ARG
1	C	29	LEU
1	C	41	VAL
1	C	55	LEU
1	C	63	LEU
1	C	79	THR
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	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	129	LYS
2	D	146	THR
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	265	LEU
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	129	LYS
2	E	146	THR
2	E	197	ASN
2	E	199	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	203	THR
2	E	214	THR
2	E	237	TRP
2	E	239	ARG
2	E	265	LEU
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	129	LYS
2	F	146	THR
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	265	LEU
2	F	288	LEU
1	G	6	ARG
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	144	PHE
1	H	6	ARG
1	H	29	LEU
1	H	41	VAL
1	H	55	LEU
1	H	63	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	144	PHE
1	I	6	ARG
1	I	29	LEU
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	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	129	LYS
2	J	146	THR
2	J	195	ASP
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	265	LEU
2	J	288	LEU
2	K	2	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	129	LYS
2	K	146	THR
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	265	LEU
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	129	LYS
2	L	146	THR
2	L	197	ASN
2	L	199	THR
2	L	203	THR
2	L	214	THR
2	L	237	TRP
2	L	239	ARG
2	L	265	LEU
2	L	288	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	30	ASN
1	A	34	ASN
1	A	61	GLN
1	A	88	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	125	GLN
1	B	19	ASN
1	B	30	ASN
1	B	34	ASN
1	B	61	GLN
1	B	88	GLN
1	B	102	GLN
1	B	125	GLN
1	C	19	ASN
1	C	30	ASN
1	C	34	ASN
1	C	61	GLN
1	C	88	GLN
1	C	102	GLN
1	C	125	GLN
2	D	41	HIS
2	D	43	ASN
2	D	65	ASN
2	D	114	ASN
2	D	121	HIS
2	D	278	GLN
2	D	285	HIS
2	E	41	HIS
2	E	43	ASN
2	E	65	ASN
2	E	114	ASN
2	E	121	HIS
2	E	278	GLN
2	E	285	HIS
2	F	41	HIS
2	F	43	ASN
2	F	65	ASN
2	F	114	ASN
2	F	121	HIS
2	F	278	GLN
2	F	285	HIS
1	G	19	ASN
1	G	30	ASN
1	G	34	ASN
1	G	61	GLN
1	G	88	GLN
1	G	125	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	19	ASN
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	30	ASN
1	I	34	ASN
1	I	61	GLN
1	I	88	GLN
1	I	125	GLN
2	J	41	HIS
2	J	43	ASN
2	J	65	ASN
2	J	114	ASN
2	J	121	HIS
2	J	278	GLN
2	J	285	HIS
2	K	41	HIS
2	K	43	ASN
2	K	65	ASN
2	K	114	ASN
2	K	121	HIS
2	K	278	GLN
2	K	285	HIS
2	L	41	HIS
2	L	43	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	K	325	2	14,14,15	0.59	0	17,19,21	0.75	0
