Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:28 pm BST

PDB ID	:	1H2I
Title	:	Human Rad52 protein, N-terminal domain
Authors	:	Singleton, M.R.; Wentzell, L.M.; Liu, Y.; West, S.C.; Wigley, D.B.
Deposited on	:	2002-08-09
Resolution	:	2.70 Å(reported)

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

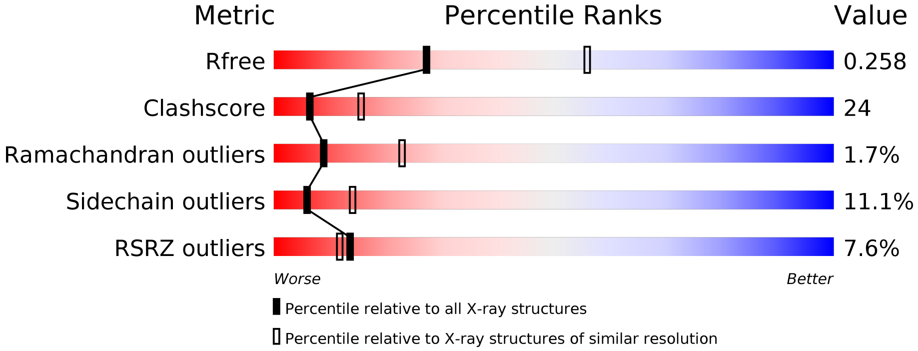
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

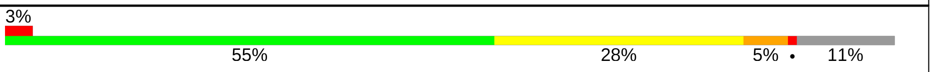
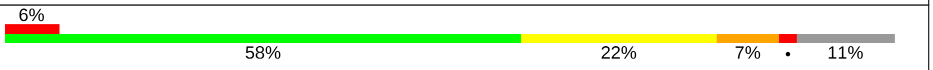
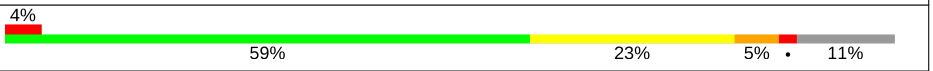
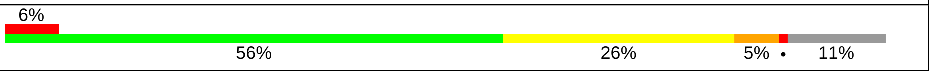
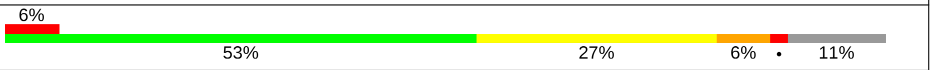
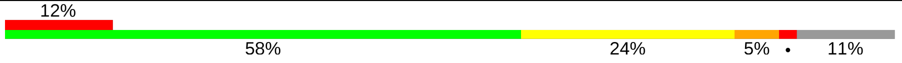
The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



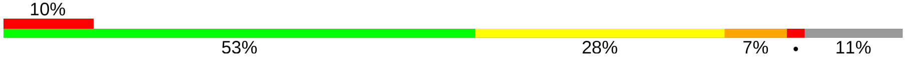
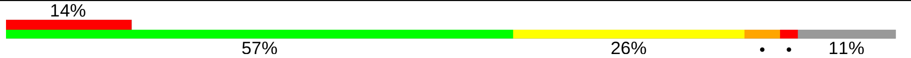
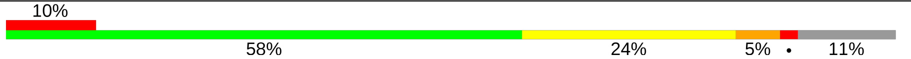
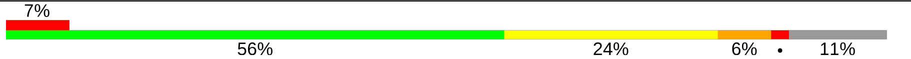
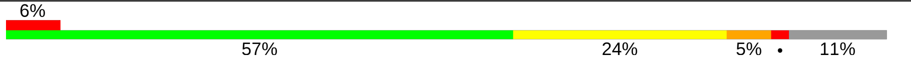
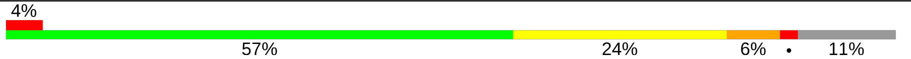
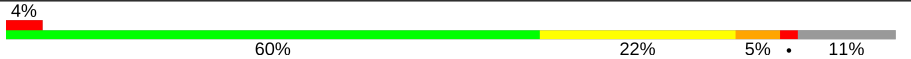
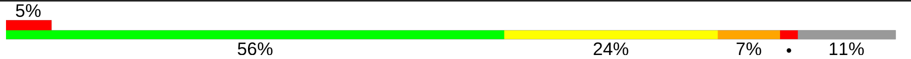
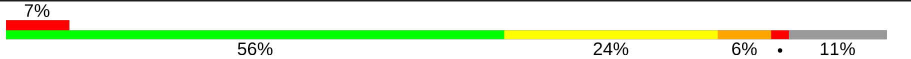
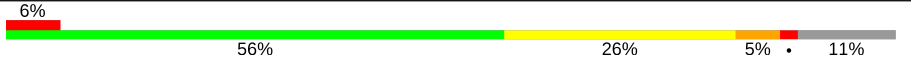
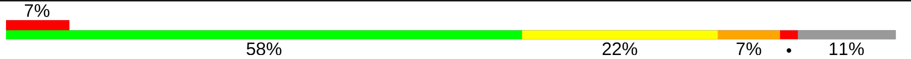
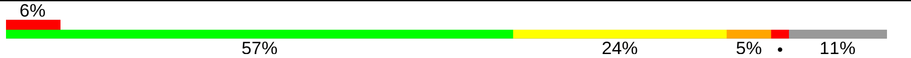
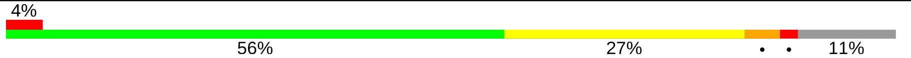
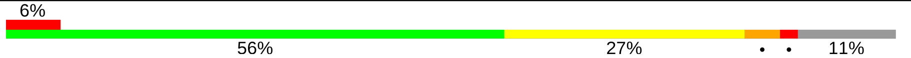
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	209	
1	B	209	
1	C	209	
1	D	209	
1	E	209	
1	F	209	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	209	 10% 53% 28% 7% • 11%
1	H	209	 14% 57% 26% • • 11%
1	I	209	 10% 58% 24% 5% • 11%
1	J	209	 7% 56% 24% 6% • 11%
1	K	209	 6% 57% 24% 5% • 11%
1	L	209	 4% 57% 24% 6% • 11%
1	M	209	 4% 60% 22% 5% • 11%
1	N	209	 5% 56% 24% 7% • 11%
1	O	209	 7% 56% 24% 6% • 11%
1	P	209	 6% 56% 26% 5% • 11%
1	Q	209	 7% 58% 22% 7% • 11%
1	R	209	 7% 60% 22% 5% • 11%
1	S	209	 7% 56% 25% 6% • 11%
1	T	209	 6% 57% 24% 5% • 11%
1	U	209	 4% 56% 27% • • 11%
1	V	209	 6% 56% 27% • • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 32802 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 DNA REPAIR PROTEIN RAD52 HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	186	1469	919	266	276	8	0	0	0
1	B	186	1469	919	266	276	8	0	0	0
1	C	186	1469	919	266	276	8	0	0	0
1	D	186	1469	919	266	276	8	0	0	0
1	E	186	1469	919	266	276	8	0	0	0
1	F	186	1469	919	266	276	8	0	0	0
1	G	186	1469	919	266	276	8	0	0	0
1	H	186	1469	919	266	276	8	0	0	0
1	I	186	1469	919	266	276	8	0	0	0
1	J	186	1469	919	266	276	8	0	0	0
1	K	186	1469	919	266	276	8	0	0	0
1	L	186	1469	919	266	276	8	0	0	0
1	M	186	1469	919	266	276	8	0	0	0
1	N	186	1469	919	266	276	8	0	0	0
1	O	186	1469	919	266	276	8	0	0	0
1	P	186	1469	919	266	276	8	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	Q	186	Total C N O S 1469 919 266 276 8	0	0	0
1	R	186	Total C N O S 1469 919 266 276 8	0	0	0
1	S	186	Total C N O S 1469 919 266 276 8	0	0	0
1	T	186	Total C N O S 1469 919 266 276 8	0	0	0
1	U	186	Total C N O S 1469 919 266 276 8	0	0	0
1	V	186	Total C N O S 1469 919 266 276 8	0	0	0

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	23	Total O 23 23	0	0
2	B	22	Total O 22 22	0	0
2	C	21	Total O 21 21	0	0
2	D	24	Total O 24 24	0	0
2	E	22	Total O 22 22	0	0
2	F	25	Total O 25 25	0	0
2	G	18	Total O 18 18	0	0
2	H	22	Total O 22 22	0	0
2	I	22	Total O 22 22	0	0
2	J	20	Total O 20 20	0	0
2	K	23	Total O 23 23	0	0
2	L	21	Total O 21 21	0	0
2	M	23	Total O 23 23	0	0

Continued on next page...

Continued from previous page...

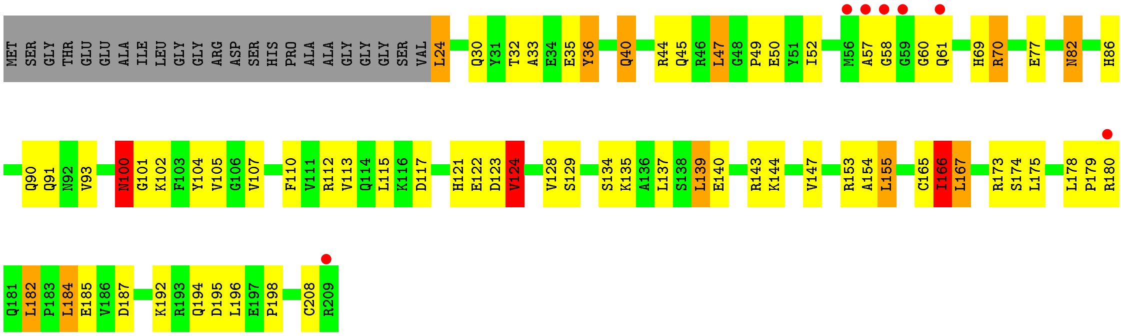
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	N	26	Total O 26 26	0	0
2	O	17	Total O 17 17	0	0
2	P	24	Total O 24 24	0	0
2	Q	21	Total O 21 21	0	0
2	R	22	Total O 22 22	0	0
2	S	22	Total O 22 22	0	0
2	T	22	Total O 22 22	0	0
2	U	23	Total O 23 23	0	0
2	V	21	Total O 21 21	0	0

3 Residue-property plots ⓘ

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

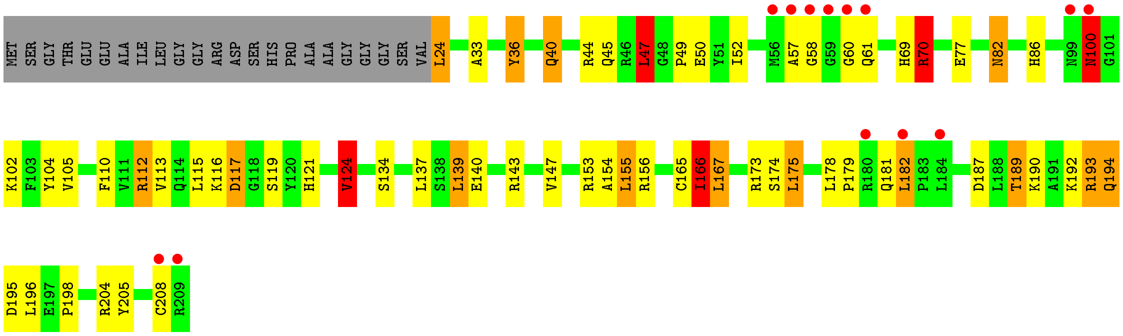
- Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

Chain A:



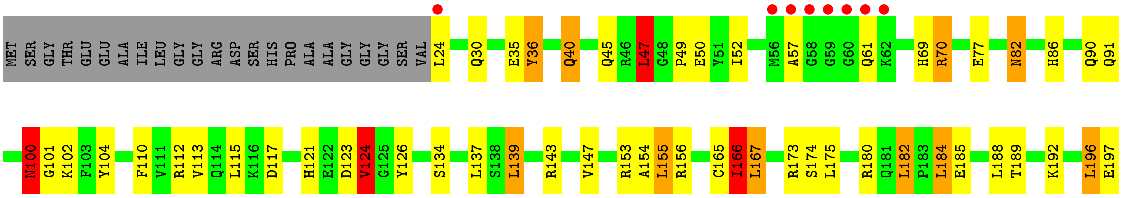
- Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

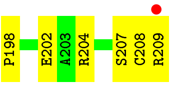
Chain B:



- Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

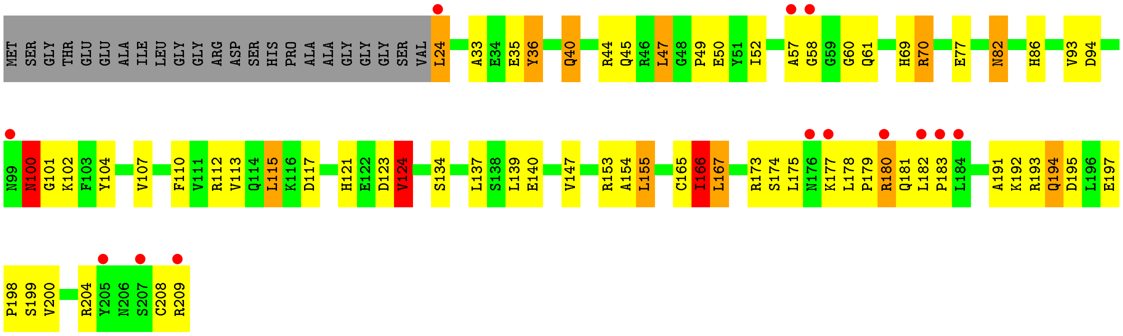
Chain C:





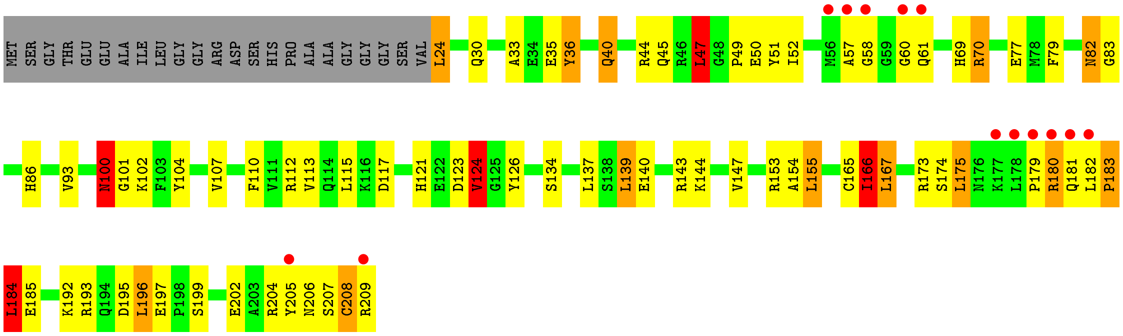
- Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

Chain D:



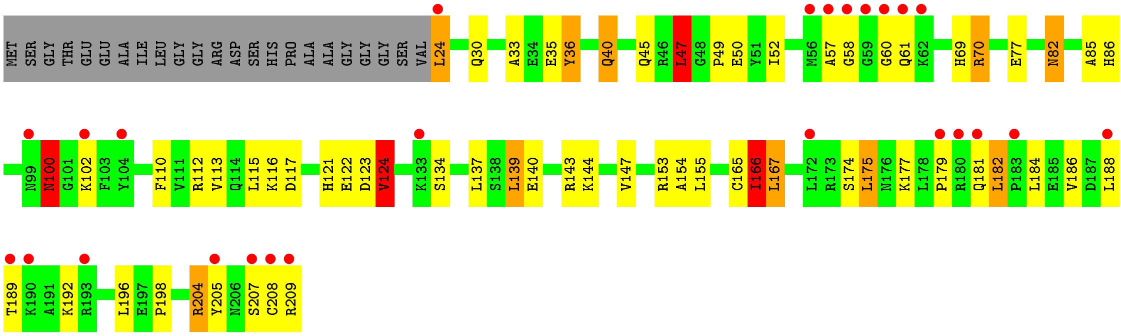
- Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

Chain E:



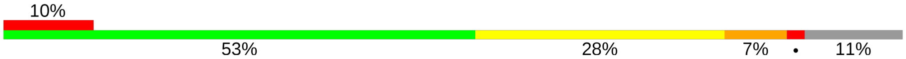
- Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

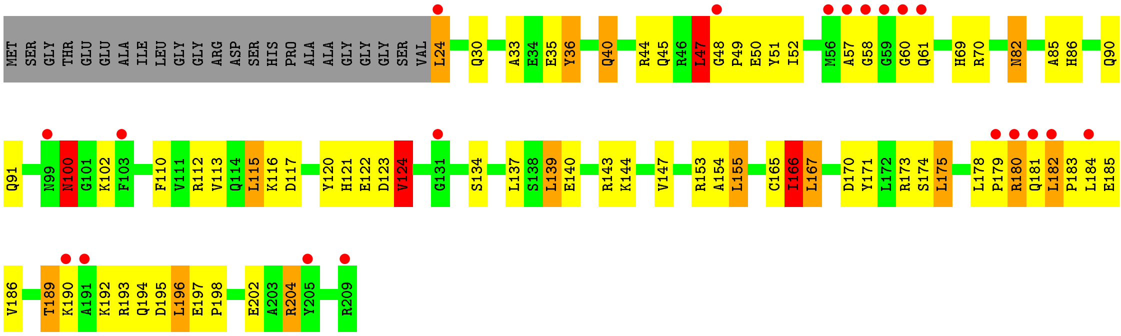
Chain F:



- Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

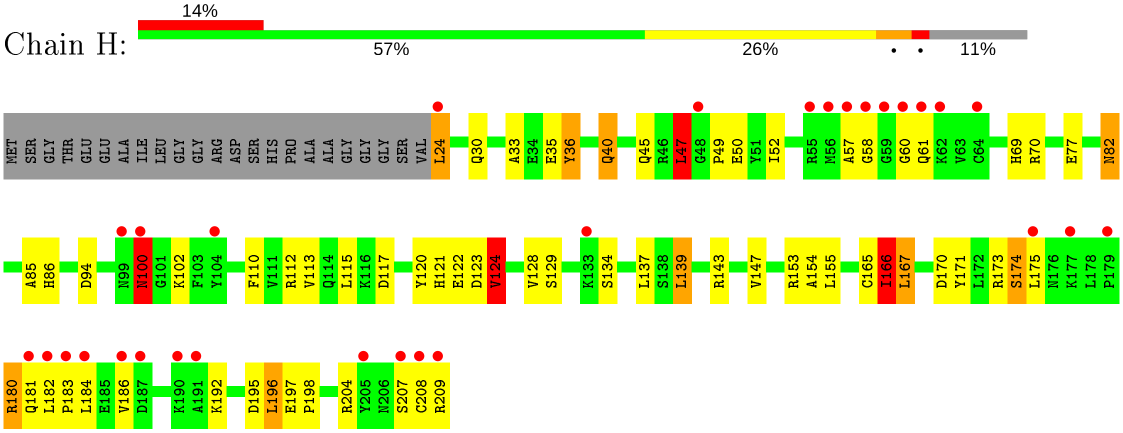
Chain G:





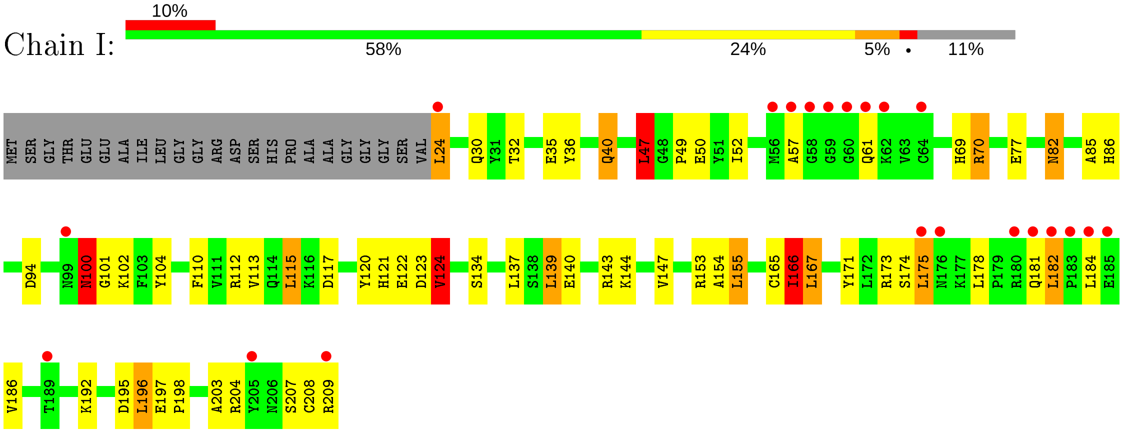
• Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

Chain H:



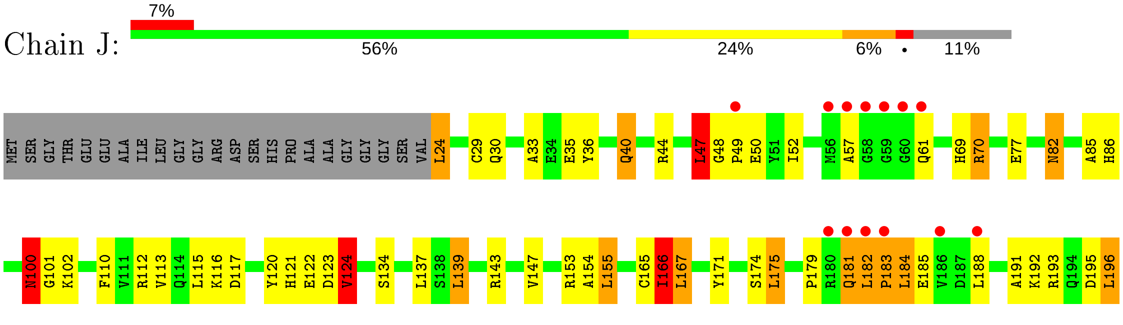
• Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

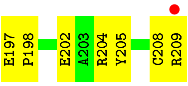
Chain I:



• Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

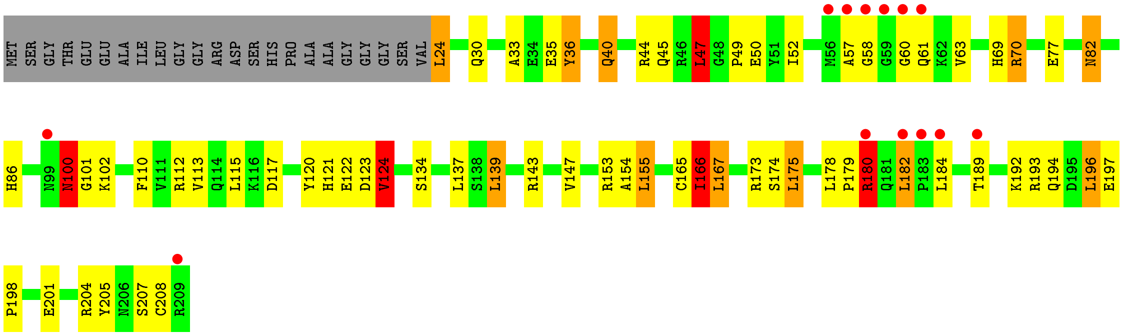
Chain J:





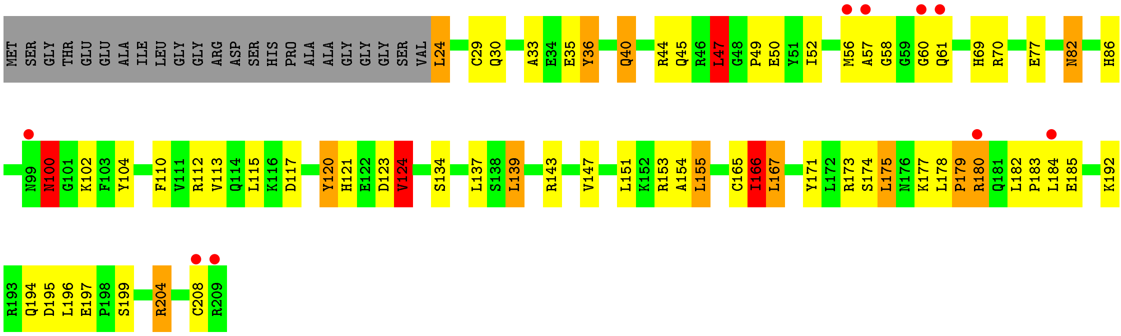
• Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

Chain K:



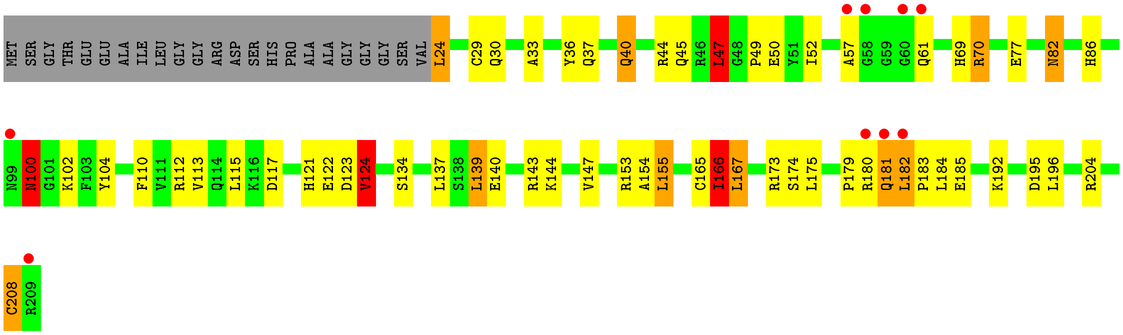
• Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

Chain L:



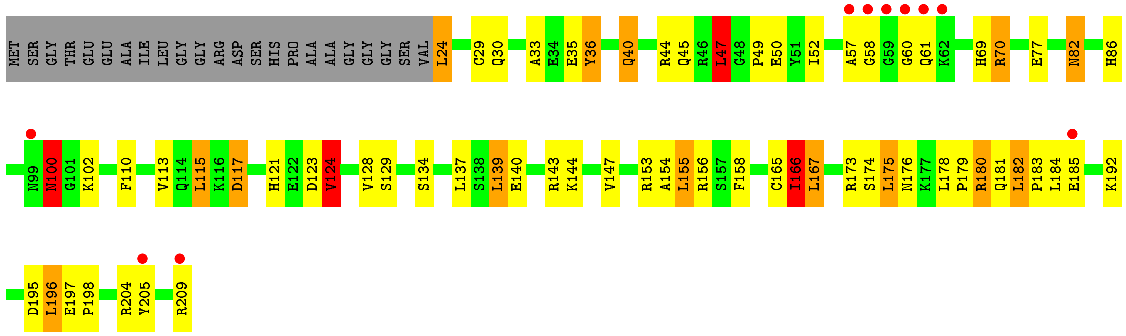
• Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

Chain M:



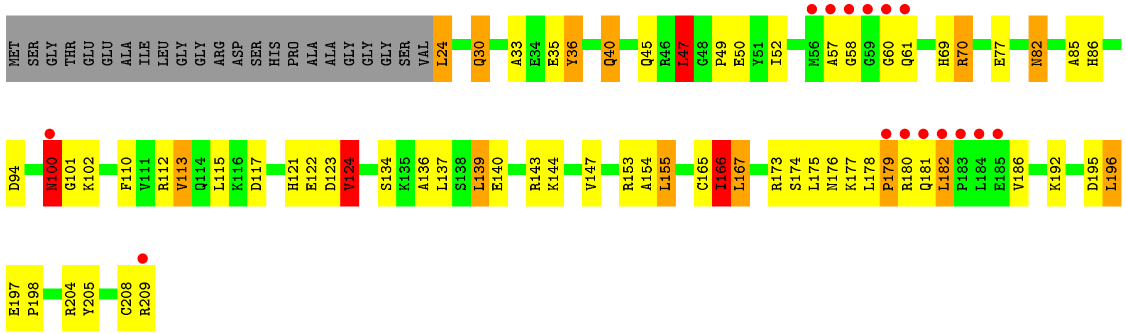
• Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

Chain N:



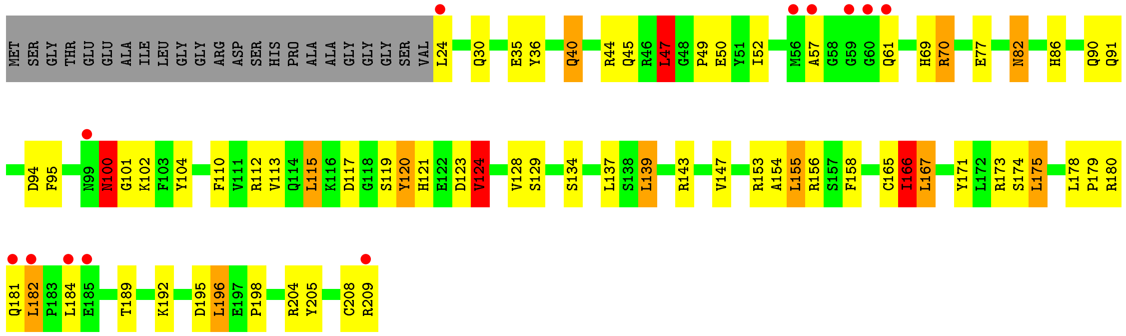
- Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

Chain O:



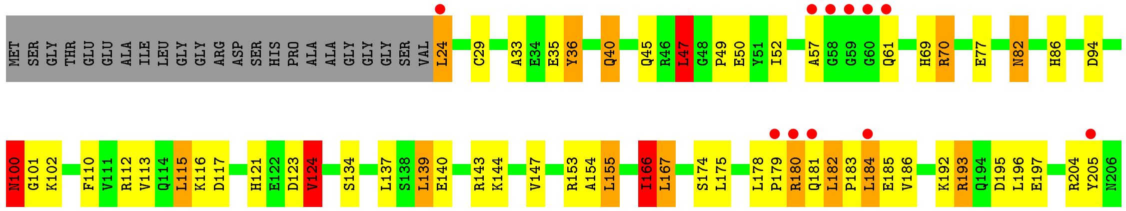
- Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

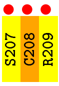
Chain P:



- Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

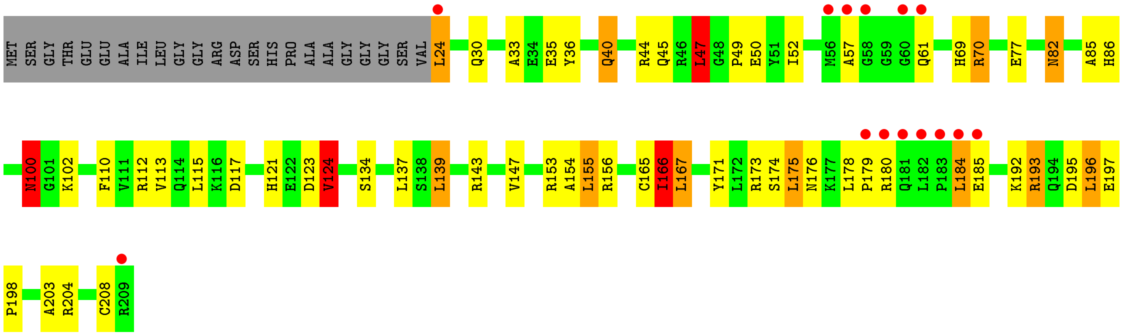
Chain Q:





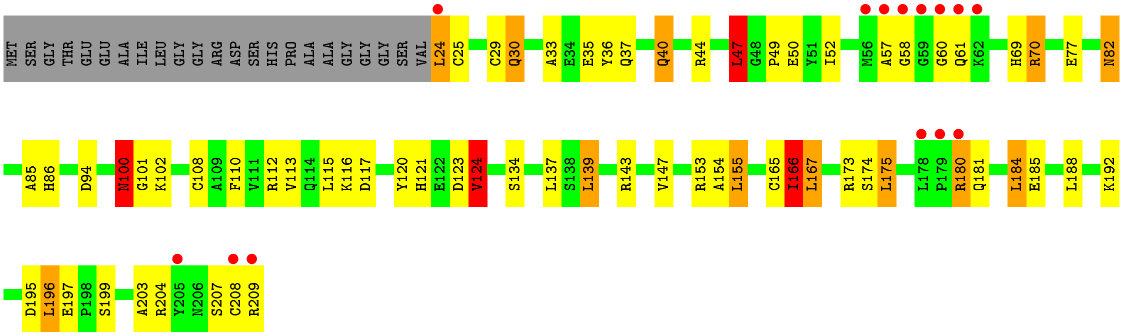
• Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

Chain R:



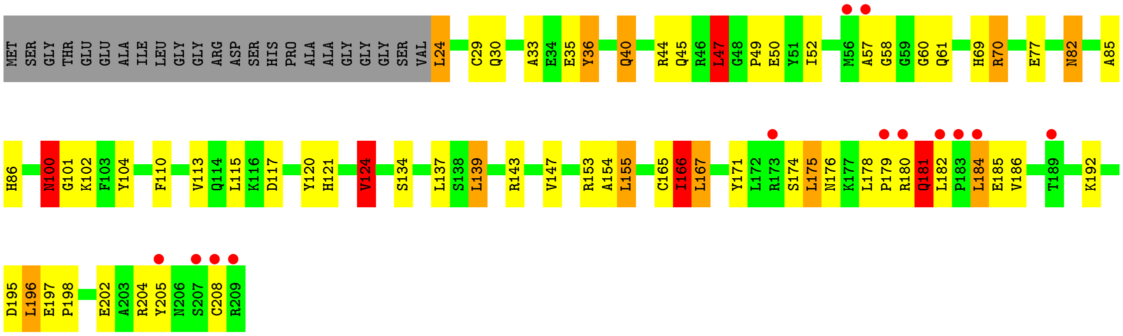
• Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

Chain S:



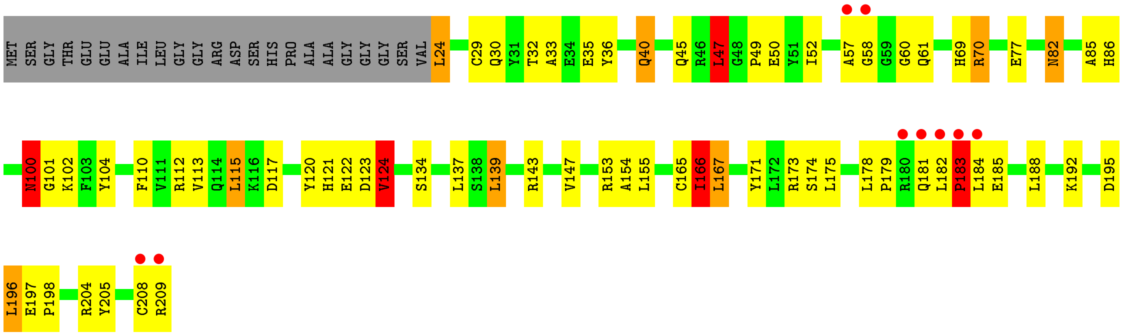
• Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

Chain T:



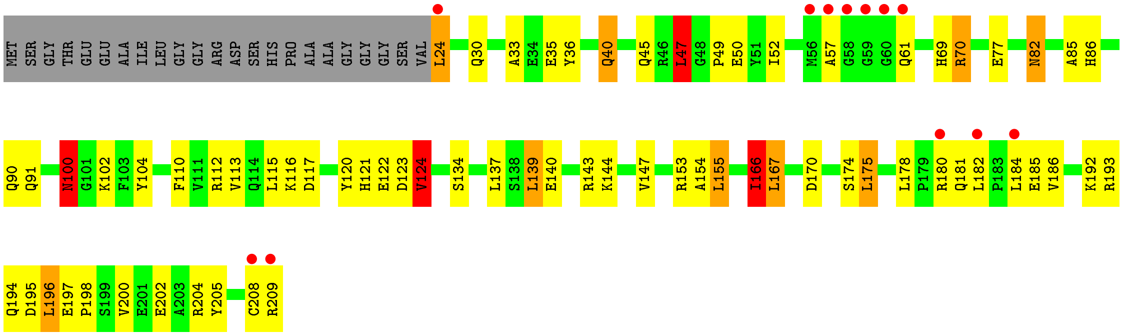
• Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

Chain U:



- Molecule 1: DNA REPAIR PROTEIN RAD52 HOMOLOG

Chain V:



4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	117.26Å 127.32Å 191.23Å 90.00° 90.29° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 29.86 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.9 (30.00-2.70) 97.0 (29.86-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.262 0.225 , 0.258	Depositor DCC
R_{free} test set	7511 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 54.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	32802	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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 ⓘ

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	0.77	0/1493	0.89	2/2006 (0.1%)
1	B	0.84	1/1493 (0.1%)	0.97	7/2006 (0.3%)
1	C	0.77	0/1493	0.94	5/2006 (0.2%)
1	D	0.69	0/1493	0.84	2/2006 (0.1%)
1	E	0.62	0/1493	0.83	3/2006 (0.1%)
1	F	0.58	0/1493	0.78	2/2006 (0.1%)
1	G	0.54	0/1493	0.79	2/2006 (0.1%)
1	H	0.54	0/1493	0.79	2/2006 (0.1%)
1	I	0.57	0/1493	0.80	2/2006 (0.1%)
1	J	0.61	1/1493 (0.1%)	0.81	3/2006 (0.1%)
1	K	0.70	1/1493 (0.1%)	0.83	2/2006 (0.1%)
1	L	0.79	1/1493 (0.1%)	0.92	3/2006 (0.1%)
1	M	0.77	1/1493 (0.1%)	0.90	2/2006 (0.1%)
1	N	0.81	2/1493 (0.1%)	0.93	5/2006 (0.2%)
1	O	0.74	1/1493 (0.1%)	0.89	4/2006 (0.2%)
1	P	0.71	0/1493	0.88	3/2006 (0.1%)
1	Q	0.71	1/1493 (0.1%)	0.86	3/2006 (0.1%)
1	R	0.71	0/1493	0.89	5/2006 (0.2%)
1	S	0.77	2/1493 (0.1%)	0.88	4/2006 (0.2%)
1	T	0.73	1/1493 (0.1%)	0.87	3/2006 (0.1%)
1	U	0.71	1/1493 (0.1%)	0.87	3/2006 (0.1%)
1	V	0.74	0/1493	0.86	3/2006 (0.1%)
All	All	0.71	13/32846 (0.0%)	0.87	70/44132 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2
1	E	0	2
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	K	0	1
1	L	0	3
1	M	0	1
1	N	0	1
1	O	0	1
1	P	0	2
1	Q	0	1
1	T	0	2
1	U	0	1
1	V	0	1
All	All	0	28

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	29	CYS	CB-SG	-7.25	1.70	1.82
1	J	29	CYS	CB-SG	-6.87	1.70	1.82
1	N	29	CYS	CB-SG	-6.86	1.70	1.82
1	L	29	CYS	CB-SG	-6.64	1.71	1.82
1	M	29	CYS	CB-SG	-6.22	1.71	1.82
1	B	117	ASP	CB-CG	-6.15	1.38	1.51
1	Q	29	CYS	CB-SG	-5.58	1.72	1.81
1	N	117	ASP	CB-CG	-5.47	1.40	1.51
1	T	29	CYS	CB-SG	-5.41	1.73	1.81
1	S	108	CYS	CB-SG	-5.32	1.73	1.81
1	U	29	CYS	CB-SG	-5.24	1.73	1.81
1	O	113	VAL	CB-CG1	-5.08	1.42	1.52
1	K	201	GLU	CG-CD	5.04	1.59	1.51

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	VAL	CB-CA-C	-6.89	98.31	111.40
1	P	124	VAL	CB-CA-C	-6.87	98.36	111.40
1	B	156	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	D	124	VAL	CB-CA-C	-6.56	98.93	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	124	VAL	CB-CA-C	-6.54	98.97	111.40
1	B	124	VAL	CB-CA-C	-6.46	99.13	111.40
1	B	117	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	L	124	VAL	CB-CA-C	-6.37	99.30	111.40
1	U	124	VAL	CB-CA-C	-6.37	99.31	111.40
1	M	124	VAL	CB-CA-C	-6.35	99.34	111.40
1	R	124	VAL	CB-CA-C	-6.34	99.35	111.40
1	A	124	VAL	CB-CA-C	-6.34	99.35	111.40
1	E	124	VAL	CB-CA-C	-6.29	99.44	111.40
1	V	124	VAL	CB-CA-C	-6.23	99.56	111.40
1	O	124	VAL	CB-CA-C	-6.20	99.63	111.40
1	F	124	VAL	CB-CA-C	-6.19	99.64	111.40
1	R	156	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	B	70	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	K	124	VAL	CB-CA-C	-6.03	99.94	111.40
1	O	47	LEU	CA-CB-CG	5.96	129.01	115.30
1	H	124	VAL	CB-CA-C	-5.96	100.08	111.40
1	P	47	LEU	CA-CB-CG	5.89	128.84	115.30
1	E	47	LEU	CA-CB-CG	5.88	128.82	115.30
1	J	47	LEU	CA-CB-CG	5.83	128.70	115.30
1	T	124	VAL	CB-CA-C	-5.79	100.39	111.40
1	Q	47	LEU	CA-CB-CG	5.78	128.59	115.30
1	N	47	LEU	CA-CB-CG	5.77	128.57	115.30
1	U	100	ASN	N-CA-C	-5.75	95.46	111.00
1	C	47	LEU	CA-CB-CG	5.73	128.49	115.30
1	V	47	LEU	CA-CB-CG	5.73	128.47	115.30
1	C	156	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	N	117	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	S	124	VAL	CB-CA-C	-5.61	100.74	111.40
1	T	47	LEU	CA-CB-CG	5.60	128.18	115.30
1	G	124	VAL	CB-CA-C	-5.59	100.78	111.40
1	Q	124	VAL	CB-CA-C	-5.58	100.80	111.40
1	N	156	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	L	47	LEU	CA-CB-CG	5.57	128.11	115.30
1	H	47	LEU	CA-CB-CG	5.56	128.08	115.30
1	M	47	LEU	CA-CB-CG	5.55	128.07	115.30
1	G	47	LEU	CA-CB-CG	5.54	128.05	115.30
1	S	47	LEU	CA-CB-CG	5.53	128.02	115.30
1	N	156	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	V	100	ASN	N-CA-C	-5.50	96.16	111.00
1	I	47	LEU	CA-CB-CG	5.39	127.70	115.30
1	F	47	LEU	CA-CB-CG	5.38	127.67	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	100	ASN	N-CA-C	-5.38	96.48	111.00
1	O	100	ASN	N-CA-C	-5.33	96.61	111.00
1	L	100	ASN	N-CA-C	-5.33	96.61	111.00
1	B	47	LEU	CA-CB-CG	5.31	127.51	115.30
1	B	100	ASN	N-CA-C	-5.28	96.75	111.00
1	U	47	LEU	CA-CB-CG	5.28	127.43	115.30
1	A	100	ASN	N-CA-C	-5.27	96.77	111.00
1	Q	100	ASN	N-CA-C	-5.25	96.81	111.00
1	B	112	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	E	100	ASN	N-CA-C	-5.20	96.97	111.00
1	R	100	ASN	N-CA-C	-5.19	96.99	111.00
1	J	124	VAL	CB-CA-C	-5.16	101.59	111.40
1	R	112	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	S	30	GLN	N-CA-C	-5.14	97.12	111.00
1	K	47	LEU	CA-CB-CG	5.11	127.06	115.30
1	S	25	CYS	CA-CB-SG	-5.10	104.82	114.00
1	J	100	ASN	N-CA-C	-5.10	97.24	111.00
1	O	30	GLN	N-CA-C	-5.10	97.24	111.00
1	C	156	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	T	181	GLN	N-CA-C	-5.06	97.35	111.00
1	R	47	LEU	CA-CB-CG	5.03	126.87	115.30
1	P	156	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	D	100	ASN	N-CA-C	-5.02	97.45	111.00
1	I	124	VAL	CB-CA-C	-5.01	101.88	111.40