3	NAG	L	326	2	14,14,15	0.92	1 (7%)	17,19,21	0.80	0
3	NAG	F	325	2	14,14,15	0.78	1 (7%)	17,19,21	0.75	1 (5%)
3	NAG	D	327	2	14,14,15	0.91	1 (7%)	17,19,21	0.90	0
3	NAG	J	326	2	14,14,15	0.92	1 (7%)	17,19,21	0.97	2 (11%)
3	NAG	J	325	2	14,14,15	0.55	0	17,19,21	0.92	1 (5%)
3	NAG	K	326	2	14,14,15	0.90	1 (7%)	17,19,21	0.92	0
3	NAG	K	327	2	14,14,15	0.95	1 (7%)	17,19,21	0.65	0
3	NAG	E	326	2	14,14,15	1.08	1 (7%)	17,19,21	1.16	1 (5%)
3	NAG	F	326	2	14,14,15	0.87	1 (7%)	17,19,21	0.68	0
3	NAG	E	325	2	14,14,15	0.57	0	17,19,21	0.83	0
3	NAG	J	327	2	14,14,15	0.73	1 (7%)	17,19,21	0.62	0
3	NAG	L	327	2	14,14,15	0.68	0	17,19,21	0.76	1 (5%)
3	NAG	F	327	2	14,14,15	0.84	1 (7%)	17,19,21	0.68	0
3	NAG	L	325	2	14,14,15	0.59	0	17,19,21	0.80	1 (5%)
3	NAG	D	325	2	14,14,15	0.62	0	17,19,21	0.89	0
3	NAG	E	327	2	14,14,15	0.80	1 (7%)	17,19,21	0.58	0
3	NAG	D	326	2	14,14,15	1.15	1 (7%)	17,19,21	0.94	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	K	325	2	-	0/6/23/26	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	D	327	2	-	6/6/23/26	0/1/1/1
3	NAG	J	326	2	-	5/6/23/26	0/1/1/1
3	NAG	J	325	2	-	3/6/23/26	0/1/1/1
3	NAG	K	326	2	-	5/6/23/26	0/1/1/1
3	NAG	K	327	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	326	2	-	3/6/23/26	0/1/1/1
3	NAG	E	325	2	-	0/6/23/26	0/1/1/1
3	NAG	J	327	2	-	4/6/23/26	0/1/1/1
3	NAG	L	327	2	-	2/6/23/26	0/1/1/1
3	NAG	F	327	2	-	4/6/23/26	0/1/1/1
3	NAG	L	325	2	-	4/6/23/26	0/1/1/1
3	NAG	D	325	2	-	2/6/23/26	0/1/1/1
3	NAG	E	327	2	-	4/6/23/26	0/1/1/1
3	NAG	D	326	2	-	3/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	326	NAG	C1-C2	3.73	1.57	1.52
3	E	326	NAG	C1-C2	3.52	1.57	1.52
3	K	327	NAG	C1-C2	3.07	1.56	1.52
3	J	326	NAG	C1-C2	3.00	1.56	1.52
3	D	327	NAG	C1-C2	2.82	1.56	1.52
3	K	326	NAG	C1-C2	2.82	1.56	1.52
3	L	326	NAG	C1-C2	2.76	1.56	1.52
3	F	326	NAG	C1-C2	2.62	1.55	1.52
3	E	327	NAG	C1-C2	2.55	1.55	1.52
3	F	327	NAG	C1-C2	2.52	1.55	1.52
3	F	325	NAG	C1-C2	2.16	1.55	1.52
3	J	327	NAG	C1-C2	2.06	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	-3.06	104.68	110.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	325	NAG	C3-C4-C5	-2.51	105.68	110.23
3	L	325	NAG	C2-N2-C7	-2.44	119.63	122.90
3	F	325	NAG	C2-N2-C7	-2.35	119.75	122.90
3	J	326	NAG	C2-N2-C7	-2.23	119.91	122.90
3	L	327	NAG	C2-N2-C7	-2.19	119.96	122.90
3	D	326	NAG	C3-C4-C5	-2.14	106.36	110.23
3	J	326	NAG	C4-C3-C2	2.09	114.09	111.02

There are no chirality outliers.