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	TYR	Sidechain
1	A	36	TYR	Sidechain
1	B	104	TYR	Sidechain
1	B	36	TYR	Sidechain
1	C	104	TYR	Sidechain
1	C	36	TYR	Sidechain
1	D	104	TYR	Sidechain
1	D	36	TYR	Sidechain
1	E	104	TYR	Sidechain
1	E	36	TYR	Sidechain
1	F	36	TYR	Sidechain
1	G	36	TYR	Sidechain
1	H	36	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	I	104	TYR	Sidechain
1	K	36	TYR	Sidechain
1	L	104	TYR	Sidechain
1	L	120	TYR	Sidechain
1	L	36	TYR	Sidechain
1	M	104	TYR	Sidechain
1	N	36	TYR	Sidechain
1	O	36	TYR	Sidechain
1	P	104	TYR	Sidechain
1	P	120	TYR	Sidechain
1	Q	36	TYR	Sidechain
1	T	104	TYR	Sidechain
1	T	36	TYR	Sidechain
1	U	104	TYR	Sidechain
1	V	104	TYR	Sidechain

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	1469	0	1457	87	0
1	B	1469	0	1457	93	0
1	C	1469	0	1457	78	0
1	D	1469	0	1457	85	0
1	E	1469	0	1457	88	0
1	F	1469	0	1457	77	0
1	G	1469	0	1457	106	0
1	H	1469	0	1457	89	0
1	I	1469	0	1457	82	0
1	J	1469	0	1457	82	0
1	K	1469	0	1457	99	0
1	L	1469	0	1457	104	0
1	M	1469	0	1457	70	0
1	N	1469	0	1457	85	0
1	O	1469	0	1457	83	0
1	P	1469	0	1457	85	0
1	Q	1469	0	1457	89	0
1	R	1469	0	1457	83	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	S	1469	0	1457	89	0
1	T	1469	0	1457	87	0
1	U	1469	0	1457	86	0
1	V	1469	0	1457	92	0
2	A	23	0	0	1	0
2	B	22	0	0	2	0
2	C	21	0	0	1	0
2	D	24	0	0	1	0
2	E	22	0	0	0	0
2	F	25	0	0	1	0
2	G	18	0	0	1	0
2	H	22	0	0	0	0
2	I	22	0	0	1	0
2	J	20	0	0	1	0
2	K	23	0	0	1	0
2	L	21	0	0	0	0
2	M	23	0	0	0	0
2	N	26	0	0	0	0
2	O	17	0	0	0	0
2	P	24	0	0	1	0
2	Q	21	0	0	1	0
2	R	22	0	0	0	0
2	S	22	0	0	1	0
2	T	22	0	0	1	0
2	U	23	0	0	2	0
2	V	21	0	0	1	0
All	All	32802	0	32054	1544	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (1544) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:193:ARG:HB3	1:L:180:ARG:NH2	1.55	1.21
1:C:182:LEU:HD23	1:C:182:LEU:H	1.01	1.17
1:B:193:ARG:HG2	1:B:193:ARG:HH11	0.98	1.14
1:K:193:ARG:HB3	1:L:180:ARG:HH21	1.02	1.07
1:C:182:LEU:H	1:C:182:LEU:CD2	1.66	1.04
1:K:193:ARG:CB	1:L:180:ARG:HH21	1.70	1.03
1:Q:182:LEU:H	1:Q:182:LEU:HD23	1.20	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:50:GLU:HA	1:I:181:GLN:HE22	1.25	1.01
1:B:189:THR:HG22	1:B:190:LYS:HG3	1.43	1.00
1:N:182:LEU:HD22	1:N:182:LEU:H	1.21	0.99
1:M:182:LEU:H	1:M:182:LEU:HD23	1.25	0.99
1:Q:182:LEU:H	1:Q:182:LEU:CD2	1.77	0.97
1:F:204:ARG:HG3	1:F:204:ARG:HH21	1.28	0.95
1:L:208:CYS:HB2	1:N:33:ALA:HB2	1.47	0.93
1:K:193:ARG:HB3	1:L:180:ARG:CZ	1.98	0.92
1:B:193:ARG:CG	1:B:193:ARG:HH11	1.79	0.92
1:G:182:LEU:HD23	1:G:182:LEU:H	1.34	0.92
1:N:182:LEU:CD2	1:N:182:LEU:H	1.83	0.91
1:N:192:LYS:HE2	1:N:197:GLU:OE2	1.71	0.90
1:U:40:GLN:HE21	1:U:40:GLN:HA	1.36	0.90
1:A:167:LEU:HD13	1:A:167:LEU:H	1.35	0.90
1:C:182:LEU:HD23	1:C:182:LEU:N	1.86	0.90
1:D:167:LEU:H	1:D:167:LEU:HD13	1.36	0.90
1:Q:40:GLN:HE21	1:Q:40:GLN:HA	1.38	0.89
1:C:167:LEU:HD13	1:C:167:LEU:H	1.36	0.89
1:P:182:LEU:H	1:P:182:LEU:HD23	1.35	0.89
1:V:40:GLN:HE21	1:V:40:GLN:HA	1.37	0.89
1:I:40:GLN:HA	1:I:40:GLN:HE21	1.39	0.88
1:J:50:GLU:HA	1:J:181:GLN:NE2	1.88	0.88
1:J:167:LEU:H	1:J:167:LEU:HD13	1.37	0.88
1:K:167:LEU:HD13	1:K:167:LEU:H	1.39	0.88
1:V:180:ARG:HG2	1:V:181:GLN:N	1.88	0.88
1:J:40:GLN:HE21	1:J:40:GLN:HA	1.38	0.88
1:A:40:GLN:HA	1:A:40:GLN:HE21	1.38	0.87
1:O:167:LEU:HD13	1:O:167:LEU:H	1.38	0.87
1:D:182:LEU:H	1:D:182:LEU:HD23	1.39	0.87
1:R:184:LEU:HD22	1:R:185:GLU:H	1.39	0.87
1:M:40:GLN:HE21	1:M:40:GLN:HA	1.40	0.87
1:L:110:PHE:CE2	1:L:124:VAL:HG13	2.09	0.87
1:T:167:LEU:H	1:T:167:LEU:HD13	1.40	0.86
1:K:40:GLN:HA	1:K:40:GLN:HE21	1.40	0.86
1:B:40:GLN:HE21	1:B:40:GLN:HA	1.40	0.86
1:L:192:LYS:HB2	1:M:45:GLN:HE21	1.41	0.86
1:N:40:GLN:HA	1:N:40:GLN:HE21	1.40	0.86
1:T:40:GLN:HE21	1:T:40:GLN:HA	1.40	0.86
1:V:100:ASN:ND2	1:V:102:LYS:HB2	1.90	0.86
1:A:100:ASN:ND2	1:A:102:LYS:HB2	1.91	0.86
1:E:167:LEU:HD13	1:E:167:LEU:H	1.39	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:167:LEU:H	1:F:167:LEU:HD13	1.39	0.86
1:B:167:LEU:HD13	1:B:167:LEU:H	1.38	0.86
1:V:180:ARG:HG2	1:V:181:GLN:H	1.41	0.86
1:Q:192:LYS:HE2	1:Q:197:GLU:OE2	1.76	0.85
1:R:167:LEU:H	1:R:167:LEU:HD13	1.39	0.85
1:O:40:GLN:HA	1:O:40:GLN:HE21	1.42	0.85
1:H:167:LEU:HD13	1:H:167:LEU:H	1.41	0.85
1:L:167:LEU:HD13	1:L:167:LEU:H	1.39	0.85
1:O:100:ASN:ND2	1:O:102:LYS:HB2	1.92	0.85
1:B:193:ARG:NH1	1:B:193:ARG:HG2	1.79	0.84
1:C:40:GLN:HA	1:C:40:GLN:HE21	1.42	0.84
1:Q:184:LEU:CD2	1:Q:185:GLU:H	1.89	0.84
1:L:192:LYS:HE2	1:L:197:GLU:OE2	1.77	0.84
1:L:40:GLN:HA	1:L:40:GLN:HE21	1.40	0.84
1:O:182:LEU:H	1:O:182:LEU:HD23	1.41	0.84
1:D:40:GLN:HE21	1:D:40:GLN:HA	1.43	0.84
1:M:167:LEU:H	1:M:167:LEU:HD13	1.42	0.84
1:P:182:LEU:H	1:P:182:LEU:CD2	1.91	0.84
1:G:184:LEU:HD23	1:G:185:GLU:N	1.92	0.84
1:U:167:LEU:H	1:U:167:LEU:HD13	1.40	0.84
1:M:100:ASN:ND2	1:M:102:LYS:HB2	1.93	0.83
1:P:147:VAL:HG21	1:Q:124:VAL:HG22	1.61	0.83
1:R:40:GLN:HA	1:R:40:GLN:HE21	1.43	0.83
1:S:40:GLN:HE21	1:S:40:GLN:HA	1.42	0.82
1:Q:167:LEU:HD13	1:Q:167:LEU:H	1.44	0.82
1:E:100:ASN:ND2	1:E:102:LYS:HB2	1.95	0.82
1:G:40:GLN:HA	1:G:40:GLN:HE21	1.44	0.82
1:E:40:GLN:HE21	1:E:40:GLN:HA	1.44	0.82
1:J:100:ASN:ND2	1:J:102:LYS:HB2	1.95	0.82
1:V:167:LEU:HD13	1:V:167:LEU:H	1.42	0.82
1:R:147:VAL:HG21	1:S:124:VAL:HG22	1.61	0.81
1:G:167:LEU:H	1:G:167:LEU:HD13	1.45	0.81
1:P:100:ASN:ND2	1:P:102:LYS:HB2	1.95	0.81
1:A:182:LEU:HD23	1:A:182:LEU:H	1.45	0.81
1:A:184:LEU:HD23	1:A:185:GLU:H	1.43	0.81
1:H:40:GLN:HE21	1:H:40:GLN:HA	1.45	0.81
1:A:184:LEU:CD2	1:A:185:GLU:H	1.94	0.80
1:I:167:LEU:H	1:I:167:LEU:HD13	1.46	0.80
1:S:100:ASN:ND2	1:S:102:LYS:HB2	1.95	0.80
1:Q:100:ASN:ND2	1:Q:102:LYS:HB2	1.96	0.80
1:P:40:GLN:HE21	1:P:40:GLN:HA	1.46	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:208:CYS:HB2	1:T:33:ALA:HB2	1.64	0.80
1:B:182:LEU:H	1:B:182:LEU:HD23	1.47	0.80
1:S:167:LEU:H	1:S:167:LEU:HD13	1.47	0.80
1:S:184:LEU:HD23	1:S:185:GLU:H	1.45	0.79
1:F:147:VAL:HG21	1:G:124:VAL:HG22	1.62	0.79
1:P:204:ARG:HG3	1:Q:35:GLU:OE1	1.82	0.79
1:L:100:ASN:ND2	1:L:102:LYS:HB2	1.97	0.79
1:U:192:LYS:HB2	1:V:45:GLN:NE2	1.97	0.79
1:C:100:ASN:ND2	1:C:102:LYS:HB2	1.96	0.78
1:D:100:ASN:ND2	1:D:102:LYS:HB2	1.98	0.78
1:K:100:ASN:ND2	1:K:102:LYS:HB2	1.98	0.78
1:F:100:ASN:ND2	1:F:102:LYS:HB2	1.99	0.78
1:U:100:ASN:ND2	1:U:102:LYS:HB2	1.99	0.78
1:F:40:GLN:HA	1:F:40:GLN:HE21	1.48	0.78
1:N:167:LEU:HD13	1:N:167:LEU:H	1.49	0.78
1:P:167:LEU:HD13	1:P:167:LEU:H	1.49	0.78
1:A:33:ALA:HB2	1:J:208:CYS:HB2	1.64	0.78
1:T:166:ILE:HG22	1:T:167:LEU:HD12	1.66	0.78
1:A:110:PHE:CE2	1:A:124:VAL:HG13	2.19	0.77
1:I:100:ASN:ND2	1:I:102:LYS:HB2	1.99	0.77
1:R:100:ASN:ND2	1:R:102:LYS:HB2	1.99	0.77
1:D:110:PHE:CE2	1:D:124:VAL:HG13	2.19	0.77
1:S:47:LEU:H	1:S:47:LEU:HD23	1.48	0.77
1:H:147:VAL:HG21	1:I:124:VAL:HG22	1.66	0.77
1:N:100:ASN:ND2	1:N:102:LYS:HB2	1.99	0.77
1:N:69:HIS:HB3	1:O:167:LEU:HD21	1.66	0.77
1:U:204:ARG:HG3	1:V:35:GLU:OE1	1.83	0.77
1:R:192:LYS:HE2	1:R:197:GLU:OE2	1.83	0.77
1:D:147:VAL:HG21	1:E:124:VAL:HG22	1.66	0.77
1:I:182:LEU:H	1:I:182:LEU:HD23	1.49	0.77
1:V:110:PHE:CE2	1:V:124:VAL:HG13	2.19	0.77
1:U:110:PHE:CE2	1:U:124:VAL:HG13	2.20	0.76
1:L:147:VAL:HG21	1:M:124:VAL:HG22	1.68	0.76
1:P:208:CYS:HB2	1:R:33:ALA:HB2	1.67	0.76
1:E:86:HIS:ND1	1:F:121:HIS:HD2	1.84	0.76
1:H:100:ASN:ND2	1:H:102:LYS:HB2	1.99	0.76
1:B:110:PHE:CE2	1:B:124:VAL:HG13	2.19	0.76
1:L:192:LYS:HB2	1:M:45:GLN:NE2	1.99	0.76
1:J:40:GLN:HE21	1:J:40:GLN:CA	1.99	0.76
1:M:208:CYS:HB3	1:O:33:ALA:HB2	1.66	0.76
1:Q:193:ARG:HG2	1:Q:193:ARG:HH11	1.50	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:147:VAL:HG21	1:V:124:VAL:HG22	1.68	0.76
1:J:204:ARG:HG3	1:K:35:GLU:OE1	1.86	0.75
1:I:50:GLU:HA	1:I:181:GLN:NE2	2.00	0.75
1:S:110:PHE:CE2	1:S:124:VAL:HG13	2.21	0.75
1:F:196:LEU:HD11	1:F:198:PRO:HG3	1.69	0.75
1:G:100:ASN:ND2	1:G:102:LYS:HB2	2.01	0.75
1:K:193:ARG:HB3	1:L:180:ARG:NE	2.01	0.75
1:I:195:ASP:HB3	1:J:77:GLU:HG3	1.68	0.75
1:M:182:LEU:N	1:M:182:LEU:HD23	2.02	0.75
1:S:147:VAL:HG21	1:T:124:VAL:HG22	1.67	0.75
1:U:205:TYR:HE2	1:U:209:ARG:NH2	1.85	0.75
1:J:147:VAL:HG21	1:K:124:VAL:HG22	1.69	0.74
1:Q:205:TYR:CE1	1:S:37:GLN:HB2	2.22	0.74
1:F:166:ILE:HG22	1:F:167:LEU:HD12	1.69	0.74
1:G:204:ARG:HG3	1:G:204:ARG:HH21	1.50	0.74
1:K:110:PHE:CE2	1:K:124:VAL:HG13	2.21	0.74
1:L:134:SER:HB3	1:L:137:LEU:HB2	1.69	0.74
1:K:192:LYS:HE2	1:K:197:GLU:OE2	1.87	0.74
1:Q:184:LEU:HD23	1:Q:185:GLU:H	1.51	0.74
1:T:110:PHE:CE2	1:T:124:VAL:HG13	2.22	0.74
1:E:110:PHE:CE2	1:E:124:VAL:HG13	2.22	0.74
1:N:147:VAL:HG21	1:O:124:VAL:HG22	1.67	0.74
1:U:182:LEU:H	1:U:182:LEU:HD23	1.51	0.74
1:H:110:PHE:CE2	1:H:124:VAL:HG13	2.23	0.74
1:I:166:ILE:HG22	1:I:167:LEU:HD12	1.70	0.74
1:C:47:LEU:HD23	1:C:47:LEU:H	1.52	0.74
1:J:184:LEU:HD13	1:J:185:GLU:H	1.53	0.74
1:F:110:PHE:CE2	1:F:124:VAL:HG13	2.23	0.73
1:D:204:ARG:HG3	1:E:35:GLU:OE1	1.88	0.73
1:F:86:HIS:ND1	1:G:121:HIS:HD2	1.87	0.73
1:C:47:LEU:N	1:C:47:LEU:HD23	2.02	0.73
1:R:166:ILE:HG22	1:R:167:LEU:HD12	1.70	0.73
1:G:186:VAL:HG11	1:H:171:TYR:HA	1.70	0.73
1:I:50:GLU:CA	1:I:181:GLN:HE22	2.01	0.73
1:G:110:PHE:CE2	1:G:124:VAL:HG13	2.24	0.73
1:H:186:VAL:HG21	1:I:171:TYR:HA	1.71	0.72
1:M:70:ARG:HH11	1:M:70:ARG:HG3	1.54	0.72
1:Q:147:VAL:HG21	1:R:124:VAL:HG22	1.71	0.72
1:U:184:LEU:HD13	1:U:185:GLU:O	1.89	0.72
1:D:82:ASN:H	1:D:82:ASN:HD22	1.36	0.72
1:D:47:LEU:HD23	1:D:47:LEU:H	1.54	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:LEU:N	1:D:47:LEU:HD23	2.04	0.72
1:K:193:ARG:HE	1:L:180:ARG:NH2	1.87	0.72
1:Q:40:GLN:CA	1:Q:40:GLN:HE21	2.02	0.72
1:B:100:ASN:ND2	1:B:102:LYS:HB2	2.03	0.72
1:B:192:LYS:HB2	1:C:45:GLN:HE21	1.55	0.72
1:O:110:PHE:CE2	1:O:124:VAL:HG13	2.24	0.72
1:A:166:ILE:HG22	1:A:167:LEU:HD12	1.70	0.72
1:P:192:LYS:HB2	1:Q:45:GLN:NE2	2.05	0.72
1:A:82:ASN:H	1:A:82:ASN:HD22	1.36	0.72
1:K:40:GLN:CA	1:K:40:GLN:HE21	2.01	0.72
1:M:110:PHE:CE2	1:M:124:VAL:HG13	2.25	0.72
1:I:147:VAL:HG21	1:J:124:VAL:HG22	1.71	0.71
1:J:181:GLN:O	1:J:181:GLN:HG3	1.90	0.71
1:P:192:LYS:HB2	1:Q:45:GLN:HE21	1.55	0.71
1:A:47:LEU:N	1:A:47:LEU:HD23	2.05	0.71
1:N:185:GLU:OE1	1:O:177:LYS:NZ	2.23	0.71
1:R:47:LEU:N	1:R:47:LEU:HD23	2.05	0.71
1:D:167:LEU:H	1:D:167:LEU:CD1	2.01	0.71
1:G:180:ARG:HG2	1:G:181:GLN:H	1.54	0.71
1:T:147:VAL:HG21	1:U:124:VAL:HG22	1.71	0.71
1:J:110:PHE:CE2	1:J:124:VAL:HG13	2.26	0.71
1:R:110:PHE:CE2	1:R:124:VAL:HG13	2.25	0.71
1:R:86:HIS:ND1	1:S:121:HIS:HD2	1.88	0.71
1:T:100:ASN:ND2	1:T:102:LYS:HB2	2.05	0.71
1:C:184:LEU:HD12	1:C:185:GLU:O	1.89	0.71
1:E:147:VAL:HG21	1:F:124:VAL:HG22	1.70	0.71
1:E:166:ILE:HG22	1:E:167:LEU:HD12	1.72	0.71
1:A:124:VAL:HG22	1:K:147:VAL:HG21	1.72	0.71
1:G:147:VAL:HG21	1:H:124:VAL:HG22	1.72	0.71
1:M:184:LEU:HD23	1:M:185:GLU:H	1.55	0.71
1:O:147:VAL:HG21	1:P:124:VAL:HG22	1.73	0.71
1:A:182:LEU:H	1:A:182:LEU:CD2	2.04	0.71
1:A:47:LEU:H	1:A:47:LEU:HD23	1.56	0.71
1:O:69:HIS:HB3	1:P:167:LEU:HD21	1.71	0.71
1:N:110:PHE:CE2	1:N:124:VAL:HG13	2.26	0.70
1:U:40:GLN:CA	1:U:40:GLN:HE21	2.03	0.70
1:D:36:TYR:OH	1:D:40:GLN:HG3	1.91	0.70
1:R:134:SER:HB3	1:R:137:LEU:HB2	1.74	0.70
1:A:40:GLN:HE21	1:A:40:GLN:CA	2.05	0.70
1:L:40:GLN:HE21	1:L:40:GLN:CA	2.04	0.70
1:R:70:ARG:HG3	1:R:70:ARG:HH11	1.56	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:182:LEU:HD23	1:L:182:LEU:H	1.55	0.70
1:Q:182:LEU:N	1:Q:182:LEU:HD23	2.02	0.70
1:G:166:ILE:HG22	1:G:167:LEU:HD12	1.73	0.70
1:R:40:GLN:CA	1:R:40:GLN:HE21	2.05	0.70
1:F:47:LEU:H	1:F:47:LEU:HD23	1.56	0.70
1:J:50:GLU:HA	1:J:181:GLN:HE22	1.57	0.70
1:S:47:LEU:N	1:S:47:LEU:HD23	2.07	0.70
1:T:204:ARG:HG3	1:U:35:GLU:OE1	1.92	0.70
1:O:47:LEU:N	1:O:47:LEU:HD23	2.07	0.69
1:P:86:HIS:ND1	1:Q:121:HIS:HD2	1.89	0.69
1:R:47:LEU:H	1:R:47:LEU:HD23	1.56	0.69
1:B:167:LEU:CD1	1:B:167:LEU:H	2.04	0.69
1:F:47:LEU:HD23	1:F:47:LEU:N	2.07	0.69
1:M:147:VAL:HG21	1:N:124:VAL:HG22	1.73	0.69
1:U:196:LEU:HD12	1:U:198:PRO:HG3	1.74	0.69
1:V:40:GLN:HE21	1:V:40:GLN:CA	2.04	0.69
1:V:47:LEU:H	1:V:47:LEU:HD23	1.56	0.69
1:B:40:GLN:CA	1:B:40:GLN:HE21	2.06	0.69
1:Q:82:ASN:H	1:Q:82:ASN:HD22	1.38	0.69
1:L:124:VAL:HG22	1:V:147:VAL:HG21	1.74	0.69
1:Q:86:HIS:ND1	1:R:121:HIS:HD2	1.90	0.69
1:V:47:LEU:N	1:V:47:LEU:HD23	2.07	0.69
1:K:193:ARG:HH12	1:L:182:LEU:HD22	1.58	0.69
1:S:184:LEU:HD23	1:S:185:GLU:N	2.08	0.69
1:C:167:LEU:CD1	1:C:167:LEU:H	2.06	0.69
1:K:182:LEU:HD23	1:K:182:LEU:H	1.57	0.69
1:U:196:LEU:CD1	1:U:198:PRO:HG3	2.23	0.69
1:D:166:ILE:HG22	1:D:167:LEU:HD12	1.75	0.69
1:G:36:TYR:OH	1:G:40:GLN:HG3	1.91	0.69
1:O:192:LYS:HB2	1:P:45:GLN:NE2	2.08	0.69
1:U:86:HIS:ND1	1:V:121:HIS:HD2	1.91	0.69
1:V:166:ILE:HG22	1:V:167:LEU:HD12	1.75	0.69
1:T:208:CYS:HB3	1:V:33:ALA:HB2	1.75	0.69
1:G:86:HIS:ND1	1:H:121:HIS:HD2	1.91	0.69
1:O:134:SER:HB3	1:O:137:LEU:HB2	1.74	0.69
1:T:47:LEU:HD23	1:T:47:LEU:H	1.58	0.69
1:V:82:ASN:HD22	1:V:82:ASN:H	1.40	0.69
1:I:40:GLN:CA	1:I:40:GLN:HE21	2.04	0.69
1:P:47:LEU:HD23	1:P:47:LEU:N	2.08	0.68
1:E:82:ASN:HD22	1:E:82:ASN:H	1.41	0.68
1:T:186:VAL:HG21	1:U:171:TYR:HA	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:192:LYS:HB3	1:G:47:LEU:HA	1.76	0.68
1:Q:36:TYR:OH	1:Q:40:GLN:HG3	1.93	0.68
1:T:47:LEU:HD23	1:T:47:LEU:N	2.08	0.68
1:L:86:HIS:ND1	1:M:121:HIS:HD2	1.92	0.68
1:C:110:PHE:CE2	1:C:124:VAL:HG13	2.28	0.68
1:L:82:ASN:H	1:L:82:ASN:HD22	1.41	0.68
1:I:86:HIS:ND1	1:J:121:HIS:HD2	1.91	0.68
1:F:204:ARG:HG3	1:F:204:ARG:NH2	2.04	0.68
1:C:184:LEU:HD13	1:C:185:GLU:N	2.09	0.68
1:U:205:TYR:CE2	1:U:209:ARG:NH2	2.62	0.68
1:A:167:LEU:H	1:A:167:LEU:CD1	2.07	0.67
1:N:82:ASN:HD22	1:N:82:ASN:H	1.42	0.67
1:C:166:ILE:HG22	1:C:167:LEU:HD12	1.76	0.67
1:A:121:HIS:HD2	1:K:86:HIS:ND1	1.91	0.67
1:B:147:VAL:HG21	1:C:124:VAL:HG22	1.76	0.67
1:G:186:VAL:HB	1:H:174:SER:HB3	1.76	0.67
1:N:179:PRO:O	1:N:180:ARG:O	2.11	0.67
1:G:180:ARG:HG2	1:G:181:GLN:N	2.08	0.67
1:H:166:ILE:HG22	1:H:167:LEU:HD12	1.75	0.67
1:L:166:ILE:HG22	1:L:167:LEU:HD12	1.75	0.67
1:L:184:LEU:HD23	1:L:185:GLU:N	2.09	0.67
1:R:113:VAL:HG12	1:R:154:ALA:HB1	1.77	0.67
1:C:147:VAL:HG21	1:D:124:VAL:HG22	1.77	0.67
1:N:70:ARG:HH11	1:N:70:ARG:HG3	1.60	0.67
1:T:50:GLU:HA	1:T:181:GLN:NE2	2.10	0.67
1:T:86:HIS:ND1	1:U:121:HIS:HD2	1.92	0.67
1:U:166:ILE:HG22	1:U:167:LEU:HD12	1.76	0.67
1:G:134:SER:HB3	1:G:137:LEU:HB2	1.77	0.67
1:R:52:ILE:HG13	1:R:175:LEU:HD11	1.77	0.67
1:G:182:LEU:H	1:G:182:LEU:CD2	2.06	0.67
1:C:184:LEU:HD13	1:C:185:GLU:H	1.59	0.67
1:C:40:GLN:CA	1:C:40:GLN:HE21	2.06	0.67
1:K:47:LEU:HD23	1:K:47:LEU:N	2.09	0.67
1:M:184:LEU:HD23	1:M:185:GLU:N	2.10	0.67
1:U:134:SER:HB3	1:U:137:LEU:HB2	1.75	0.67
1:H:69:HIS:HB3	1:I:167:LEU:HD21	1.77	0.66
1:N:166:ILE:HG22	1:N:167:LEU:HD12	1.77	0.66
1:U:47:LEU:HD23	1:U:47:LEU:N	2.10	0.66
1:O:192:LYS:HE2	1:O:197:GLU:OE2	1.95	0.66
1:Q:134:SER:HB3	1:Q:137:LEU:HB2	1.76	0.66
1:T:181:GLN:O	1:T:181:GLN:HG3	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:VAL:HG21	1:B:124:VAL:HG22	1.78	0.66
1:K:167:LEU:CD1	1:K:167:LEU:H	2.07	0.66
1:M:49:PRO:HD2	1:M:50:GLU:OE1	1.96	0.66
1:O:167:LEU:H	1:O:167:LEU:CD1	2.07	0.66
1:D:208:CYS:HB2	1:F:33:ALA:HB2	1.77	0.66
1:G:47:LEU:HD23	1:G:47:LEU:H	1.61	0.66
1:O:40:GLN:CA	1:O:40:GLN:HE21	2.09	0.66
1:O:195:ASP:HB3	1:P:77:GLU:HG3	1.78	0.66
1:Q:110:PHE:CE2	1:Q:124:VAL:HG13	2.30	0.66
1:S:113:VAL:HG12	1:S:154:ALA:HB1	1.77	0.66
1:E:47:LEU:N	1:E:47:LEU:HD23	2.10	0.66
1:L:69:HIS:HB3	1:M:167:LEU:HD21	1.78	0.66
1:F:192:LYS:HG2	1:G:51:TYR:CE1	2.31	0.66
1:T:69:HIS:HB3	1:U:167:LEU:HD21	1.76	0.66
1:A:86:HIS:ND1	1:B:121:HIS:HD2	1.93	0.66
1:B:47:LEU:HD23	1:B:47:LEU:N	2.11	0.66
1:B:69:HIS:HB3	1:C:167:LEU:HD21	1.78	0.66
1:H:134:SER:HB3	1:H:137:LEU:HB2	1.77	0.66
1:K:139:LEU:O	1:K:143:ARG:HG3	1.95	0.66
1:N:184:LEU:O	1:O:173:ARG:NH2	2.28	0.66
1:O:49:PRO:HD2	1:O:50:GLU:OE1	1.96	0.66
1:A:184:LEU:CD2	1:A:185:GLU:N	2.59	0.65
1:R:196:LEU:HD12	1:R:198:PRO:HG3	1.77	0.65
1:K:166:ILE:HG22	1:K:167:LEU:HD12	1.76	0.65
1:M:47:LEU:H	1:M:47:LEU:HD23	1.61	0.65
1:T:134:SER:HB3	1:T:137:LEU:HB2	1.78	0.65
1:H:86:HIS:ND1	1:I:121:HIS:HD2	1.94	0.65
1:S:86:HIS:ND1	1:T:121:HIS:HD2	1.94	0.65
1:N:182:LEU:N	1:N:182:LEU:CD2	2.55	0.65
1:N:40:GLN:HE21	1:N:40:GLN:CA	2.09	0.65
1:C:86:HIS:ND1	1:D:121:HIS:HD2	1.95	0.65
1:J:166:ILE:HG22	1:J:167:LEU:HD12	1.79	0.65
1:K:193:ARG:HB3	1:L:180:ARG:HE	1.61	0.65
1:P:52:ILE:HG13	1:P:175:LEU:HD11	1.77	0.65
1:J:167:LEU:H	1:J:167:LEU:CD1	2.09	0.65
1:K:193:ARG:NE	1:L:180:ARG:CZ	2.59	0.65
1:L:184:LEU:HD23	1:L:185:GLU:H	1.62	0.65
1:M:69:HIS:HB3	1:N:167:LEU:HD21	1.79	0.65
1:S:204:ARG:HG3	1:T:35:GLU:OE1	1.97	0.65
1:C:82:ASN:HB2	1:D:117:ASP:OD1	1.96	0.65
1:D:49:PRO:HD2	1:D:50:GLU:OE1	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:40:GLN:HE21	1:H:40:GLN:CA	2.10	0.65
1:I:110:PHE:CE2	1:I:124:VAL:HG13	2.32	0.65
1:O:166:ILE:HG22	1:O:167:LEU:HD12	1.78	0.65
1:V:100:ASN:HD21	1:V:102:LYS:HB2	1.61	0.65
1:L:167:LEU:CD1	1:L:167:LEU:H	2.10	0.64
1:U:167:LEU:CD1	1:U:167:LEU:H	2.09	0.64
1:D:182:LEU:H	1:D:182:LEU:CD2	2.10	0.64
1:J:134:SER:HB3	1:J:137:LEU:HB2	1.80	0.64
1:Q:166:ILE:HG22	1:Q:167:LEU:HD12	1.77	0.64
1:Q:184:LEU:HD22	1:Q:185:GLU:H	1.62	0.64
1:F:196:LEU:C	1:F:196:LEU:HD13	2.18	0.64
1:M:47:LEU:N	1:M:47:LEU:HD23	2.13	0.64
1:M:82:ASN:HD22	1:M:82:ASN:H	1.45	0.64
1:T:182:LEU:H	1:T:182:LEU:HD23	1.60	0.64
1:B:47:LEU:HD23	1:B:47:LEU:H	1.62	0.64
1:O:82:ASN:H	1:O:82:ASN:HD22	1.45	0.64
1:P:50:GLU:HA	1:P:181:GLN:HE22	1.63	0.64
1:S:134:SER:HB3	1:S:137:LEU:HB2	1.78	0.64
1:G:69:HIS:HB3	1:H:167:LEU:HD21	1.79	0.64
1:S:40:GLN:HE21	1:S:40:GLN:CA	2.10	0.64
1:F:167:LEU:H	1:F:167:LEU:CD1	2.11	0.64
1:C:182:LEU:N	1:C:182:LEU:CD2	2.47	0.64
1:K:82:ASN:HD22	1:K:82:ASN:H	1.44	0.64
1:T:70:ARG:HH11	1:T:70:ARG:HG3	1.63	0.64
1:A:167:LEU:N	1:A:167:LEU:HD13	2.11	0.64
1:M:86:HIS:ND1	1:N:121:HIS:HD2	1.96	0.64
1:U:47:LEU:HD23	1:U:47:LEU:H	1.62	0.64
1:E:167:LEU:H	1:E:167:LEU:CD1	2.09	0.64
1:Q:207:SER:C	1:Q:209:ARG:H	2.00	0.64
1:E:40:GLN:CA	1:E:40:GLN:HE21	2.11	0.64
1:H:204:ARG:HG3	1:I:35:GLU:OE1	1.98	0.64
1:Q:192:LYS:HB2	1:R:45:GLN:HE21	1.63	0.64
1:K:47:LEU:HD23	1:K:47:LEU:H	1.61	0.63
1:Q:52:ILE:HG13	1:Q:175:LEU:HD11	1.80	0.63
1:B:70:ARG:HH11	1:B:70:ARG:HG3	1.64	0.63
1:C:204:ARG:HG3	1:C:204:ARG:HH21	1.63	0.63
1:C:36:TYR:OH	1:C:40:GLN:HG3	1.98	0.63
1:P:47:LEU:HD23	1:P:47:LEU:H	1.61	0.63
1:T:40:GLN:CA	1:T:40:GLN:HE21	2.11	0.63
1:J:47:LEU:H	1:J:47:LEU:HD23	1.63	0.63
1:M:166:ILE:HG22	1:M:167:LEU:HD12	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:166:ILE:HG22	1:S:167:LEU:HD12	1.80	0.63
1:O:47:LEU:H	1:O:47:LEU:HD23	1.61	0.63
1:V:167:LEU:CD1	1:V:167:LEU:H	2.12	0.63
1:P:69:HIS:HB3	1:Q:167:LEU:HD21	1.81	0.63
1:D:167:LEU:N	1:D:167:LEU:CD1	2.62	0.63
1:G:82:ASN:HD22	1:G:82:ASN:H	1.47	0.63
1:U:205:TYR:HE2	1:U:209:ARG:HH22	1.46	0.63
1:M:123:ASP:OD1	1:M:153:ARG:NH1	2.32	0.63
1:R:82:ASN:H	1:R:82:ASN:HD22	1.44	0.63
1:E:52:ILE:HG13	1:E:175:LEU:HD11	1.81	0.62
1:G:40:GLN:CA	1:G:40:GLN:HE21	2.12	0.62
1:Q:193:ARG:NH1	1:Q:193:ARG:HG2	2.10	0.62
1:R:193:ARG:HH11	1:R:193:ARG:HG2	1.64	0.62
1:B:82:ASN:HD22	1:B:82:ASN:H	1.47	0.62
1:G:195:ASP:HB3	1:H:77:GLU:HG3	1.80	0.62
1:P:70:ARG:HH11	1:P:70:ARG:HG3	1.64	0.62
1:Q:204:ARG:HG3	1:R:35:GLU:OE1	1.99	0.62
1:G:47:LEU:HD23	1:G:47:LEU:N	2.13	0.62
1:G:52:ILE:HG13	1:G:175:LEU:HD11	1.79	0.62
1:F:208:CYS:HB3	1:H:33:ALA:HB2	1.81	0.62
1:J:70:ARG:HG3	1:J:70:ARG:HH11	1.64	0.62
1:S:180:ARG:HG2	1:S:180:ARG:HH11	1.64	0.62
1:S:82:ASN:H	1:S:82:ASN:HD22	1.47	0.62
1:K:193:ARG:NE	1:L:180:ARG:NH2	2.47	0.62
1:R:167:LEU:CD1	1:R:167:LEU:H	2.12	0.62
1:U:82:ASN:H	1:U:82:ASN:HD22	1.47	0.62
1:V:197:GLU:O	1:V:200:VAL:HB	1.99	0.62
1:I:134:SER:HB3	1:I:137:LEU:HB2	1.82	0.62
1:K:193:ARG:CB	1:L:180:ARG:HE	2.13	0.62
1:P:182:LEU:N	1:P:182:LEU:HD23	2.12	0.62
1:P:82:ASN:HD22	1:P:82:ASN:H	1.48	0.62
1:H:167:LEU:CD1	1:H:167:LEU:H	2.13	0.62
1:K:134:SER:HB3	1:K:137:LEU:HB2	1.82	0.62
1:A:100:ASN:HD22	1:A:102:LYS:HB2	1.64	0.62
1:A:196:LEU:CD1	1:A:198:PRO:HG3	2.30	0.62
1:C:134:SER:HB3	1:C:137:LEU:HB2	1.80	0.62
1:I:24:LEU:HB3	1:J:30:GLN:NE2	2.14	0.62
1:J:47:LEU:N	1:J:47:LEU:HD23	2.15	0.62
1:O:70:ARG:HH11	1:O:70:ARG:HG3	1.64	0.62
1:P:110:PHE:CE2	1:P:124:VAL:HG13	2.34	0.62
1:L:47:LEU:HD23	1:L:47:LEU:H	1.65	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:LEU:HD13	1:C:167:LEU:N	2.12	0.62
1:T:24:LEU:HB3	1:U:30:GLN:NE2	2.13	0.62
1:E:207:SER:C	1:E:209:ARG:H	2.04	0.61
1:I:47:LEU:H	1:I:47:LEU:HD23	1.65	0.61
1:K:182:LEU:N	1:K:182:LEU:HD23	2.15	0.61
1:H:82:ASN:HD22	1:H:82:ASN:H	1.46	0.61
1:L:47:LEU:HD23	1:L:47:LEU:N	2.14	0.61
1:N:47:LEU:HD23	1:N:47:LEU:H	1.64	0.61
1:F:82:ASN:H	1:F:82:ASN:HD22	1.46	0.61
1:Q:167:LEU:CD1	1:Q:167:LEU:H	2.14	0.61
1:A:70:ARG:HG3	1:A:70:ARG:HH11	1.64	0.61
1:B:86:HIS:ND1	1:C:121:HIS:HD2	1.98	0.61
1:Q:47:LEU:N	1:Q:47:LEU:HD23	2.15	0.61
1:F:113:VAL:HG12	1:F:154:ALA:HB1	1.82	0.61
1:H:204:ARG:HH21	1:H:204:ARG:HG3	1.65	0.61
1:Q:24:LEU:HB3	1:R:30:GLN:NE2	2.16	0.61
1:V:52:ILE:HG13	1:V:175:LEU:HD11	1.82	0.61
1:A:113:VAL:HG12	1:A:154:ALA:HB1	1.82	0.61
1:B:196:LEU:CD1	1:B:198:PRO:HG3	2.29	0.61
1:D:86:HIS:ND1	1:E:121:HIS:HD2	1.98	0.61
1:F:52:ILE:HG13	1:F:175:LEU:HD11	1.81	0.61
1:H:195:ASP:HB3	1:I:77:GLU:HG3	1.83	0.61
1:B:166:ILE:HG22	1:B:167:LEU:HD12	1.81	0.61
1:B:182:LEU:H	1:B:182:LEU:CD2	2.12	0.61
1:S:204:ARG:HG3	1:S:204:ARG:HH21	1.65	0.61
1:T:208:CYS:CB	1:V:33:ALA:HB2	2.31	0.61
1:T:49:PRO:HD2	1:T:50:GLU:OE1	2.00	0.61
1:B:187:ASP:OD2	1:B:189:THR:HB	2.01	0.61
1:C:192:LYS:HB2	1:D:45:GLN:NE2	2.15	0.61
1:A:36:TYR:OH	1:A:40:GLN:HG3	2.01	0.61
1:C:167:LEU:N	1:C:167:LEU:CD1	2.64	0.61
1:J:195:ASP:HB3	1:K:77:GLU:HG3	1.81	0.61
1:N:47:LEU:HD23	1:N:47:LEU:N	2.15	0.61
1:T:165:CYS:HA	2:T:2022:HOH:O	2.00	0.61
1:U:192:LYS:HB2	1:V:45:GLN:HE21	1.63	0.61
1:Q:113:VAL:HG12	1:Q:154:ALA:HB1	1.83	0.60
1:S:208:CYS:HB2	1:U:33:ALA:HB2	1.83	0.60
1:A:82:ASN:HB2	1:B:117:ASP:OD1	2.01	0.60
1:H:52:ILE:HG13	1:H:175:LEU:HD11	1.83	0.60
1:N:86:HIS:ND1	1:O:121:HIS:HD2	1.99	0.60
1:C:70:ARG:HG3	1:C:70:ARG:HH11	1.64	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:LEU:HD23	1:H:47:LEU:N	2.16	0.60
1:G:192:LYS:HE2	1:H:45:GLN:HE22	1.65	0.60
1:Q:205:TYR:HE1	1:S:37:GLN:HB2	1.63	0.60
1:L:121:HIS:HD2	1:V:86:HIS:ND1	1.99	0.60
1:E:195:ASP:HB3	1:F:77:GLU:HG3	1.83	0.60
1:I:182:LEU:H	1:I:182:LEU:CD2	2.13	0.60
1:M:40:GLN:CA	1:M:40:GLN:HE21	2.12	0.60
1:N:124:VAL:O	1:N:153:ARG:HD3	2.01	0.60
1:O:100:ASN:HD21	1:O:102:LYS:HB2	1.62	0.60
1:T:196:LEU:HD13	1:T:198:PRO:HG3	1.82	0.60
1:U:100:ASN:HD21	1:U:102:LYS:HB2	1.66	0.60
1:D:69:HIS:HB3	1:E:167:LEU:HD21	1.83	0.60
1:G:113:VAL:HG12	1:G:154:ALA:HB1	1.82	0.60
1:M:167:LEU:CD1	1:M:167:LEU:H	2.14	0.60
1:P:166:ILE:HG22	1:P:167:LEU:HD12	1.82	0.60
1:A:134:SER:HB3	1:A:137:LEU:HB2	1.84	0.60
1:I:47:LEU:N	1:I:47:LEU:HD23	2.16	0.60
1:L:35:GLU:OE1	1:V:204:ARG:HG3	2.02	0.60
1:N:36:TYR:OH	1:N:40:GLN:HG3	2.01	0.60
1:V:192:LYS:NZ	1:V:197:GLU:OE2	2.34	0.60
1:C:49:PRO:HD2	1:C:50:GLU:OE1	2.02	0.60
1:D:52:ILE:HG13	1:D:175:LEU:HD11	1.83	0.60
1:J:167:LEU:HD13	1:J:167:LEU:N	2.14	0.60
1:G:70:ARG:HH11	1:G:70:ARG:HG3	1.66	0.60
1:J:52:ILE:HG13	1:J:175:LEU:HD11	1.83	0.60
1:J:86:HIS:ND1	1:K:121:HIS:HD2	2.00	0.60
1:D:134:SER:HB3	1:D:137:LEU:HB2	1.83	0.59
1:F:36:TYR:OH	1:F:40:GLN:HG3	2.01	0.59
1:L:82:ASN:HB2	1:M:117:ASP:OD1	2.02	0.59
1:U:52:ILE:HG13	1:U:175:LEU:HD11	1.84	0.59
1:E:47:LEU:H	1:E:47:LEU:HD23	1.65	0.59
1:K:52:ILE:HG13	1:K:175:LEU:HD11	1.83	0.59
1:L:45:GLN:HE21	1:V:192:LYS:HB2	1.67	0.59
1:F:134:SER:HB3	1:F:137:LEU:HB2	1.83	0.59
1:O:167:LEU:N	1:O:167:LEU:CD1	2.65	0.59