All (62) 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	D	327	NAG	C8-C7-N2-C2
3	D	327	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	E	327	NAG	C3-C2-N2-C7
3	E	327	NAG	C8-C7-N2-C2
3	E	327	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	F	327	NAG	C8-C7-N2-C2
3	F	327	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	J	327	NAG	C8-C7-N2-C2
3	J	327	NAG	O7-C7-N2-C2
3	K	326	NAG	C3-C2-N2-C7
3	K	326	NAG	C8-C7-N2-C2
3	K	326	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	L	327	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	L	327	NAG	O7-C7-N2-C2
3	J	326	NAG	O5-C5-C6-O6
3	L	325	NAG	O5-C5-C6-O6
3	K	326	NAG	O5-C5-C6-O6
3	F	325	NAG	O5-C5-C6-O6
3	J	326	NAG	C4-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	L	326	NAG	O5-C5-C6-O6
3	F	325	NAG	C8-C7-N2-C2
3	E	326	NAG	O5-C5-C6-O6
3	D	327	NAG	C4-C5-C6-O6
3	F	325	NAG	O7-C7-N2-C2
3	D	327	NAG	O5-C5-C6-O6
3	E	327	NAG	O5-C5-C6-O6
3	K	327	NAG	C3-C2-N2-C7
3	E	326	NAG	C4-C5-C6-O6
3	F	327	NAG	C4-C5-C6-O6
3	J	325	NAG	C4-C5-C6-O6
3	D	327	NAG	C3-C2-N2-C7
3	F	327	NAG	C3-C2-N2-C7
3	J	327	NAG	C3-C2-N2-C7
3	D	325	NAG	C4-C5-C6-O6
3	J	325	NAG	O5-C5-C6-O6
3	L	325	NAG	C8-C7-N2-C2
3	D	327	NAG	C1-C2-N2-C7
3	J	325	NAG	C1-C2-N2-C7
3	J	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	L	326	NAG	5	0
3	D	327	NAG	2	0
3	J	326	NAG	1	0
3	J	325	NAG	2	0
3	K	326	NAG	3	0

Continued on next page...

Continued from previous page...

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.49	19 (12%) 8 6	31, 56, 172, 191	0
1	B	152/161 (94%)	0.37	14 (9%) 14 10	28, 53, 170, 200	0
1	C	152/161 (94%)	0.51	23 (15%) 5 4	28, 56, 176, 195	0
1	G	152/161 (94%)	0.44	19 (12%) 8 6	27, 56, 176, 195	0
1	H	152/161 (94%)	0.63	18 (11%) 9 7	33, 65, 169, 194	0
1	I	152/161 (94%)	0.51	17 (11%) 10 7	31, 59, 172, 201	0
2	D	299/324 (92%)	0.87	48 (16%) 4 4	29, 58, 138, 201	0
2	E	299/324 (92%)	0.68	35 (11%) 9 7	32, 59, 134, 199	0
2	F	299/324 (92%)	0.80	33 (11%) 10 8	35, 74, 144, 201	0
2	J	299/324 (92%)	0.66	42 (14%) 6 5	31, 57, 130, 189	0
2	K	299/324 (92%)	0.70	44 (14%) 6 4	26, 59, 136, 201	0
2	L	299/324 (92%)	1.08	45 (15%) 5 4	39, 90, 153, 201	0
All	All	2706/2910 (92%)	0.69	357 (13%) 7 6	26, 63, 159, 201	0

All (357) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	16	LEU	10.5
2	D	15	GLY	7.4
2	K	193	LEU	7.2
2	D	193	LEU	6.9
2	J	193	LEU	6.7