1:K:182:LEU:CD2	1:K:182:LEU:H	2.14	0.59
1:T:167:LEU:H	1:T:167:LEU:CD1	2.14	0.59
1:D:70:ARG:HH11	1:D:70:ARG:HG3	1.68	0.59
1:F:70:ARG:HG3	1:F:70:ARG:HH11	1.67	0.59
1:G:186:VAL:HG21	1:H:170:ASP:C	2.22	0.59
1:N:70:ARG:NH1	1:N:70:ARG:HG3	2.17	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:182:LEU:N	1:Q:182:LEU:CD2	2.57	0.59
1:B:204:ARG:HG3	1:C:35:GLU:OE1	2.01	0.59
1:H:47:LEU:HD23	1:H:47:LEU:H	1.66	0.59
1:I:82:ASN:HD22	1:I:82:ASN:H	1.50	0.59
1:M:167:LEU:N	1:M:167:LEU:HD13	2.17	0.59
1:Q:69:HIS:HB3	1:R:167:LEU:HD21	1.84	0.59
1:V:196:LEU:O	1:V:198:PRO:HD3	2.03	0.59
1:A:100:ASN:HD21	1:A:102:LYS:HB2	1.67	0.59
1:A:167:LEU:N	1:A:167:LEU:CD1	2.65	0.59
1:D:123:ASP:OD1	1:D:153:ARG:NH1	2.36	0.59
1:R:193:ARG:HG2	1:S:50:GLU:OE2	2.02	0.59
1:R:196:LEU:CD1	1:R:198:PRO:HG3	2.32	0.59
1:A:52:ILE:HG13	1:A:175:LEU:HD11	1.85	0.59
1:B:167:LEU:CD1	1:B:167:LEU:N	2.65	0.59
1:I:52:ILE:HG13	1:I:175:LEU:HD11	1.84	0.59
1:M:134:SER:HB3	1:M:137:LEU:HB2	1.84	0.59
1:M:36:TYR:OH	1:M:40:GLN:HG3	2.02	0.59
1:M:192:LYS:HG3	1:N:45:GLN:NE2	2.17	0.59
1:U:183:PRO:HB3	1:V:170:ASP:OD1	2.02	0.59
1:A:45:GLN:HE21	1:K:192:LYS:HB2	1.68	0.59
1:C:52:ILE:HG13	1:C:175:LEU:HD11	1.84	0.59
1:E:100:ASN:HD21	1:E:102:LYS:HB2	1.65	0.59
1:E:182:LEU:O	1:E:184:LEU:N	2.36	0.59
1:L:52:ILE:HG13	1:L:175:LEU:HD11	1.84	0.59
1:J:82:ASN:HD22	1:J:82:ASN:H	1.50	0.59
1:B:192:LYS:HB2	1:C:45:GLN:NE2	2.18	0.58
1:K:36:TYR:OH	1:K:40:GLN:HG3	2.03	0.58
1:U:69:HIS:HB3	1:V:167:LEU:HD21	1.85	0.58
1:V:192:LYS:HE2	1:V:197:GLU:OE2	2.02	0.58
1:H:113:VAL:HG12	1:H:154:ALA:HB1	1.85	0.58
1:J:192:LYS:HB2	1:K:45:GLN:HE21	1.67	0.58
1:H:208:CYS:HB3	1:J:33:ALA:HB2	1.84	0.58
1:L:139:LEU:O	1:L:143:ARG:HG3	2.03	0.58
1:M:52:ILE:HG13	1:M:175:LEU:HD11	1.85	0.58
1:Q:47:LEU:HD23	1:Q:47:LEU:H	1.67	0.58
1:V:70:ARG:HH11	1:V:70:ARG:HG3	1.66	0.58
1:B:52:ILE:HG13	1:B:175:LEU:HD11	1.86	0.58
1:G:196:LEU:HD13	1:G:197:GLU:H	1.66	0.58
1:M:100:ASN:HD22	1:M:102:LYS:HB2	1.66	0.58
1:L:117:ASP:OD1	1:V:82:ASN:HB2	2.03	0.58
1:E:204:ARG:HH21	1:E:204:ARG:HG3	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:179:PRO:C	1:N:180:ARG:O	2.42	0.58
1:O:86:HIS:ND1	1:P:121:HIS:HD2	2.00	0.58
1:Q:70:ARG:HH11	1:Q:70:ARG:HG3	1.68	0.58
1:L:50:GLU:CD	1:V:193:ARG:HG2	2.24	0.58
1:M:70:ARG:NH1	1:M:70:ARG:HG3	2.18	0.58
1:Q:100:ASN:HD21	1:Q:102:LYS:HB2	1.66	0.58
1:V:134:SER:HB3	1:V:137:LEU:HB2	1.85	0.58
1:M:33:ALA:HB2	1:V:208:CYS:HB2	1.84	0.58
1:B:113:VAL:HG12	1:B:154:ALA:HB1	1.85	0.58
1:H:36:TYR:OH	1:H:40:GLN:HG3	2.04	0.58
1:U:49:PRO:HD2	1:U:50:GLU:OE1	2.03	0.58
1:D:192:LYS:HG3	1:E:45:GLN:HE22	1.69	0.58
1:B:57:ALA:HB3	1:B:61:GLN:HG3	1.86	0.58
1:J:100:ASN:HD21	1:J:102:LYS:HB2	1.66	0.58
1:T:124:VAL:O	1:T:153:ARG:HD3	2.04	0.58
1:D:192:LYS:HB2	1:E:45:GLN:HE21	1.69	0.58
1:G:184:LEU:HD23	1:G:185:GLU:H	1.68	0.58
1:J:69:HIS:HB3	1:K:167:LEU:HD21	1.84	0.58
1:R:49:PRO:HD2	1:R:50:GLU:OE1	2.04	0.58
1:F:123:ASP:OD1	1:F:153:ARG:NH1	2.37	0.57
1:I:204:ARG:HG3	1:J:35:GLU:OE1	2.04	0.57
1:N:205:TYR:HE2	1:N:209:ARG:NH2	2.02	0.57
1:T:204:ARG:HH21	1:T:204:ARG:HG3	1.68	0.57
1:F:182:LEU:O	1:F:182:LEU:HG	2.02	0.57
1:J:139:LEU:O	1:J:143:ARG:HG3	2.03	0.57
1:N:204:ARG:HG3	1:N:204:ARG:HH21	1.69	0.57
1:R:167:LEU:CD1	1:R:167:LEU:N	2.67	0.57
1:T:192:LYS:HB2	1:U:45:GLN:HE21	1.69	0.57
1:R:204:ARG:HD2	1:T:36:TYR:CZ	2.38	0.57
1:E:139:LEU:O	1:E:143:ARG:HG3	2.04	0.57
1:E:70:ARG:HG3	1:E:70:ARG:HH11	1.67	0.57
1:I:100:ASN:HD21	1:I:102:LYS:HB2	1.68	0.57
1:C:184:LEU:CD1	1:C:185:GLU:O	2.52	0.57
1:F:40:GLN:HE21	1:F:40:GLN:CA	2.15	0.57
1:K:167:LEU:N	1:K:167:LEU:CD1	2.68	0.57
1:R:139:LEU:O	1:R:143:ARG:HG3	2.04	0.57
1:U:70:ARG:HG3	1:U:70:ARG:HH11	1.69	0.57
1:D:179:PRO:O	1:D:180:ARG:C	2.42	0.57
1:E:36:TYR:OH	1:E:40:GLN:HG3	2.04	0.57
1:B:208:CYS:HB2	1:D:33:ALA:HB2	1.87	0.57
1:E:167:LEU:N	1:E:167:LEU:CD1	2.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:VAL:HG21	1:G:124:VAL:CG2	2.32	0.57
1:O:52:ILE:HG13	1:O:175:LEU:HD11	1.85	0.57
1:R:69:HIS:HB3	1:S:167:LEU:HD21	1.85	0.57
1:S:100:ASN:HD22	1:S:102:LYS:HB2	1.68	0.57
1:U:167:LEU:CD1	1:U:167:LEU:N	2.68	0.57
1:E:192:LYS:NZ	1:E:195:ASP:O	2.38	0.57
1:G:24:LEU:HB3	1:H:30:GLN:NE2	2.19	0.57
1:L:182:LEU:CD2	1:L:182:LEU:H	2.16	0.57
1:R:184:LEU:HD22	1:R:185:GLU:N	2.17	0.57
1:O:204:ARG:HD2	1:Q:36:TYR:CZ	2.40	0.57
1:T:167:LEU:N	1:T:167:LEU:HD13	2.15	0.57
1:F:167:LEU:CD1	1:F:167:LEU:N	2.68	0.57
1:Q:49:PRO:HD2	1:Q:50:GLU:OE1	2.04	0.57
1:Q:82:ASN:HB2	1:R:117:ASP:OD1	2.05	0.57
1:U:40:GLN:NE2	1:U:40:GLN:HA	2.15	0.57
1:A:40:GLN:HA	1:A:40:GLN:NE2	2.16	0.56
1:I:124:VAL:O	1:I:153:ARG:HD3	2.04	0.56
1:K:196:LEU:HD13	1:K:198:PRO:HG3	1.87	0.56
1:L:36:TYR:OH	1:L:40:GLN:HG3	2.05	0.56
1:E:192:LYS:HB2	1:F:45:GLN:HE21	1.70	0.56
1:E:49:PRO:HD2	1:E:50:GLU:OE1	2.04	0.56
1:I:70:ARG:HG3	1:I:70:ARG:HH11	1.70	0.56
1:M:192:LYS:HG3	1:N:45:GLN:HE22	1.68	0.56
1:P:40:GLN:HE21	1:P:40:GLN:CA	2.17	0.56
1:T:184:LEU:HD23	1:T:185:GLU:H	1.69	0.56
1:D:100:ASN:HD21	1:D:102:LYS:HB2	1.70	0.56
1:L:167:LEU:HD21	1:V:69:HIS:HB3	1.87	0.56
1:P:100:ASN:HD22	1:P:102:LYS:HB2	1.70	0.56
1:S:192:LYS:HB2	1:T:45:GLN:HE21	1.69	0.56
1:S:195:ASP:HB3	1:T:77:GLU:HG3	1.86	0.56
1:E:113:VAL:HG12	1:E:154:ALA:HB1	1.86	0.56
1:J:167:LEU:N	1:J:167:LEU:CD1	2.68	0.56
1:S:70:ARG:HG3	1:S:70:ARG:HH11	1.69	0.56
1:E:69:HIS:HB3	1:F:167:LEU:HD21	1.87	0.56
1:P:113:VAL:HG12	1:P:154:ALA:HB1	1.87	0.56
1:O:24:LEU:HB3	1:P:30:GLN:NE2	2.20	0.56
1:T:176:ASN:C	1:T:178:LEU:H	2.08	0.56
1:S:204:ARG:HD2	1:U:36:TYR:CZ	2.40	0.56
1:C:207:SER:C	1:C:209:ARG:H	2.07	0.56
1:L:113:VAL:HG12	1:L:154:ALA:HB1	1.86	0.56
1:K:193:ARG:NE	1:L:180:ARG:NE	2.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:192:LYS:HB2	1:P:45:GLN:HE21	1.70	0.56
1:P:134:SER:HB3	1:P:137:LEU:HB2	1.87	0.56
1:P:124:VAL:O	1:P:153:ARG:HD3	2.06	0.56
1:V:124:VAL:O	1:V:153:ARG:HD3	2.06	0.56
1:H:186:VAL:HG21	1:I:171:TYR:CA	2.36	0.56
1:L:167:LEU:HD13	1:L:167:LEU:N	2.16	0.56
1:N:100:ASN:HD22	1:N:102:LYS:HB2	1.71	0.56
1:V:180:ARG:CG	1:V:181:GLN:N	2.67	0.56
1:J:123:ASP:OD1	1:J:153:ARG:NH1	2.38	0.56
1:K:113:VAL:HG12	1:K:154:ALA:HB1	1.88	0.56
1:K:179:PRO:O	1:K:180:ARG:O	2.24	0.56
1:N:49:PRO:HD2	1:N:50:GLU:OE1	2.04	0.56
1:E:123:ASP:OD1	1:E:153:ARG:NH1	2.39	0.56
1:G:192:LYS:HE2	1:H:45:GLN:NE2	2.21	0.56
1:A:49:PRO:HG3	1:A:178:LEU:HD12	1.88	0.56
1:E:184:LEU:CD2	1:E:185:GLU:H	2.19	0.56
1:G:124:VAL:O	1:G:153:ARG:HD3	2.05	0.56
1:P:113:VAL:HG21	1:P:155:LEU:HD13	1.87	0.56
1:P:167:LEU:CD1	1:P:167:LEU:H	2.18	0.56
1:O:196:LEU:HD12	1:O:198:PRO:HG3	1.88	0.56
1:P:49:PRO:HD2	1:P:50:GLU:OE1	2.06	0.56
1:E:167:LEU:N	1:E:167:LEU:HD13	2.16	0.55
1:L:204:ARG:HD2	1:N:36:TYR:CZ	2.41	0.55
1:P:82:ASN:HB2	1:Q:117:ASP:OD1	2.06	0.55
1:E:204:ARG:HD2	1:G:36:TYR:CZ	2.41	0.55
1:G:167:LEU:H	1:G:167:LEU:CD1	2.16	0.55
1:K:193:ARG:CB	1:L:180:ARG:NH2	2.43	0.55
1:S:124:VAL:O	1:S:153:ARG:HD3	2.06	0.55
1:C:100:ASN:HD21	1:C:102:LYS:HB2	1.70	0.55
1:C:57:ALA:HB3	1:C:61:GLN:HG3	1.88	0.55
1:E:57:ALA:HB3	1:E:61:GLN:HG3	1.88	0.55
1:I:36:TYR:OH	1:I:40:GLN:HG3	2.05	0.55
1:H:167:LEU:N	1:H:167:LEU:CD1	2.70	0.55
1:A:30:GLN:NE2	1:K:24:LEU:HB3	2.22	0.55
1:L:123:ASP:OD1	1:L:153:ARG:NH1	2.40	0.55
1:M:139:LEU:O	1:M:143:ARG:HG3	2.07	0.55
1:O:204:ARG:HG3	1:P:35:GLU:OE1	2.06	0.55
1:R:70:ARG:HG3	1:R:70:ARG:NH1	2.20	0.55
1:C:204:ARG:HG3	1:D:35:GLU:OE1	2.07	0.55
1:H:100:ASN:HD21	1:H:102:LYS:HB2	1.70	0.55
1:N:167:LEU:CD1	1:N:167:LEU:H	2.19	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:139:LEU:O	1:V:143:ARG:HG3	2.06	0.55
1:A:77:GLU:OE2	1:B:44:ARG:NH1	2.40	0.55
1:R:124:VAL:O	1:R:153:ARG:HD3	2.07	0.55
1:V:100:ASN:HD22	1:V:102:LYS:HB2	1.69	0.55
1:F:100:ASN:HD21	1:F:102:LYS:HB2	1.70	0.55
1:I:167:LEU:H	1:I:167:LEU:CD1	2.18	0.55
1:M:124:VAL:O	1:M:153:ARG:HD3	2.06	0.55
1:S:49:PRO:HD2	1:S:50:GLU:OE1	2.07	0.55
1:V:82:ASN:HD22	1:V:82:ASN:N	2.02	0.55
1:E:134:SER:HB3	1:E:137:LEU:HB2	1.88	0.55
1:G:100:ASN:HD21	1:G:102:LYS:HB2	1.72	0.55
1:J:49:PRO:HD2	1:J:50:GLU:OE1	2.07	0.55
1:T:186:VAL:HG21	1:U:171:TYR:CA	2.37	0.55
1:I:69:HIS:HB3	1:J:167:LEU:HD21	1.88	0.55
1:Q:192:LYS:HB2	1:R:45:GLN:NE2	2.22	0.55
1:R:86:HIS:ND1	1:S:121:HIS:CD2	2.73	0.55
1:B:134:SER:HB3	1:B:137:LEU:HB2	1.89	0.54
1:B:205:TYR:CE1	1:D:33:ALA:HB1	2.42	0.54
1:K:100:ASN:HD21	1:K:102:LYS:HB2	1.70	0.54
1:L:167:LEU:N	1:L:167:LEU:CD1	2.69	0.54
1:Q:195:ASP:HB3	1:R:77:GLU:HG3	1.89	0.54
1:S:69:HIS:HB3	1:T:167:LEU:HD21	1.88	0.54
1:U:50:GLU:HA	1:U:181:GLN:HE21	1.71	0.54
1:A:49:PRO:HD2	1:A:50:GLU:OE1	2.07	0.54
1:B:36:TYR:OH	1:B:40:GLN:HG3	2.07	0.54
1:C:82:ASN:H	1:C:82:ASN:HD22	1.54	0.54
1:U:24:LEU:HB3	1:V:30:GLN:NE2	2.21	0.54
1:C:113:VAL:HG12	1:C:154:ALA:HB1	1.89	0.54
1:C:192:LYS:HB2	1:D:45:GLN:HE21	1.70	0.54
1:J:40:GLN:HA	1:J:40:GLN:NE2	2.16	0.54
1:M:182:LEU:CD2	1:M:182:LEU:H	2.01	0.54
1:R:36:TYR:OH	1:R:40:GLN:HG3	2.07	0.54
1:S:192:LYS:HG3	1:T:45:GLN:HE22	1.72	0.54
1:S:52:ILE:HG13	1:S:175:LEU:HD11	1.88	0.54
1:E:208:CYS:HB2	1:G:33:ALA:HB2	1.90	0.54
1:H:167:LEU:N	1:H:167:LEU:HD13	2.16	0.54
1:H:70:ARG:HH11	1:H:70:ARG:HG3	1.71	0.54
1:L:100:ASN:HD21	1:L:102:LYS:HB2	1.70	0.54
1:M:167:LEU:CD1	1:M:167:LEU:N	2.70	0.54
1:P:147:VAL:HG21	1:Q:124:VAL:CG2	2.36	0.54
1:T:113:VAL:HG12	1:T:154:ALA:HB1	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:52:ILE:HG13	1:T:175:LEU:HD11	1.89	0.54
1:T:82:ASN:H	1:T:82:ASN:HD22	1.55	0.54
1:V:205:TYR:CE2	1:V:209:ARG:NH2	2.76	0.54
1:G:196:LEU:HD13	1:G:197:GLU:N	2.23	0.54
1:K:40:GLN:HA	1:K:40:GLN:NE2	2.16	0.54
1:K:70:ARG:HG3	1:K:70:ARG:HH11	1.71	0.54
1:F:57:ALA:HB3	1:F:61:GLN:HG3	1.89	0.54
1:N:50:GLU:HB3	1:N:181:GLN:HE21	1.72	0.54
1:O:123:ASP:OD1	1:O:153:ARG:NH1	2.41	0.54
1:R:123:ASP:OD1	1:R:153:ARG:NH1	2.41	0.54
1:S:100:ASN:HD21	1:S:102:LYS:HB2	1.69	0.54
1:T:167:LEU:N	1:T:167:LEU:CD1	2.71	0.54
1:U:123:ASP:OD1	1:U:153:ARG:NH1	2.41	0.54
1:U:178:LEU:HD23	1:U:179:PRO:HD3	1.90	0.54
1:E:204:ARG:HG3	1:F:35:GLU:OE1	2.07	0.54
1:I:40:GLN:HA	1:I:40:GLN:NE2	2.16	0.54
1:L:124:VAL:O	1:L:153:ARG:HD3	2.08	0.54
1:M:113:VAL:HG12	1:M:154:ALA:HB1	1.90	0.54
1:O:82:ASN:HD22	1:O:82:ASN:N	2.06	0.54
1:V:167:LEU:CD1	1:V:167:LEU:N	2.71	0.54
1:V:70:ARG:HG3	1:V:70:ARG:NH1	2.23	0.54
1:A:184:LEU:HD22	1:A:185:GLU:N	2.24	0.54
1:E:124:VAL:O	1:E:153:ARG:HD3	2.08	0.54
1:F:49:PRO:HD2	1:F:50:GLU:OE1	2.08	0.54
1:H:85:ALA:HB1	1:I:120:TYR:O	2.09	0.54
1:O:113:VAL:HG21	1:O:155:LEU:HD13	1.90	0.54
1:R:24:LEU:HB3	1:S:30:GLN:NE2	2.23	0.54
1:U:188:LEU:HD12	1:V:178:LEU:HD11	1.90	0.54
1:T:195:ASP:HB3	1:U:77:GLU:HG3	1.89	0.54
1:C:124:VAL:O	1:C:153:ARG:HD3	2.08	0.53
1:J:192:LYS:HB2	1:K:45:GLN:NE2	2.22	0.53
1:K:49:PRO:HD2	1:K:50:GLU:OE1	2.08	0.53
1:N:134:SER:HB3	1:N:137:LEU:HB2	1.89	0.53
1:P:100:ASN:HD21	1:P:102:LYS:HB2	1.69	0.53
1:U:182:LEU:CD2	1:U:182:LEU:H	2.21	0.53
1:A:49:PRO:HD2	1:L:180:ARG:NH1	2.24	0.53
1:C:139:LEU:O	1:C:143:ARG:HG3	2.07	0.53
1:R:100:ASN:HD21	1:R:102:LYS:HB2	1.69	0.53
1:C:113:VAL:HG21	1:C:155:LEU:HD13	1.91	0.53
1:J:205:TYR:CE2	1:J:209:ARG:NH2	2.76	0.53
1:K:123:ASP:OD1	1:K:153:ARG:NH1	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:113:VAL:HG12	1:O:154:ALA:HB1	1.91	0.53
1:P:86:HIS:ND1	1:Q:121:HIS:CD2	2.74	0.53
1:R:147:VAL:HG21	1:S:124:VAL:CG2	2.35	0.53
1:C:184:LEU:O	1:D:173:ARG:NH2	2.40	0.53
1:K:167:LEU:HD13	1:K:167:LEU:N	2.17	0.53
1:N:113:VAL:HG12	1:N:154:ALA:HB1	1.90	0.53
1:A:70:ARG:HG3	1:A:70:ARG:NH1	2.24	0.53
1:J:124:VAL:O	1:J:153:ARG:HD3	2.07	0.53
1:Q:86:HIS:ND1	1:R:121:HIS:CD2	2.76	0.53
1:R:193:ARG:HG2	1:R:193:ARG:NH1	2.22	0.53
1:T:70:ARG:NH1	1:T:70:ARG:HG3	2.23	0.53
1:V:180:ARG:CG	1:V:181:GLN:H	2.17	0.53
1:D:82:ASN:HB2	1:E:117:ASP:OD1	2.09	0.53
1:H:49:PRO:HD2	1:H:50:GLU:OE1	2.09	0.53
1:H:57:ALA:HB3	1:H:61:GLN:HG3	1.91	0.53
1:I:113:VAL:HG12	1:I:154:ALA:HB1	1.90	0.53
1:P:179:PRO:O	1:P:180:ARG:C	2.45	0.53
1:P:180:ARG:HG3	1:P:180:ARG:O	2.08	0.53
1:Q:167:LEU:N	1:Q:167:LEU:CD1	2.71	0.53
1:R:195:ASP:HB3	1:S:77:GLU:HG3	1.90	0.53
1:F:112:ARG:HG3	1:F:122:GLU:HB2	1.90	0.53
1:F:69:HIS:HB3	1:G:167:LEU:HD21	1.90	0.53
1:A:45:GLN:NE2	1:K:192:LYS:HB2	2.23	0.53
1:F:139:LEU:O	1:F:143:ARG:HG3	2.09	0.53
1:O:100:ASN:HD22	1:O:102:LYS:HB2	1.71	0.53
1:O:180:ARG:O	1:O:180:ARG:HD2	2.09	0.53
1:P:70:ARG:NH1	1:P:70:ARG:HG3	2.24	0.53
1:Q:57:ALA:HB3	1:Q:61:GLN:HG3	1.91	0.53
1:S:167:LEU:CD1	1:S:167:LEU:H	2.19	0.53
1:S:180:ARG:HG2	1:S:180:ARG:NH1	2.23	0.53
1:T:100:ASN:HD21	1:T:102:LYS:HB2	1.74	0.53
1:B:124:VAL:O	1:B:153:ARG:HD3	2.09	0.53
1:H:124:VAL:O	1:H:153:ARG:HD3	2.09	0.53
1:N:40:GLN:HA	1:N:40:GLN:NE2	2.18	0.53
1:P:165:CYS:HA	2:P:2023:HOH:O	2.09	0.53
1:S:196:LEU:HD22	1:S:197:GLU:N	2.24	0.53
1:D:113:VAL:HG12	1:D:154:ALA:HB1	1.91	0.52
1:P:57:ALA:HB3	1:P:61:GLN:HG3	1.90	0.52
1:C:100:ASN:HD22	1:C:102:LYS:HB2	1.71	0.52
1:H:139:LEU:O	1:H:143:ARG:HG3	2.08	0.52
1:L:70:ARG:HH11	1:L:70:ARG:HG3	1.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:179:PRO:O	1:Q:180:ARG:O	2.27	0.52
1:U:178:LEU:CD2	1:U:179:PRO:HD3	2.40	0.52
1:C:112:ARG:HD2	2:C:2005:HOH:O	2.09	0.52
1:D:177:LYS:O	1:D:178:LEU:HD23	2.09	0.52
1:O:36:TYR:OH	1:O:40:GLN:HG3	2.10	0.52
1:P:36:TYR:OH	1:P:40:GLN:HG3	2.09	0.52
1:T:36:TYR:OH	1:T:40:GLN:HG3	2.10	0.52
1:A:184:LEU:HD23	1:A:185:GLU:N	2.18	0.52
1:G:186:VAL:HG21	1:H:171:TYR:N	2.25	0.52
1:H:180:ARG:CG	1:H:181:GLN:N	2.72	0.52
1:H:196:LEU:HD12	1:H:198:PRO:HD3	1.90	0.52
1:Q:40:GLN:NE2	1:Q:40:GLN:HA	2.16	0.52
1:A:182:LEU:N	1:A:182:LEU:CD2	2.72	0.52
1:C:69:HIS:HB3	1:D:167:LEU:HD21	1.91	0.52
1:G:167:LEU:N	1:G:167:LEU:CD1	2.73	0.52
1:G:167:LEU:N	1:G:167:LEU:HD13	2.20	0.52
1:H:82:ASN:HD22	1:H:82:ASN:N	2.06	0.52
1:L:195:ASP:HB3	1:M:77:GLU:HG3	1.90	0.52
1:N:182:LEU:HB2	1:N:183:PRO:HD2	1.90	0.52
1:Q:140:GLU:HG3	1:Q:144:LYS:HE3	1.90	0.52
1:A:77:GLU:OE1	1:B:44:ARG:HD3	2.09	0.52
1:J:181:GLN:O	1:J:181:GLN:CG	2.58	0.52
1:R:204:ARG:HG3	1:S:35:GLU:OE1	2.10	0.52
1:C:47:LEU:CD2	1:C:47:LEU:N	2.71	0.52
1:E:192:LYS:HE2	1:E:197:GLU:OE2	2.10	0.52
1:G:196:LEU:HD12	1:G:198:PRO:HD3	1.90	0.52
1:H:207:SER:HB2	1:I:32:THR:HG21	1.92	0.52
1:J:113:VAL:HG12	1:J:154:ALA:HB1	1.91	0.52
1:U:192:LYS:HE2	1:U:197:GLU:OE2	2.10	0.52
1:V:182:LEU:HD23	1:V:182:LEU:H	1.75	0.52
1:G:49:PRO:HD2	1:G:50:GLU:OE1	2.09	0.52
1:N:82:ASN:HD22	1:N:82:ASN:N	2.07	0.52
1:O:124:VAL:O	1:O:153:ARG:HD3	2.09	0.52
1:L:77:GLU:HG3	1:V:195:ASP:HB3	1.91	0.52
1:V:36:TYR:OH	1:V:40:GLN:HG3	2.10	0.52
1:I:49:PRO:HD2	1:I:50:GLU:OE1	2.10	0.52
1:L:120:TYR:O	1:V:85:ALA:HB1	2.09	0.52
1:R:57:ALA:HB3	1:R:61:GLN:HG3	1.91	0.52
1:A:82:ASN:N	1:A:82:ASN:HD22	2.01	0.52
1:A:192:LYS:HD2	1:B:45:GLN:NE2	2.25	0.52
1:J:196:LEU:HD13	1:J:198:PRO:HG3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:166:ILE:HD13	1:N:166:ILE:O	2.10	0.52
1:S:167:LEU:N	1:S:167:LEU:HD13	2.22	0.52
1:S:139:LEU:O	1:S:143:ARG:HG3	2.09	0.51
1:B:49:PRO:HD2	1:B:50:GLU:OE1	2.10	0.51
1:D:165:CYS:HA	2:D:2024:HOH:O	2.09	0.51
1:E:100:ASN:HD22	1:E:102:LYS:HB2	1.73	0.51
1:N:204:ARG:HG3	1:O:35:GLU:OE1	2.10	0.51
1:O:70:ARG:NH1	1:O:70:ARG:HG3	2.25	0.51
1:U:70:ARG:HG3	1:U:70:ARG:NH1	2.25	0.51
1:D:124:VAL:O	1:D:153:ARG:HD3	2.09	0.51
1:E:183:PRO:O	1:E:184:LEU:O	2.28	0.51
1:I:181:GLN:HG3	1:I:181:GLN:O	2.09	0.51
1:J:70:ARG:HG3	1:J:70:ARG:NH1	2.23	0.51
1:A:135:LYS:HE2	2:A:2014:HOH:O	2.10	0.51
1:B:70:ARG:NH1	1:B:70:ARG:HG3	2.23	0.51
1:O:82:ASN:HB2	1:P:117:ASP:OD1	2.11	0.51
1:Q:123:ASP:OD1	1:Q:153:ARG:NH1	2.43	0.51
1:S:40:GLN:NE2	1:S:40:GLN:HA	2.20	0.51
1:S:85:ALA:HB1	1:T:120:TYR:O	2.09	0.51
1:V:40:GLN:NE2	1:V:40:GLN:HA	2.16	0.51
1:F:86:HIS:ND1	1:G:121:HIS:CD2	2.75	0.51
1:G:196:LEU:HD12	1:G:198:PRO:CD	2.41	0.51
1:H:123:ASP:OD1	1:H:153:ARG:NH1	2.44	0.51
1:S:47:LEU:CD2	1:S:47:LEU:N	2.72	0.51
1:F:100:ASN:HD22	1:F:102:LYS:HB2	1.75	0.51
1:F:192:LYS:HE2	1:G:45:GLN:NE2	2.26	0.51
1:G:204:ARG:CG	1:G:204:ARG:HH21	2.18	0.51
1:H:207:SER:HB2	1:I:32:THR:CG2	2.40	0.51
1:N:52:ILE:HG13	1:N:175:LEU:HD11	1.92	0.51
1:P:82:ASN:HD22	1:P:82:ASN:N	2.09	0.51
1:T:57:ALA:HB3	1:T:61:GLN:HG3	1.92	0.51
1:V:57:ALA:HB3	1:V:61:GLN:HG3	1.92	0.51
1:B:33:ALA:HB2	1:K:208:CYS:HB2	1.92	0.51
1:H:24:LEU:HB3	1:I:30:GLN:NE2	2.25	0.51
1:A:179:PRO:HD3	1:L:183:PRO:HG3	1.93	0.51
1:O:179:PRO:O	1:O:180:ARG:C	2.49	0.51
1:P:196:LEU:CD1	1:P:198:PRO:HG3	2.40	0.51
1:Q:50:GLU:HA	1:Q:181:GLN:HE22	1.75	0.51
1:V:100:ASN:ND2	1:V:102:LYS:CB	2.71	0.51
1:A:100:ASN:HD22	1:A:102:LYS:CB	2.24	0.51
1:A:195:ASP:HB3	1:B:77:GLU:HG3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:LEU:HD23	1:E:185:GLU:H	1.75	0.51
1:F:124:VAL:O	1:F:153:ARG:HD3	2.11	0.51
1:F:196:LEU:HD13	1:F:198:PRO:HD3	1.93	0.51
1:J:100:ASN:HD22	1:J:102:LYS:HB2	1.72	0.51
1:M:57:ALA:HB3	1:M:61:GLN:HG3	1.93	0.51
1:T:113:VAL:HG21	1:T:155:LEU:HD13	1.93	0.51
1:T:192:LYS:HG3	1:U:45:GLN:HE22	1.76	0.51
1:A:117:ASP:OD1	1:K:82:ASN:HB2	2.10	0.51
1:A:49:PRO:CD	1:L:180:ARG:NH1	2.74	0.51
1:B:182:LEU:HD23	1:B:182:LEU:N	2.21	0.51
1:K:124:VAL:O	1:K:153:ARG:HD3	2.11	0.51
1:M:40:GLN:NE2	1:M:40:GLN:HA	2.18	0.51
1:N:196:LEU:HD13	1:N:197:GLU:N	2.25	0.51
1:O:173:ARG:HG2	1:O:173:ARG:HH11	1.75	0.51
1:Q:139:LEU:O	1:Q:143:ARG:HG3	2.11	0.51
1:S:123:ASP:OD1	1:S:153:ARG:NH1	2.44	0.51
1:B:189:THR:HG22	1:B:190:LYS:CG	2.28	0.51
1:F:47:LEU:CD2	1:F:47:LEU:N	2.74	0.51
1:A:167:LEU:HD21	1:K:69:HIS:HB3	1.92	0.51
1:O:205:TYR:CE2	1:O:209:ARG:NH2	2.79	0.51
1:V:192:LYS:NZ	1:V:194:GLN:O	2.36	0.51
1:M:100:ASN:HD21	1:M:102:LYS:HB2	1.68	0.50
1:N:192:LYS:CE	1:N:197:GLU:OE2	2.52	0.50
1:P:167:LEU:CD1	1:P:167:LEU:N	2.74	0.50
1:S:57:ALA:HB3	1:S:61:GLN:HG3	1.93	0.50
1:V:100:ASN:HD22	1:V:102:LYS:CB	2.24	0.50
1:V:192:LYS:CE	1:V:197:GLU:OE2	2.58	0.50
1:F:82:ASN:N	1:F:82:ASN:HD22	2.07	0.50
1:J:204:ARG:HH21	1:J:204:ARG:HG3	1.76	0.50
1:K:165:CYS:HA	2:K:2023:HOH:O	2.10	0.50
1:G:193:ARG:HG2	1:G:193:ARG:HH11	1.76	0.50
1:G:183:PRO:HB2	1:H:170:ASP:OD1	2.11	0.50
1:H:182:LEU:HD23	1:H:182:LEU:H	1.77	0.50
1:K:193:ARG:NH1	1:L:182:LEU:HD22	2.25	0.50
1:L:45:GLN:NE2	1:V:192:LYS:HB2	2.26	0.50
1:R:47:LEU:N	1:R:47:LEU:CD2	2.73	0.50
1:S:167:LEU:CD1	1:S:167:LEU:N	2.75	0.50
1:S:203:ALA:HB1	1:T:35:GLU:N	2.26	0.50
1:C:184:LEU:CD1	1:C:185:GLU:N	2.74	0.50
1:D:113:VAL:HG21	1:D:155:LEU:HD13	1.92	0.50
1:N:24:LEU:HB3	1:O:30:GLN:NE2	2.27	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:47:LEU:HD23	1:S:165:CYS:SG	2.51	0.50
1:T:86:HIS:ND1	1:U:121:HIS:CD2	2.77	0.50
1:U:50:GLU:HA	1:U:181:GLN:NE2	2.26	0.50
1:E:82:ASN:HB2	1:F:117:ASP:OD1	2.11	0.50
1:E:192:LYS:HB2	1:F:45:GLN:NE2	2.26	0.50
1:I:204:ARG:HG3	1:I:204:ARG:HH21	1.75	0.50
1:J:188:LEU:HB3	1:J:191:ALA:HB2	1.92	0.50
1:V:196:LEU:C	1:V:198:PRO:HD3	2.32	0.50
1:A:124:VAL:O	1:A:153:ARG:HD3	2.12	0.50
1:C:196:LEU:HD12	1:C:198:PRO:HG3	1.92	0.50
1:L:30:GLN:NE2	1:V:24:LEU:HB3	2.27	0.50
1:O:57:ALA:HB3	1:O:61:GLN:HG3	1.94	0.50
1:U:112:ARG:HG3	1:U:122:GLU:HB2	1.94	0.50
1:B:40:GLN:NE2	1:B:40:GLN:HA	2.19	0.50
1:F:192:LYS:O	1:G:48:GLY:N	2.35	0.50
1:L:57:ALA:HB3	1:L:61:GLN:HG3	1.94	0.50
1:T:40:GLN:NE2	1:T:40:GLN:HA	2.20	0.50
1:B:193:ARG:NH1	1:C:50:GLU:OE2	2.43	0.50
1:G:112:ARG:HG3	1:G:122:GLU:HB2	1.93	0.50
1:B:82:ASN:N	1:B:82:ASN:HD22	2.07	0.50
1:D:40:GLN:NE2	1:D:40:GLN:HA	2.20	0.50
1:D:57:ALA:HB3	1:D:61:GLN:HG3	1.93	0.50
1:J:36:TYR:OH	1:J:40:GLN:HG3	2.12	0.50
1:A:121:HIS:CD2	1:K:86:HIS:ND1	2.77	0.50
1:N:192:LYS:HB2	1:O:45:GLN:HE21	1.77	0.50
1:Q:167:LEU:N	1:Q:167:LEU:HD13	2.19	0.50
1:R:82:ASN:HB2	1:S:117:ASP:OD1	2.12	0.50
1:G:139:LEU:O	1:G:143:ARG:HG3	2.12	0.49
1:M:100:ASN:HD22	1:M:102:LYS:CB	2.25	0.49
1:S:36:TYR:OH	1:S:40:GLN:HG3	2.11	0.49
1:B:189:THR:CG2	1:B:190:LYS:HG3	2.30	0.49
1:M:47:LEU:HD23	1:M:165:CYS:SG	2.52	0.49
1:P:117:ASP:HB3	1:P:119:SER:H	1.77	0.49
1:A:47:LEU:N	1:A:47:LEU:CD2	2.75	0.49
1:A:69:HIS:HB3	1:B:167:LEU:HD21	1.94	0.49
1:D:147:VAL:HG21	1:E:124:VAL:CG2	2.40	0.49
1:G:182:LEU:N	1:G:182:LEU:HD23	2.16	0.49
1:G:116:LYS:HE2	2:G:2004:HOH:O	2.11	0.49
1:L:177:LYS:NZ	1:V:185:GLU:OE1	2.45	0.49
1:L:40:GLN:HA	1:L:40:GLN:NE2	2.18	0.49
1:L:86:HIS:ND1	1:M:121:HIS:CD2	2.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:124:VAL:O	1:Q:153:ARG:HD3	2.11	0.49
1:Q:166:ILE:HD13	1:Q:166:ILE:O	2.13	0.49
1:S:184:LEU:CD2	1:S:185:GLU:N	2.75	0.49
1:T:47:LEU:HD23	1:T:165:CYS:SG	2.53	0.49
1:B:192:LYS:HG3	1:C:45:GLN:HE22	1.76	0.49
1:D:192:LYS:HG3	1:E:45:GLN:NE2	2.28	0.49
1:F:24:LEU:HB3	1:G:30:GLN:NE2	2.28	0.49
1:F:70:ARG:HG3	1:F:70:ARG:NH1	2.27	0.49
1:N:139:LEU:O	1:N:143:ARG:HG3	2.11	0.49
1:R:176:ASN:C	1:R:178:LEU:H	2.16	0.49
1:D:182:LEU:N	1:D:182:LEU:HD23	2.19	0.49
1:G:82:ASN:HD22	1:G:82:ASN:N	2.06	0.49
1:L:100:ASN:HD22	1:L:102:LYS:HB2	1.72	0.49
1:Q:184:LEU:CD2	1:Q:185:GLU:N	2.68	0.49
1:D:82:ASN:N	1:D:82:ASN:HD22	2.00	0.49
1:I:203:ALA:HB1	1:J:35:GLU:HA	1.95	0.49
1:M:113:VAL:HG21	1:M:155:LEU:HD13	1.93	0.49
1:N:167:LEU:CD1	1:N:167:LEU:N	2.76	0.49
1:S:82:ASN:HB2	1:T:117:ASP:OD1	2.13	0.49
1:U:192:LYS:CE	1:U:197:GLU:OE2	2.60	0.49
1:B:100:ASN:HD21	1:B:102:LYS:HB2	1.77	0.49
1:E:82:ASN:HD22	1:E:82:ASN:N	2.04	0.49
1:G:57:ALA:HB3	1:G:61:GLN:HG3	1.94	0.49
1:J:184:LEU:HD13	1:J:185:GLU:N	2.26	0.49
1:K:47:LEU:N	1:K:47:LEU:CD2	2.76	0.49
1:L:77:GLU:OE2	1:M:44:ARG:NH1	2.46	0.49
1:S:147:VAL:HG21	1:T:124:VAL:CG2	2.40	0.49
1:T:139:LEU:O	1:T:143:ARG:HG3	2.13	0.49
1:A:182:LEU:HB2	1:L:56:MET:HE3	1.94	0.49
1:B:100:ASN:HD22	1:B:102:LYS:HB2	1.76	0.49
1:D:47:LEU:N	1:D:47:LEU:CD2	2.74	0.49
1:E:86:HIS:ND1	1:F:121:HIS:CD2	2.73	0.49
1:H:112:ARG:HG3	1:H:122:GLU:HB2	1.94	0.49
1:N:113:VAL:HG21	1:N:155:LEU:HD13	1.95	0.49
1:R:113:VAL:HG21	1:R:155:LEU:HD13	1.94	0.49
1:B:33:ALA:HB2	1:K:208:CYS:CB	2.43	0.49
1:D:24:LEU:HB3	1:E:30:GLN:NE2	2.27	0.49
1:J:24:LEU:HB3	1:K:30:GLN:NE2	2.28	0.49
1:Q:100:ASN:HD22	1:Q:102:LYS:CB	2.26	0.49
1:U:165:CYS:HA	2:U:2023:HOH:O	2.11	0.49
1:C:70:ARG:NH1	1:C:70:ARG:HG3	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:ASN:HD22	1:D:102:LYS:HB2	1.74	0.48
1:K:57:ALA:HB3	1:K:61:GLN:HG3	1.94	0.48
1:O:100:ASN:HD22	1:O:102:LYS:CB	2.26	0.48
1:O:186:VAL:HG21	1:P:171:TYR:HA	1.95	0.48
1:E:100:ASN:HD22	1:E:102:LYS:CB	2.26	0.48
1:E:185:GLU:OE1	1:F:177:LYS:NZ	2.47	0.48
1:G:204:ARG:NH2	1:H:35:GLU:OE1	2.47	0.48
1:I:113:VAL:HG21	1:I:155:LEU:HD13	1.94	0.48
1:Q:82:ASN:HD22	1:Q:82:ASN:N	2.02	0.48
1:S:70:ARG:NH1	1:S:70:ARG:HG3	2.28	0.48
1:T:175:LEU:O	1:T:178:LEU:HD12	2.13	0.48
1:V:49:PRO:HD2	1:V:50:GLU:OE1	2.13	0.48
1:U:195:ASP:HB3	1:V:77:GLU:HG3	1.95	0.48
1:D:140:GLU:HB2	1:E:126:TYR:CD2	2.47	0.48
1:E:70:ARG:NH1	1:E:70:ARG:HG3	2.28	0.48
1:I:167:LEU:N	1:I:167:LEU:CD1	2.74	0.48
1:I:86:HIS:ND1	1:J:121:HIS:CD2	2.79	0.48
1:O:139:LEU:O	1:O:143:ARG:HG3	2.12	0.48
1:P:167:LEU:HD13	1:P:167:LEU:N	2.23	0.48
1:P:47:LEU:CD2	1:P:47:LEU:N	2.76	0.48
1:E:207:SER:O	1:E:209:ARG:N	2.46	0.48
1:F:116:LYS:HE2	2:F:2005:HOH:O	2.13	0.48
1:H:70:ARG:NH1	1:H:70:ARG:HG3	2.29	0.48
1:R:193:ARG:HG2	1:S:50:GLU:CD	2.34	0.48
1:R:40:GLN:HA	1:R:40:GLN:NE2	2.20	0.48
1:T:182:LEU:H	1:T:182:LEU:CD2	2.24	0.48
1:B:116:LYS:HE2	2:B:2001:HOH:O	2.12	0.48
1:C:47:LEU:HD23	1:C:165:CYS:SG	2.54	0.48
1:H:196:LEU:HD13	1:H:197:GLU:N	2.29	0.48
1:J:100:ASN:HD22	1:J:102:LYS:CB	2.27	0.48
1:V:116:LYS:HE2	2:V:2003:HOH:O	2.14	0.48
1:D:191:ALA:O	1:D:193:ARG:HG3	2.14	0.48
1:D:195:ASP:HB3	1:E:77:GLU:HG3	1.95	0.48
1:G:123:ASP:OD1	1:G:153:ARG:NH1	2.47	0.48
1:J:182:LEU:H	1:J:182:LEU:CD2	2.26	0.48
1:V:47:LEU:N	1:V:47:LEU:CD2	2.75	0.48
1:F:196:LEU:CD1	1:F:198:PRO:HG3	2.42	0.48
1:F:205:TYR:CE2	1:F:209:ARG:NH2	2.81	0.48
1:G:204:ARG:HG3	1:H:35:GLU:OE1	2.13	0.48
1:G:204:ARG:HG2	1:G:204:ARG:O	2.12	0.48