2	E	13	ASP	6.5
2	L	193	LEU	6.2
2	F	193	LEU	6.0
2	K	196	GLY	5.9
2	K	15	GLY	5.8
2	K	12	LYS	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	13	ASP	5.7
2	K	299	CYS	5.3
2	J	41	HIS	5.2
2	K	271	THR	5.1
2	K	191	ASN	5.1
1	A	102	GLN	5.1
2	D	11	LEU	4.9
2	J	62	ASN	4.8
2	K	195	ASP	4.8
2	D	258	LYS	4.7
2	K	13	ASP	4.7
2	K	14	ASP	4.6
2	J	296	SER	4.6
2	F	299	CYS	4.6
1	C	102	GLN	4.6
2	D	299	CYS	4.5
2	D	13	ASP	4.5
2	K	296	SER	4.4
2	D	296	SER	4.4
1	H	146	GLU	4.4
1	G	102	GLN	4.4
2	E	296	SER	4.4
1	A	101	CYS	4.4
2	E	198	MET	4.3
2	E	273	SER	4.3
1	C	146	GLU	4.2
2	L	121	HIS	4.1
1	A	8	PRO	4.1
2	L	34	SER	4.1
1	G	53	GLU	4.0
1	I	6	ARG	4.0
2	E	299	CYS	4.0
2	D	259	ASP	3.8
2	F	124	ASP	3.8
2	K	198	MET	3.8
1	A	6	ARG	3.8
2	D	257	ASP	3.8
1	H	33	ALA	3.8
2	D	196	GLY	3.8
1	B	101	CYS	3.8
1	B	8	PRO	3.8
2	J	237	TRP	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	274	LYS	3.8
2	E	197	ASN	3.8
2	E	12	LYS	3.7
2	E	14	ASP	3.7
2	F	259	ASP	3.7
1	I	101	CYS	3.7
2	K	16	LEU	3.7
2	J	177	LYS	3.7
2	K	63	ASP	3.7
2	J	208	TYR	3.7
1	A	53	GLU	3.7
1	I	7	THR	3.7
2	J	299	CYS	3.7
2	J	198	MET	3.6
2	J	14	ASP	3.6
2	D	237	TRP	3.6
1	C	33	ALA	3.6
1	I	110	GLU	3.6
2	L	296	SER	3.5
1	B	146	GLU	3.5
2	F	296	SER	3.5
2	D	89	THR	3.5
1	C	53	GLU	3.5
2	D	187	LYS	3.5
2	D	14	ASP	3.5
2	J	40	ARG	3.5
2	K	295	CYS	3.5
2	K	224	GLY	3.5
2	F	16	LEU	3.5
2	J	297	GLU	3.5
2	J	86	THR	3.4
1	G	101	CYS	3.4
1	H	72	THR	3.4
1	B	102	GLN	3.4
2	F	143	VAL	3.4
1	B	53	GLU	3.4
2	E	268	LEU	3.4
2	F	126	ARG	3.4
1	I	8	PRO	3.4
2	L	142	THR	3.4
2	J	190	GLY	3.3
1	G	33	ALA	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	K	197	ASN	3.3
2	J	12	LYS	3.3
1	H	102	GLN	3.3
2	F	142	THR	3.3
1	A	146	GLU	3.3
1	H	70	PRO	3.3
2	J	195	ASP	3.3
2	L	208	TYR	3.3
2	E	193	LEU	3.3
2	E	278	GLN	3.3
2	K	272	THR	3.2
2	F	208	TYR	3.2
2	D	63	ASP	3.2
1	C	6	ARG	3.2
2	L	169	ASP	3.2
2	K	187	LYS	3.2
2	L	274	LYS	3.2
2	D	10	THR	3.2
1	A	71	SER	3.2
2	D	17	TYR	3.2
2	L	273	SER	3.2
1	A	73	HIS	3.2
1	C	8	PRO	3.2
1	C	101	CYS	3.1
1	B	73	HIS	3.1
2	D	37	HIS	3.1
1	H	73	HIS	3.1
1	I	73	HIS	3.1
1	H	101	CYS	3.1
1	I	71	SER	3.1
1	C	73	HIS	3.1
2	D	132	HIS	3.1
1	H	71	SER	3.1
2	E	277	SER	3.1
2	D	253	ASN	3.1
1	C	71	SER	3.0
1	C	103	ARG	3.0
1	G	8	PRO	3.0
1	A	72	THR	3.0
1	I	72	THR	3.0
1	C	70	PRO	3.0
2	E	272	THR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	16	LEU	3.0
1	G	146	GLU	3.0
2	K	258	LYS	3.0
1	B	6	ARG	3.0