1:Q:113:VAL:HG21	1:Q:155:LEU:HD13	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:82:ASN:H	1:Q:82:ASN:ND2	2.10	0.48
1:V:182:LEU:N	1:V:182:LEU:HD23	2.29	0.48
1:B:195:ASP:HB3	1:C:77:GLU:HG3	1.95	0.48
1:G:140:GLU:HG3	1:G:144:LYS:HE3	1.95	0.48
1:L:182:LEU:HD23	1:L:182:LEU:N	2.25	0.48
1:M:166:ILE:HD13	1:M:166:ILE:O	2.14	0.48
1:M:82:ASN:HB2	1:N:117:ASP:OD1	2.14	0.48
1:N:57:ALA:HB3	1:N:61:GLN:HG3	1.96	0.48
1:O:40:GLN:HA	1:O:40:GLN:NE2	2.21	0.48
1:T:166:ILE:HD13	1:T:166:ILE:O	2.14	0.48
1:T:192:LYS:NZ	1:T:197:GLU:OE2	2.45	0.48
1:U:47:LEU:CD2	1:U:47:LEU:N	2.77	0.48
1:V:167:LEU:N	1:V:167:LEU:HD13	2.19	0.48
1:G:70:ARG:NH1	1:G:70:ARG:HG3	2.26	0.48
1:L:40:GLN:NE2	1:L:40:GLN:CA	2.76	0.48
1:L:82:ASN:N	1:L:82:ASN:HD22	2.06	0.48
1:Q:207:SER:C	1:Q:209:ARG:N	2.66	0.48
1:Q:70:ARG:HG3	1:Q:70:ARG:NH1	2.29	0.48
1:H:100:ASN:HD22	1:H:102:LYS:HB2	1.76	0.48
1:I:139:LEU:O	1:I:143:ARG:HG3	2.14	0.48
1:A:35:GLU:OE1	1:K:204:ARG:HG3	2.13	0.48
1:N:123:ASP:OD1	1:N:153:ARG:NH1	2.47	0.47
1:I:57:ALA:HB3	1:I:61:GLN:HG3	1.96	0.47
1:N:100:ASN:HD21	1:N:102:LYS:HB2	1.75	0.47
1:T:47:LEU:N	1:T:47:LEU:CD2	2.75	0.47
1:J:116:LYS:HE2	2:J:2001:HOH:O	2.13	0.47
1:V:113:VAL:HG12	1:V:154:ALA:HB1	1.96	0.47
1:A:192:LYS:HB2	1:B:45:GLN:HE21	1.80	0.47
1:B:82:ASN:HB2	1:C:117:ASP:OD1	2.14	0.47
1:M:112:ARG:HG3	1:M:122:GLU:HB2	1.96	0.47
1:N:184:LEU:C	1:O:173:ARG:HH22	2.15	0.47
1:C:123:ASP:OD1	1:C:153:ARG:NH1	2.48	0.47
1:L:49:PRO:HD2	1:L:50:GLU:OE1	2.14	0.47
1:O:47:LEU:N	1:O:47:LEU:CD2	2.76	0.47
1:R:196:LEU:HD13	1:R:197:GLU:N	2.29	0.47
1:U:166:ILE:O	1:U:166:ILE:HD13	2.14	0.47
1:E:140:GLU:HG3	1:E:144:LYS:HE3	1.95	0.47
1:E:40:GLN:NE2	1:E:40:GLN:HA	2.22	0.47
1:F:192:LYS:HE2	1:G:45:GLN:HE22	1.79	0.47
1:U:182:LEU:O	1:U:183:PRO:C	2.52	0.47
1:F:100:ASN:HD22	1:F:102:LYS:CB	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:70:ARG:NH1	1:I:70:ARG:HG3	2.29	0.47
1:N:47:LEU:HD23	1:N:165:CYS:SG	2.55	0.47
1:U:82:ASN:HB2	1:V:117:ASP:OD1	2.15	0.47
1:V:182:LEU:CD2	1:V:182:LEU:H	2.28	0.47
1:H:208:CYS:C	1:H:209:ARG:HG3	2.34	0.47
1:M:182:LEU:O	1:M:183:PRO:C	2.52	0.47
1:T:175:LEU:HA	1:T:178:LEU:HD12	1.97	0.47
1:A:128:VAL:HG12	1:A:129:SER:N	2.29	0.47
1:B:175:LEU:O	1:B:178:LEU:HB2	2.15	0.47
1:J:85:ALA:HB1	1:K:120:TYR:O	2.15	0.47
1:L:50:GLU:OE1	1:V:193:ARG:HG2	2.15	0.47
1:M:82:ASN:N	1:M:82:ASN:HD22	2.07	0.47
1:N:182:LEU:N	1:N:182:LEU:HD22	2.06	0.47
1:Q:100:ASN:HD22	1:Q:102:LYS:HB2	1.74	0.47
1:D:40:GLN:HE21	1:D:40:GLN:CA	2.19	0.47
1:D:70:ARG:HG3	1:D:70:ARG:NH1	2.29	0.47
1:G:100:ASN:HD22	1:G:102:LYS:HB2	1.78	0.47
1:H:147:VAL:HG21	1:I:124:VAL:CG2	2.41	0.47
1:I:100:ASN:HB2	1:I:101:GLY:H	1.49	0.47
1:K:113:VAL:HG21	1:K:155:LEU:HD13	1.96	0.47
1:A:57:ALA:HB3	1:A:61:GLN:HG3	1.96	0.46
1:G:113:VAL:HG21	1:G:155:LEU:HD13	1.97	0.46
1:J:82:ASN:HB2	1:K:117:ASP:OD1	2.15	0.46
1:U:124:VAL:O	1:U:153:ARG:HD3	2.14	0.46
1:U:40:GLN:CA	1:U:40:GLN:NE2	2.75	0.46
1:B:86:HIS:ND1	1:C:121:HIS:CD2	2.83	0.46
1:D:100:ASN:HB2	1:D:101:GLY:H	1.57	0.46
1:E:47:LEU:HD23	1:E:165:CYS:SG	2.54	0.46
1:I:123:ASP:OD1	1:I:153:ARG:NH1	2.48	0.46
1:J:100:ASN:HB2	1:J:101:GLY:H	1.51	0.46
1:K:173:ARG:HG2	1:K:173:ARG:HH11	1.80	0.46
1:L:100:ASN:HD22	1:L:102:LYS:CB	2.27	0.46
1:C:86:HIS:ND1	1:D:121:HIS:CD2	2.80	0.46
1:D:36:TYR:CZ	1:D:40:GLN:HG3	2.51	0.46
1:J:57:ALA:HB3	1:J:61:GLN:HG3	1.97	0.46
1:O:69:HIS:HB3	1:P:167:LEU:CD2	2.44	0.46
1:C:192:LYS:HE2	1:C:197:GLU:OE2	2.15	0.46
1:N:50:GLU:HA	1:N:181:GLN:HG2	1.96	0.46
1:O:134:SER:OG	1:O:137:LEU:HD23	2.15	0.46
1:S:100:ASN:HB2	1:S:101:GLY:H	1.59	0.46
1:U:57:ALA:HB3	1:U:61:GLN:HG3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:LEU:O	1:B:143:ARG:HG3	2.15	0.46
1:H:100:ASN:HD22	1:H:102:LYS:CB	2.29	0.46
1:K:193:ARG:CZ	1:L:180:ARG:CZ	2.93	0.46
1:L:24:LEU:HB3	1:M:30:GLN:NE2	2.31	0.46
1:O:24:LEU:HA	1:O:24:LEU:HD22	1.80	0.46
1:P:134:SER:OG	1:P:137:LEU:HD23	2.16	0.46
1:P:139:LEU:O	1:P:143:ARG:HG3	2.16	0.46
1:A:139:LEU:O	1:A:143:ARG:HG3	2.15	0.46
1:E:207:SER:C	1:E:209:ARG:N	2.68	0.46
1:D:194:GLN:C	1:E:51:TYR:OH	2.53	0.46
1:E:24:LEU:HB3	1:F:30:GLN:NE2	2.30	0.46
1:L:33:ALA:HB2	1:U:208:CYS:HB2	1.96	0.46
1:N:82:ASN:HB2	1:O:117:ASP:OD1	2.16	0.46
1:D:180:ARG:O	1:D:180:ARG:HG3	2.15	0.46
1:G:196:LEU:HD12	1:G:198:PRO:HG3	1.97	0.46
1:H:134:SER:OG	1:H:137:LEU:HD23	2.15	0.46
1:L:173:ARG:HG2	1:L:173:ARG:HH11	1.81	0.46
1:N:173:ARG:HH11	1:N:173:ARG:HG2	1.81	0.46
1:V:40:GLN:NE2	1:V:40:GLN:CA	2.76	0.46
1:I:173:ARG:HH11	1:I:173:ARG:HG2	1.81	0.46
1:P:192:LYS:NZ	1:P:195:ASP:O	2.49	0.46
1:A:49:PRO:CG	1:A:178:LEU:HD12	2.46	0.46
1:A:86:HIS:ND1	1:B:121:HIS:CD2	2.80	0.46
1:F:140:GLU:HG3	1:F:144:LYS:HE3	1.98	0.46
1:K:100:ASN:HD22	1:K:102:LYS:CB	2.27	0.46
1:K:193:ARG:CZ	1:L:180:ARG:NE	2.79	0.46
1:M:47:LEU:N	1:M:47:LEU:CD2	2.79	0.46
1:S:77:GLU:OE2	1:T:44:ARG:NH1	2.49	0.46
1:B:47:LEU:CD2	1:B:47:LEU:N	2.78	0.46
1:D:173:ARG:HG2	1:D:173:ARG:HH11	1.81	0.46
1:E:184:LEU:HD22	1:E:185:GLU:N	2.31	0.46
1:O:112:ARG:HG3	1:O:122:GLU:HB2	1.98	0.46
1:P:100:ASN:HD22	1:P:102:LYS:CB	2.28	0.46
1:A:77:GLU:CD	1:B:44:ARG:HH11	2.20	0.45
1:D:194:GLN:HB2	1:D:194:GLN:HE21	1.48	0.45
1:N:147:VAL:HG21	1:O:124:VAL:CG2	2.40	0.45
1:N:196:LEU:HD12	1:N:198:PRO:HG3	1.98	0.45
1:O:176:ASN:C	1:O:178:LEU:H	2.20	0.45
1:O:204:ARG:HH21	1:O:204:ARG:HG3	1.82	0.45
1:P:182:LEU:CD2	1:P:182:LEU:N	2.67	0.45
1:S:100:ASN:HD22	1:S:102:LYS:CB	2.27	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:113:VAL:HG21	1:S:155:LEU:HD13	1.99	0.45
1:U:85:ALA:HB1	1:V:120:TYR:O	2.15	0.45
1:H:86:HIS:ND1	1:I:121:HIS:CD2	2.81	0.45
1:I:175:LEU:O	1:I:178:LEU:HB2	2.15	0.45
1:K:70:ARG:HG3	1:K:70:ARG:NH1	2.31	0.45
1:T:182:LEU:N	1:T:182:LEU:HD23	2.30	0.45
1:H:24:LEU:HA	1:H:24:LEU:HD22	1.82	0.45
1:K:112:ARG:HG3	1:K:122:GLU:HB2	1.97	0.45
1:K:193:ARG:CA	1:L:180:ARG:HH21	2.28	0.45
1:O:100:ASN:HB2	1:O:101:GLY:H	1.54	0.45
1:B:113:VAL:HG21	1:B:155:LEU:HD13	1.98	0.45
1:F:82:ASN:HB2	1:G:117:ASP:OD1	2.17	0.45
1:K:192:LYS:NZ	1:K:194:GLN:O	2.47	0.45
1:O:85:ALA:HB1	1:P:120:TYR:O	2.16	0.45
1:Q:204:ARG:HG3	1:R:35:GLU:CD	2.37	0.45
1:B:196:LEU:HD13	1:B:198:PRO:HD3	1.99	0.45
1:D:82:ASN:H	1:D:82:ASN:ND2	2.10	0.45
1:M:113:VAL:HG21	1:M:155:LEU:CD1	2.47	0.45
1:R:82:ASN:N	1:R:82:ASN:HD22	2.09	0.45
1:U:192:LYS:NZ	1:U:197:GLU:OE2	2.49	0.45
1:V:82:ASN:H	1:V:82:ASN:ND2	2.10	0.45
1:B:40:GLN:NE2	1:B:40:GLN:CA	2.78	0.45
1:H:180:ARG:HG3	1:H:181:GLN:N	2.32	0.45
1:I:100:ASN:HD22	1:I:102:LYS:CB	2.29	0.45
1:E:184:LEU:CD2	1:E:185:GLU:N	2.78	0.45
1:E:47:LEU:CD2	1:E:47:LEU:N	2.78	0.45
1:G:143:ARG:NH1	1:H:94:ASP:OD2	2.49	0.45
1:I:40:GLN:CA	1:I:40:GLN:NE2	2.75	0.45
1:M:140:GLU:HG3	1:M:144:LYS:HE3	1.98	0.45
1:M:86:HIS:ND1	1:N:121:HIS:CD2	2.82	0.45
1:O:166:ILE:HD13	1:O:166:ILE:O	2.17	0.45
1:P:47:LEU:HD23	1:P:165:CYS:SG	2.57	0.45
1:B:196:LEU:HD13	1:B:198:PRO:CD	2.46	0.45
1:G:47:LEU:HD23	1:G:165:CYS:SG	2.57	0.45
1:K:47:LEU:HD23	1:K:165:CYS:SG	2.57	0.45
1:L:24:LEU:HD22	1:L:24:LEU:HA	1.82	0.45
1:N:100:ASN:HD22	1:N:102:LYS:CB	2.30	0.45
1:T:192:LYS:HB2	1:U:45:GLN:NE2	2.31	0.45
1:G:204:ARG:CG	1:G:204:ARG:NH2	2.79	0.45
1:H:192:LYS:HE2	1:H:197:GLU:OE2	2.16	0.45
1:I:47:LEU:HD23	1:I:165:CYS:SG	2.57	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:85:ALA:HB1	1:J:120:TYR:O	2.16	0.45
1:O:47:LEU:HD23	1:O:165:CYS:SG	2.57	0.45
1:T:192:LYS:HG3	1:U:45:GLN:NE2	2.32	0.45
1:A:40:GLN:NE2	1:A:40:GLN:CA	2.76	0.45
1:G:40:GLN:HA	1:G:40:GLN:NE2	2.22	0.45
1:H:173:ARG:HG2	1:H:173:ARG:HH11	1.80	0.45
1:N:195:ASP:HB3	1:O:77:GLU:HG3	1.97	0.45
1:S:40:GLN:NE2	1:S:40:GLN:CA	2.80	0.45
1:U:36:TYR:OH	1:U:40:GLN:HG3	2.17	0.45
1:M:37:GLN:OE1	1:V:205:TYR:CE1	2.70	0.45
1:C:100:ASN:HD22	1:C:102:LYS:CB	2.28	0.44
1:E:193:ARG:HG2	1:F:50:GLU:CD	2.38	0.44
1:H:128:VAL:HG12	1:H:129:SER:N	2.32	0.44
1:I:208:CYS:HB2	1:K:33:ALA:HB2	1.99	0.44
1:Q:181:GLN:HG3	1:Q:181:GLN:O	2.18	0.44
1:S:192:LYS:HG3	1:T:45:GLN:NE2	2.32	0.44
1:A:173:ARG:HG2	1:A:173:ARG:HH11	1.82	0.44
1:B:181:GLN:O	1:B:181:GLN:HG3	2.17	0.44
1:C:173:ARG:HH11	1:C:173:ARG:HG2	1.81	0.44
1:D:192:LYS:HB2	1:E:45:GLN:NE2	2.32	0.44
1:D:208:CYS:C	1:D:209:ARG:HG3	2.38	0.44
1:I:192:LYS:O	1:J:48:GLY:N	2.36	0.44
1:N:128:VAL:HG12	1:N:129:SER:N	2.33	0.44
1:P:100:ASN:HB2	1:P:101:GLY:H	1.56	0.44
1:R:47:LEU:HD23	1:R:165:CYS:SG	2.57	0.44
1:B:47:LEU:HD23	1:B:165:CYS:SG	2.57	0.44
1:G:173:ARG:HH11	1:G:173:ARG:HG2	1.81	0.44
1:G:179:PRO:C	1:G:180:ARG:O	2.56	0.44
1:G:47:LEU:CD2	1:G:47:LEU:N	2.79	0.44
1:Q:186:VAL:HG21	1:R:171:TYR:HA	2.00	0.44
1:D:100:ASN:HD22	1:D:102:LYS:CB	2.30	0.44
1:J:112:ARG:HG3	1:J:122:GLU:HB2	2.00	0.44
1:K:100:ASN:HB2	1:K:101:GLY:H	1.54	0.44
1:S:207:SER:C	1:S:209:ARG:H	2.21	0.44
1:I:100:ASN:HD22	1:I:102:LYS:HB2	1.77	0.44
1:I:196:LEU:HD13	1:I:197:GLU:H	1.82	0.44
1:M:204:ARG:HG3	1:N:35:GLU:OE1	2.16	0.44
1:A:113:VAL:HG21	1:A:155:LEU:HD13	2.00	0.44
1:B:113:VAL:HG21	1:B:155:LEU:CD1	2.48	0.44
1:C:208:CYS:HB2	1:E:33:ALA:HB2	1.98	0.44
1:G:166:ILE:HD13	1:G:166:ILE:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:86:HIS:ND1	1:H:121:HIS:CD2	2.79	0.44
1:P:40:GLN:NE2	1:P:40:GLN:HA	2.25	0.44
1:Q:116:LYS:HE2	2:Q:2001:HOH:O	2.18	0.44
1:S:24:LEU:HB3	1:T:30:GLN:NE2	2.33	0.44
1:U:100:ASN:HD22	1:U:102:LYS:CB	2.30	0.44
1:T:82:ASN:HB2	1:U:117:ASP:OD1	2.18	0.44
1:V:50:GLU:HA	1:V:181:GLN:NE2	2.33	0.44
1:B:192:LYS:NZ	1:B:194:GLN:O	2.46	0.44
1:C:40:GLN:CA	1:C:40:GLN:NE2	2.78	0.44
1:E:100:ASN:ND2	1:E:102:LYS:CB	2.74	0.44
1:E:113:VAL:HG21	1:E:155:LEU:HD13	1.99	0.44
1:F:77:GLU:OE2	1:G:44:ARG:NH1	2.51	0.44
1:L:47:LEU:CD2	1:L:47:LEU:N	2.80	0.44
1:T:82:ASN:N	1:T:82:ASN:HD22	2.14	0.44
1:D:77:GLU:OE2	1:E:44:ARG:NH1	2.51	0.44
1:E:202:GLU:HG2	1:E:206:ASN:HD21	1.83	0.44
1:F:186:VAL:HG21	1:G:171:TYR:HA	2.00	0.44
1:F:204:ARG:HG3	1:G:35:GLU:OE1	2.18	0.44
1:H:58:GLY:C	1:H:60:GLY:H	2.22	0.44
1:B:33:ALA:HB1	1:K:205:TYR:CE1	2.53	0.44
1:A:49:PRO:HD3	1:L:180:ARG:HH12	1.83	0.44
1:M:77:GLU:OE2	1:N:44:ARG:NH1	2.51	0.44
1:T:58:GLY:C	1:T:60:GLY:H	2.21	0.44
1:U:173:ARG:HH11	1:U:173:ARG:HG2	1.83	0.44
1:A:192:LYS:HB2	1:B:45:GLN:NE2	2.32	0.43
1:K:178:LEU:HB3	1:K:179:PRO:CD	2.48	0.43
1:L:151:LEU:CD1	1:L:155:LEU:HD22	2.48	0.43
1:L:192:LYS:NZ	1:L:194:GLN:O	2.40	0.43
1:O:77:GLU:OE2	1:P:44:ARG:NH1	2.51	0.43
1:U:47:LEU:HD23	1:U:165:CYS:SG	2.57	0.43
1:D:113:VAL:HG21	1:D:155:LEU:CD1	2.48	0.43
1:E:93:VAL:HA	1:E:107:VAL:HG22	2.00	0.43
1:E:179:PRO:C	1:E:180:ARG:O	2.56	0.43
1:G:186:VAL:HG21	1:H:171:TYR:HA	2.00	0.43
1:N:140:GLU:HG3	1:N:144:LYS:HE3	1.99	0.43
1:U:58:GLY:C	1:U:60:GLY:H	2.22	0.43
1:I:166:ILE:O	1:I:166:ILE:HD13	2.19	0.43
1:J:113:VAL:HG21	1:J:155:LEU:HD13	2.00	0.43
1:N:40:GLN:NE2	1:N:40:GLN:CA	2.79	0.43
1:P:173:ARG:HG2	1:P:173:ARG:HH11	1.83	0.43
1:R:166:ILE:O	1:R:166:ILE:HD13	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:ASN:HD22	1:G:102:LYS:CB	2.30	0.43
1:O:113:VAL:HG21	1:O:155:LEU:CD1	2.48	0.43
1:P:143:ARG:NH1	1:Q:94:ASP:OD2	2.51	0.43
1:D:24:LEU:HA	1:D:24:LEU:HD22	1.81	0.43
1:G:115:LEU:C	1:G:117:ASP:H	2.22	0.43
1:G:186:VAL:HG21	1:H:171:TYR:CA	2.49	0.43
1:I:115:LEU:C	1:I:117:ASP:H	2.21	0.43
1:L:178:LEU:O	1:L:179:PRO:C	2.57	0.43
1:L:178:LEU:O	1:L:179:PRO:O	2.36	0.43
1:M:204:ARG:HH21	1:M:204:ARG:HG3	1.83	0.43
1:N:143:ARG:NH1	1:O:94:ASP:OD2	2.51	0.43
1:N:175:LEU:O	1:N:178:LEU:HB2	2.18	0.43
1:T:202:GLU:O	1:T:205:TYR:N	2.51	0.43
1:A:105:VAL:HG11	1:A:139:LEU:HD13	1.99	0.43
1:B:193:ARG:HH12	1:C:50:GLU:CD	2.22	0.43
1:B:24:LEU:HB3	1:C:30:GLN:NE2	2.34	0.43
1:A:32:THR:CG2	1:K:207:SER:HB2	2.48	0.43
1:L:58:GLY:C	1:L:60:GLY:H	2.22	0.43
1:L:70:ARG:NH1	1:L:70:ARG:HG3	2.31	0.43
1:M:173:ARG:HH11	1:M:173:ARG:HG2	1.83	0.43
1:R:143:ARG:NH1	1:S:94:ASP:OD2	2.52	0.43
1:B:140:GLU:HB2	1:C:126:TYR:CD2	2.53	0.43
1:D:179:PRO:O	1:D:180:ARG:O	2.37	0.43
1:G:178:LEU:HA	1:G:178:LEU:HD23	1.78	0.43