2	E	190	GLY	3.0
1	H	74	VAL	2.9
2	K	237	TRP	2.9
2	F	192	GLU	2.9
2	L	181	ASP	2.9
2	D	260	ALA	2.9
2	D	272	THR	2.9
2	E	177	LYS	2.9
2	F	137	LYS	2.9
1	G	6	ARG	2.9
2	F	237	TRP	2.9
2	K	226	TYR	2.9
1	I	146	GLU	2.9
2	E	297	GLU	2.9
1	B	71	SER	2.9
1	C	147	SER	2.9
2	E	270	ARG	2.9
2	J	277	SER	2.9
2	K	288	LEU	2.9
2	D	274	LYS	2.8
1	H	31	ARG	2.8
2	D	230	ASN	2.8
2	J	49	ASP	2.8
1	A	70	PRO	2.8
2	K	208	TYR	2.8
1	B	72	THR	2.8
1	H	9	SER	2.8
2	L	202	CYS	2.8
2	L	299	CYS	2.8
2	J	194	GLU	2.8
1	G	73	HIS	2.8
2	F	187	LYS	2.8
1	H	8	PRO	2.8
1	G	104	GLU	2.8
2	D	270	ARG	2.8
1	A	33	ALA	2.8
1	C	72	THR	2.8
2	E	258	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	99	SER	2.8
2	K	251	PRO	2.8
1	C	104	GLU	2.7
1	I	33	ALA	2.7
2	D	289	GLU	2.7
1	C	7	THR	2.7
2	J	197	ASN	2.7
2	J	261	ASN	2.7
1	G	71	SER	2.7
2	J	236	GLU	2.7
2	D	133	LYS	2.7
2	D	271	THR	2.7
2	E	195	ASP	2.7
2	F	273	SER	2.7
2	J	258	LYS	2.6
2	F	10	THR	2.6
2	L	272	THR	2.6
1	G	21	GLN	2.6
1	I	53	GLU	2.6
2	D	195	ASP	2.6
2	J	11	LEU	2.6
2	J	192	GLU	2.6
1	B	33	ALA	2.6
1	B	9	SER	2.6
1	H	21	GLN	2.6
1	C	105	THR	2.6
2	E	289	GLU	2.6
1	I	108	GLY	2.5
2	E	201	GLU	2.5
2	D	191	ASN	2.5
2	F	191	ASN	2.5
2	J	132	HIS	2.5
2	J	137	LYS	2.5
2	J	175	LYS	2.5
2	L	90	SER	2.5
2	K	17	TYR	2.5
2	D	225	GLU	2.5
2	F	297	GLU	2.5
1	B	74	VAL	2.5
2	E	225	GLU	2.5
2	K	194	GLU	2.5
2	E	86	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	191	ASN	2.5
2	J	289	GLU	2.5
2	K	192	GLU	2.5
1	G	103	ARG	2.5
1	G	72	THR	2.5
2	D	262	THR	2.5
2	D	181	ASP	2.4
1	H	24	GLY	2.4
2	L	19	GLY	2.4
2	D	78	GLU	2.4
2	F	258	LYS	2.4
1	H	7	THR	2.4
2	J	271	THR	2.4
2	L	131	THR	2.4
2	D	288	LEU	2.4
1	B	147	SER	2.4
2	K	206	SER	2.4
1	A	104	GLU	2.4
2	L	297	GLU	2.4
1	G	74	VAL	2.4
2	E	196	GLY	2.4
1	A	103	ARG	2.4
2	J	187	LYS	2.4
2	K	270	ARG	2.4
2	F	289	GLU	2.4
2	E	237	TRP	2.4
2	D	208	TYR	2.4
2	F	272	THR	2.4
2	L	132	HIS	2.4
2	D	197	ASN	2.4
1	G	7	THR	2.4
2	D	275	MET	2.4
2	K	132	HIS	2.4
2	D	251	PRO	2.4
2	L	261	ASN	2.3
1	G	10	ASP	2.3
2	L	295	CYS	2.3
1	A	9	SER	2.3
1	G	147	SER	2.3
1	A	7	THR	2.3
2	E	142	THR	2.3
2	L	137	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	180	LYS	2.3
2	L	187	LYS	2.3
2	K	239	ARG	2.3
1	C	21	GLN	2.3
1	C	67	GLN	2.3
2	J	268	LEU	2.3
1	A	105	THR	2.3
2	F	239	ARG	2.3
2	J	239	ARG	2.3
1	A	74	VAL	2.3
2	L	260	ALA	2.3
2	L	130	MET	2.3
2	E	288	LEU	2.3
2	D	177	LYS	2.3
2	K	137	LYS	2.3
1	A	108	GLY	2.3
1	H	53	GLU	2.3
2	D	295	CYS	2.3
2	F	132	HIS	2.3
2	F	8	THR	2.3
1	I	70	PRO	2.3
1	B	108	GLY	2.3
2	L	275	MET	2.2
2	J	38	GLU	2.2
2	E	11	LEU	2.2
2	E	200	LEU	2.2
2	K	181	ASP	2.2
1	H	6	ARG	2.2
1	I	112	LYS	2.2
2	D	121	HIS	2.2
2	L	138	VAL	2.2
1	C	109	ALA	2.2
2	K	297	GLU	2.2
2	L	11	LEU	2.2
2	F	197	ASN	2.2
2	E	239	ARG	2.2
2	F	251	PRO	2.2
2	J	200	LEU	2.2
2	K	201	GLU	2.2
2	L	244	GLU	2.2
1	C	131	ARG	2.2
2	F	270	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	K	41	HIS	2.2
2	J	179	PRO	2.2
2	E	208	TYR	2.2
2	K	78	GLU	2.2
1	I	131	ARG	2.1
2	J	36	ASN	2.1
2	L	37	HIS	2.1
2	J	272	THR	2.1
2	L	89	THR	2.1
2	L	288	LEU	2.1
2	L	22	TYR	2.1
2	L	111	GLU	2.1
1	I	102	GLN	2.1
2	D	62	ASN	2.1
2	E	275	MET	2.1
2	F	140	MET	2.1
2	K	112	THR	2.1
1	G	131	ARG	2.1
1	C	9	SER	2.1
1	C	127	GLU	2.1
2	D	201	GLU	2.1
2	E	78	GLU	2.1
2	E	187	LYS	2.1
2	J	251	PRO	2.1
2	L	152	LYS	2.1
1	H	105	THR	2.1
2	D	49	ASP	2.1
2	F	271	THR	2.1
2	D	126	ARG	2.1
1	A	21	GLN	2.1
2	K	177	LYS	2.1
2	L	191	ASN	2.1
2	F	91	LEU	2.1
2	K	49	ASP	2.1
2	K	89	THR	2.1
1	C	111	ALA	2.1
1	G	111	ALA	2.1
2	F	277	SER	2.0
2	L	258	LYS	2.0
2	F	37	HIS	2.0
2	L	188	VAL	2.0
2	L	269	VAL	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	112	THR	2.0
2	L	203	THR	2.0
2	K	289	GLU	2.0
2	D	175	LYS	2.0
2	L	33	ILE	2.0
2	K	225	GLU	2.0
2	L	124	ASP	2.0
2	L	149	LYS	2.0
2	J	275	MET	2.0
2	F	70	TYR	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 oligosaccharides 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	J	327	14/15	0.26	0.18	140,140,140,140	0
3	NAG	K	327	14/15	0.27	0.17	140,140,140,140	0
3	NAG	F	327	14/15	0.30	0.19	140,140,140,140	0
3	NAG	E	327	14/15	0.42	0.18	140,140,140,140	0
3	NAG	L	326	14/15	0.42	0.15	128,128,128,128	0
3	NAG	D	327	14/15	0.46	0.16	140,140,140,140	0
3	NAG	F	326	14/15	0.47	0.18	141,141,141,141	0
3	NAG	L	327	14/15	0.54	0.18	140,140,140,140	0
3	NAG	D	326	14/15	0.57	0.17	112,112,112,112	0
3	NAG	K	326	14/15	0.60	0.18	122,122,122,122	0
3	NAG	E	326	14/15	0.74	0.18	81,81,81,81	0
3	NAG	J	326	14/15	0.80	0.17	96,96,96,96	0
3	NAG	F	325	14/15	0.86	0.13	79,79,79,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	L	325	14/15	0.87	0.13	90,90,90,90	0
3	NAG	D	325	14/15	0.88	0.12	57,57,57,57	0
3	NAG	K	325	14/15	0.92	0.10	54,54,54,54	0
3	NAG	E	325	14/15	0.92	0.10	56,56,56,56	0
3	NAG	J	325	14/15	0.93	0.08	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.