1:G:36:TYR:CZ	1:G:40:GLN:HG3	2.53	0.43
1:G:85:ALA:HB1	1:H:120:TYR:O	2.19	0.43
1:I:186:VAL:HG21	1:J:171:TYR:HA	2.00	0.43
1:K:24:LEU:HA	1:K:24:LEU:HD22	1.81	0.43
1:A:166:ILE:HD13	1:A:166:ILE:O	2.18	0.43
1:B:192:LYS:CB	1:C:45:GLN:NE2	2.81	0.43
1:D:93:VAL:HA	1:D:107:VAL:HG22	2.00	0.43
1:I:77:GLU:OE1	1:J:44:ARG:HD3	2.18	0.43
1:J:113:VAL:HG21	1:J:155:LEU:CD1	2.49	0.43
1:L:44:ARG:HD3	1:V:77:GLU:OE1	2.19	0.43
1:O:100:ASN:HD22	1:O:102:LYS:H	1.67	0.43
1:Q:186:VAL:HG21	1:R:171:TYR:CA	2.49	0.43
1:R:113:VAL:CG1	1:R:154:ALA:HB1	2.47	0.43
1:R:178:LEU:HA	1:R:178:LEU:HD23	1.79	0.43
1:S:196:LEU:HD22	1:S:197:GLU:H	1.82	0.43
1:Q:208:CYS:HB3	1:S:33:ALA:HB2	2.01	0.43
1:A:123:ASP:OD1	1:A:153:ARG:NH1	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ILE:HD13	1:B:166:ILE:O	2.18	0.43
1:D:204:ARG:HG3	1:E:35:GLU:CD	2.39	0.43
1:F:100:ASN:ND2	1:F:102:LYS:CB	2.77	0.43
1:P:128:VAL:HG12	1:P:129:SER:N	2.33	0.43
1:Q:100:ASN:HB2	1:Q:101:GLY:H	1.55	0.43
1:R:70:ARG:NH1	1:R:70:ARG:CG	2.82	0.43
1:T:85:ALA:HB1	1:U:120:TYR:O	2.19	0.43
1:V:112:ARG:HG3	1:V:122:GLU:HB2	2.00	0.43
1:V:140:GLU:HG3	1:V:144:LYS:HE3	2.01	0.43
1:C:113:VAL:HG21	1:C:155:LEU:CD1	2.49	0.43
1:C:77:GLU:OE2	1:D:44:ARG:NH1	2.51	0.43
1:F:40:GLN:HA	1:F:40:GLN:NE2	2.26	0.43
1:G:58:GLY:C	1:G:60:GLY:H	2.22	0.43
1:G:82:ASN:HB2	1:H:117:ASP:OD1	2.19	0.43
1:K:58:GLY:C	1:K:60:GLY:H	2.22	0.43
1:P:205:TYR:CE2	1:P:209:ARG:NH2	2.86	0.43
1:P:90:GLN:HG2	1:P:91:GLN:N	2.34	0.43
1:Q:40:GLN:CA	1:Q:40:GLN:NE2	2.75	0.43
1:S:192:LYS:HB2	1:T:45:GLN:NE2	2.34	0.43
1:T:134:SER:OG	1:T:137:LEU:HD23	2.18	0.43
1:V:50:GLU:HA	1:V:181:GLN:HE21	1.83	0.43
1:F:58:GLY:C	1:F:60:GLY:H	2.21	0.42
1:H:69:HIS:HB3	1:I:167:LEU:CD2	2.47	0.42
1:R:175:LEU:O	1:R:178:LEU:HB2	2.18	0.42
1:M:40:GLN:CA	1:M:40:GLN:NE2	2.81	0.42
1:P:189:THR:HG22	1:P:189:THR:O	2.19	0.42
1:R:36:TYR:CE1	1:R:40:GLN:HG2	2.54	0.42
1:S:166:ILE:O	1:S:166:ILE:HD13	2.18	0.42
1:K:179:PRO:C	1:K:180:ARG:O	2.58	0.42
1:R:113:VAL:HG21	1:R:155:LEU:CD1	2.49	0.42
1:U:139:LEU:O	1:U:143:ARG:HG3	2.19	0.42
1:L:44:ARG:NH1	1:V:77:GLU:OE2	2.52	0.42
1:B:50:GLU:HA	1:B:181:GLN:HE22	1.85	0.42
1:D:197:GLU:HB3	1:D:200:VAL:HB	2.01	0.42
1:E:205:TYR:CE2	1:E:209:ARG:NH2	2.87	0.42
1:G:198:PRO:O	1:G:202:GLU:HG3	2.20	0.42
1:I:112:ARG:NH1	2:I:2007:HOH:O	2.51	0.42
1:J:47:LEU:N	1:J:47:LEU:CD2	2.80	0.42
1:K:134:SER:OG	1:K:137:LEU:HD23	2.19	0.42
1:N:47:LEU:N	1:N:47:LEU:CD2	2.80	0.42
1:S:58:GLY:C	1:S:60:GLY:H	2.22	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:188:LEU:HD21	1:T:171:TYR:CE1	2.54	0.42
1:U:86:HIS:HA	1:U:112:ARG:O	2.19	0.42
1:B:196:LEU:HD13	1:B:198:PRO:HG3	1.99	0.42
1:F:204:ARG:CG	1:F:204:ARG:NH2	2.75	0.42
1:Q:184:LEU:HD22	1:Q:185:GLU:N	2.32	0.42
1:B:173:ARG:HH11	1:B:173:ARG:HG2	1.84	0.42
1:E:100:ASN:HB2	1:E:101:GLY:H	1.57	0.42
1:G:90:GLN:HG2	1:G:91:GLN:N	2.35	0.42
1:I:147:VAL:HG21	1:J:124:VAL:CG2	2.43	0.42
1:J:77:GLU:OE2	1:K:44:ARG:NH1	2.52	0.42
1:L:113:VAL:HG21	1:L:155:LEU:HD13	2.00	0.42
1:L:36:TYR:CE1	1:L:40:GLN:HG2	2.55	0.42
1:M:180:ARG:O	1:M:181:GLN:HB3	2.19	0.42
1:O:40:GLN:CA	1:O:40:GLN:NE2	2.80	0.42
1:T:100:ASN:HB2	1:T:101:GLY:H	1.57	0.42
1:A:82:ASN:ND2	1:A:82:ASN:H	2.10	0.42
1:D:115:LEU:C	1:D:117:ASP:N	2.72	0.42
1:D:134:SER:OG	1:D:137:LEU:HD23	2.20	0.42
1:I:112:ARG:HG3	1:I:122:GLU:HB2	2.02	0.42
1:I:207:SER:C	1:I:209:ARG:H	2.21	0.42
1:K:100:ASN:ND2	1:K:102:LYS:CB	2.77	0.42
1:J:77:GLU:OE1	1:K:44:ARG:HD3	2.20	0.42
1:Q:77:GLU:OE2	1:R:44:ARG:NH1	2.52	0.42
1:R:173:ARG:HG2	1:R:173:ARG:HH11	1.84	0.42
1:S:24:LEU:HD22	1:S:24:LEU:HA	1.82	0.42
1:B:165:CYS:HA	2:B:2021:HOH:O	2.19	0.42
1:G:36:TYR:CE1	1:G:40:GLN:HG2	2.55	0.42
1:J:82:ASN:HD22	1:J:82:ASN:N	2.11	0.42
1:L:134:SER:OG	1:L:137:LEU:HD23	2.20	0.42
1:N:176:ASN:C	1:N:178:LEU:H	2.22	0.42
1:M:24:LEU:HB3	1:N:30:GLN:NE2	2.34	0.42
1:Q:24:LEU:HD22	1:Q:24:LEU:HA	1.89	0.42
1:R:85:ALA:HB1	1:S:120:TYR:O	2.20	0.42
1:U:100:ASN:HB2	1:U:101:GLY:H	1.53	0.42
1:V:113:VAL:HG21	1:V:155:LEU:HD13	2.02	0.42
1:I:115:LEU:C	1:I:117:ASP:N	2.73	0.42
1:N:204:ARG:HD2	1:P:36:TYR:CZ	2.55	0.42
1:Q:182:LEU:O	1:Q:183:PRO:C	2.58	0.42
1:U:32:THR:HG23	2:U:2002:HOH:O	2.19	0.42
1:D:204:ARG:HG3	1:D:204:ARG:HH21	1.85	0.42
1:F:186:VAL:HG21	1:G:170:ASP:C	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:204:ARG:HG3	1:I:35:GLU:CD	2.41	0.42
1:K:192:LYS:CE	1:K:197:GLU:OE2	2.65	0.42
1:L:179:PRO:O	1:L:180:ARG:O	2.38	0.42
1:S:82:ASN:HD22	1:S:82:ASN:N	2.11	0.42
1:A:140:GLU:HG3	1:A:144:LYS:HE3	2.01	0.41
1:B:193:ARG:NH1	1:B:193:ARG:CG	2.51	0.41
1:D:86:HIS:ND1	1:E:121:HIS:CD2	2.85	0.41
1:G:192:LYS:HB2	1:H:45:GLN:HE21	1.85	0.41
1:H:40:GLN:NE2	1:H:40:GLN:HA	2.23	0.41
1:I:140:GLU:HG3	1:I:144:LYS:HE3	2.01	0.41
1:K:113:VAL:HG21	1:K:155:LEU:CD1	2.50	0.41
1:O:136:ALA:HB2	1:P:95:PHE:HZ	1.85	0.41
1:R:100:ASN:HD22	1:R:102:LYS:CB	2.32	0.41
1:R:77:GLU:OE1	1:S:44:ARG:HD3	2.20	0.41
1:E:173:ARG:HG2	1:E:173:ARG:HH11	1.85	0.41
1:F:181:GLN:O	1:F:181:GLN:HG3	2.20	0.41
1:G:24:LEU:HA	1:G:24:LEU:HD22	1.82	0.41
1:O:192:LYS:CE	1:O:197:GLU:OE2	2.66	0.41
1:P:178:LEU:HA	1:P:178:LEU:HD23	1.78	0.41
1:O:143:ARG:NH1	1:P:94:ASP:OD2	2.53	0.41
1:Q:86:HIS:HA	1:Q:112:ARG:O	2.20	0.41
1:V:90:GLN:HG2	1:V:91:GLN:N	2.35	0.41
1:B:178:LEU:HD22	1:B:179:PRO:HD3	2.02	0.41
1:E:40:GLN:CA	1:E:40:GLN:NE2	2.81	0.41
1:I:113:VAL:HG21	1:I:155:LEU:CD1	2.50	0.41
1:I:182:LEU:HD23	1:I:182:LEU:N	2.24	0.41
1:O:140:GLU:HG3	1:O:144:LYS:HE3	2.01	0.41
1:Q:36:TYR:CE1	1:Q:40:GLN:HG2	2.55	0.41
1:S:203:ALA:CB	1:T:35:GLU:HA	2.51	0.41
1:S:208:CYS:CB	1:U:33:ALA:HB2	2.49	0.41
1:A:100:ASN:HB2	1:A:101:GLY:H	1.55	0.41
1:A:112:ARG:HG3	1:A:122:GLU:HB2	2.03	0.41
1:A:47:LEU:HD23	1:A:165:CYS:SG	2.61	0.41
1:E:193:ARG:HH11	1:E:193:ARG:HG2	1.85	0.41
1:F:47:LEU:HD23	1:F:165:CYS:SG	2.61	0.41
1:H:40:GLN:NE2	1:H:40:GLN:CA	2.81	0.41
1:J:184:LEU:HA	1:J:184:LEU:HD22	1.75	0.41
1:V:204:ARG:HG3	1:V:204:ARG:HH21	1.84	0.41
1:B:105:VAL:HG11	1:B:139:LEU:HD13	2.02	0.41
1:D:58:GLY:C	1:D:60:GLY:H	2.24	0.41
1:J:47:LEU:HD23	1:J:165:CYS:SG	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:208:CYS:CB	1:J:33:ALA:HB2	2.50	0.41
1:K:193:ARG:CD	1:L:180:ARG:HE	2.32	0.41
1:O:58:GLY:C	1:O:60:GLY:H	2.23	0.41
1:R:100:ASN:HD22	1:R:102:LYS:H	1.68	0.41
1:U:204:ARG:HG3	1:U:204:ARG:HH21	1.84	0.41
1:C:188:LEU:HD23	1:C:188:LEU:HA	1.69	0.41
1:E:58:GLY:C	1:E:60:GLY:H	2.24	0.41
1:J:50:GLU:CD	1:J:50:GLU:H	2.24	0.41
1:K:57:ALA:HB2	1:K:63:VAL:CG2	2.51	0.41
1:M:195:ASP:HB3	1:N:77:GLU:HG3	2.02	0.41
1:R:77:GLU:OE2	1:S:44:ARG:NH1	2.54	0.41
1:V:123:ASP:OD1	1:V:153:ARG:NH1	2.54	0.41
1:A:24:LEU:HD22	1:A:24:LEU:HA	1.81	0.41
1:C:100:ASN:HB2	1:C:101:GLY:H	1.56	0.41
1:D:36:TYR:CE1	1:D:40:GLN:HG2	2.55	0.41
1:E:166:ILE:O	1:E:166:ILE:HD13	2.21	0.41
1:P:36:TYR:CE1	1:P:40:GLN:HG2	2.56	0.41
1:V:24:LEU:HA	1:V:24:LEU:HD22	1.88	0.41
1:B:117:ASP:HB3	1:B:119:SER:H	1.86	0.41
1:B:70:ARG:NH1	1:B:70:ARG:CG	2.81	0.41
1:C:188:LEU:O	1:C:189:THR:C	2.58	0.41
1:E:79:PHE:O	1:E:83:GLY:HA3	2.21	0.41
1:H:143:ARG:NH1	1:I:94:ASP:OD2	2.54	0.41
1:I:100:ASN:ND2	1:I:102:LYS:CB	2.77	0.41
1:J:182:LEU:N	1:J:182:LEU:HD23	2.35	0.41
1:K:165:CYS:O	1:K:167:LEU:N	2.54	0.41
1:K:178:LEU:HA	1:K:178:LEU:HD23	1.90	0.41
1:N:115:LEU:HD22	1:N:158:PHE:CE2	2.56	0.41
1:Q:77:GLU:OE1	1:R:44:ARG:HD3	2.21	0.41
1:T:113:VAL:HG21	1:T:155:LEU:CD1	2.50	0.41
1:S:203:ALA:HB1	1:T:35:GLU:CA	2.51	0.41
1:L:45:GLN:HE22	1:V:192:LYS:HG3	1.85	0.41
1:A:194:GLN:HE21	1:A:194:GLN:HB3	1.57	0.41
1:A:44:ARG:HD3	1:K:77:GLU:OE1	2.21	0.41
1:A:93:VAL:HA	1:A:107:VAL:HG22	2.02	0.41
1:H:182:LEU:HD23	1:H:182:LEU:N	2.36	0.41
1:H:47:LEU:HD23	1:H:165:CYS:SG	2.61	0.41
1:H:47:LEU:CD2	1:H:47:LEU:N	2.83	0.41
1:J:191:ALA:O	1:J:193:ARG:HG3	2.20	0.41
1:J:196:LEU:HD22	1:J:197:GLU:H	1.85	0.41
1:J:192:LYS:HG3	1:K:45:GLN:HE22	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:47:LEU:HD23	1:L:165:CYS:SG	2.61	0.41
1:N:82:ASN:ND2	1:N:82:ASN:H	2.15	0.41
1:P:165:CYS:O	1:P:167:LEU:N	2.54	0.41
1:S:134:SER:OG	1:S:137:LEU:HD23	2.21	0.41
1:T:50:GLU:HA	1:T:181:GLN:HE22	1.82	0.41
1:A:90:GLN:HG2	1:A:91:GLN:N	2.35	0.41
1:B:58:GLY:C	1:B:60:GLY:H	2.23	0.41
1:C:90:GLN:HG2	1:C:91:GLN:N	2.34	0.41
1:R:204:ARG:HG3	1:R:204:ARG:HH21	1.85	0.41
1:U:115:LEU:C	1:U:117:ASP:H	2.24	0.41
1:U:113:VAL:HG12	1:U:154:ALA:HB1	2.02	0.41
1:L:121:HIS:CD2	1:V:86:HIS:ND1	2.85	0.41
1:G:113:VAL:HG21	1:G:155:LEU:CD1	2.51	0.41
1:G:192:LYS:HB2	1:H:45:GLN:NE2	2.36	0.41
1:H:182:LEU:HA	1:H:183:PRO:HD3	1.98	0.41
1:B:36:TYR:CZ	1:K:204:ARG:HD2	2.56	0.41
1:L:166:ILE:O	1:L:166:ILE:HD13	2.20	0.41
1:N:192:LYS:HB2	1:O:45:GLN:NE2	2.36	0.41
1:P:195:ASP:HB3	1:Q:77:GLU:HG3	2.02	0.41
1:Q:115:LEU:C	1:Q:117:ASP:H	2.24	0.41
1:R:203:ALA:HB1	1:S:35:GLU:HA	2.03	0.41
1:S:116:LYS:HE2	2:S:2001:HOH:O	2.21	0.41
1:U:184:LEU:HD13	1:U:185:GLU:C	2.41	0.41
1:B:178:LEU:HA	1:B:178:LEU:HD23	1.88	0.40
1:D:166:ILE:HD13	1:D:166:ILE:O	2.21	0.40
1:F:166:ILE:O	1:F:166:ILE:HD13	2.21	0.40
1:O:208:CYS:HB2	1:Q:33:ALA:HB2	2.01	0.40
1:P:184:LEU:HA	1:P:184:LEU:HD23	1.87	0.40
1:T:110:PHE:CD2	1:T:124:VAL:HG13	2.54	0.40
1:V:166:ILE:O	1:V:166:ILE:HD13	2.21	0.40
1:L:171:TYR:HA	1:V:186:VAL:HG21	2.04	0.40
1:A:58:GLY:C	1:A:60:GLY:H	2.25	0.40
1:C:143:ARG:NH1	1:D:94:ASP:OD2	2.55	0.40
1:F:207:SER:C	1:F:209:ARG:H	2.24	0.40
1:F:85:ALA:HB1	1:G:120:TYR:O	2.22	0.40
1:H:82:ASN:ND2	1:H:82:ASN:H	2.15	0.40
1:N:36:TYR:CE1	1:N:40:GLN:HG2	2.56	0.40
1:S:173:ARG:HH11	1:S:173:ARG:HG2	1.86	0.40
1:T:24:LEU:HD22	1:T:24:LEU:HA	1.74	0.40
1:C:166:ILE:HD13	1:C:166:ILE:O	2.22	0.40
1:G:189:THR:HG22	1:G:190:LYS:N	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:82:ASN:HB2	1:J:117:ASP:OD1	2.21	0.40
1:J:166:ILE:O	1:J:166:ILE:HD13	2.21	0.40
1:K:100:ASN:HD22	1:K:102:LYS:HB2	1.73	0.40
1:N:58:GLY:C	1:N:60:GLY:H	2.24	0.40
1:Q:175:LEU:O	1:Q:178:LEU:HB2	2.22	0.40
1:N:113:VAL:HG21	1:N:155:LEU:CD1	2.51	0.40
1:O:86:HIS:ND1	1:P:121:HIS:CD2	2.86	0.40
1:P:123:ASP:OD1	1:P:153:ARG:NH1	2.55	0.40
1:P:115:LEU:HD22	1:P:158:PHE:CE2	2.56	0.40
1:S:86:HIS:HA	1:S:112:ARG:O	2.22	0.40
1:B:178:LEU:HD22	1:B:179:PRO:CD	2.52	0.40
1:D:115:LEU:C	1:D:117:ASP:H	2.23	0.40
1:G:184:LEU:CD2	1:G:185:GLU:O	2.69	0.40
1:I:196:LEU:HD12	1:I:198:PRO:HG3	2.03	0.40
1:A:187:ASP:OD1	1:L:177:LYS:CE	2.70	0.40
1:M:24:LEU:HD22	1:M:24:LEU:HA	1.82	0.40
1:P:50:GLU:CA	1:P:181:GLN:HE22	2.30	0.40
1:P:50:GLU:H	1:P:50:GLU:CD	2.24	0.40
1:R:179:PRO:O	1:R:180:ARG:C	2.59	0.40
1:V:181:GLN:OE1	1:V:181:GLN:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	184/209 (88%)	177 (96%)	4 (2%)	3 (2%)	9	24
1	B	184/209 (88%)	178 (97%)	4 (2%)	2 (1%)	14	34
1	C	184/209 (88%)	172 (94%)	9 (5%)	3 (2%)	9	24
1	D	184/209 (88%)	173 (94%)	6 (3%)	5 (3%)	5	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	184/209 (88%)	171 (93%)	6 (3%)	7 (4%)	3	7
1	F	184/209 (88%)	171 (93%)	8 (4%)	5 (3%)	5	12
1	G	184/209 (88%)	169 (92%)	12 (6%)	3 (2%)	9	24
1	H	184/209 (88%)	171 (93%)	11 (6%)	2 (1%)	14	34
1	I	184/209 (88%)	174 (95%)	8 (4%)	2 (1%)	14	34
1	J	184/209 (88%)	175 (95%)	5 (3%)	4 (2%)	6	17
1	K	184/209 (88%)	176 (96%)	5 (3%)	3 (2%)	9	24
1	L	184/209 (88%)	175 (95%)	5 (3%)	4 (2%)	6	17
1	M	184/209 (88%)	173 (94%)	6 (3%)	5 (3%)	5	12
1	N	184/209 (88%)	173 (94%)	8 (4%)	3 (2%)	9	24
1	O	184/209 (88%)	173 (94%)	9 (5%)	2 (1%)	14	34
1	P	184/209 (88%)	179 (97%)	3 (2%)	2 (1%)	14	34
1	Q	184/209 (88%)	173 (94%)	8 (4%)	3 (2%)	9	24
1	R	184/209 (88%)	178 (97%)	4 (2%)	2 (1%)	14	34
1	S	184/209 (88%)	175 (95%)	7 (4%)	2 (1%)	14	34
1	T	184/209 (88%)	173 (94%)	8 (4%)	3 (2%)	9	24
1	U	184/209 (88%)	175 (95%)	6 (3%)	3 (2%)	9	24
1	V	184/209 (88%)	173 (94%)	9 (5%)	2 (1%)	14	34
All	All	4048/4598 (88%)	3827 (94%)	151 (4%)	70 (2%)	9	23

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	166	ILE
1	E	184	LEU
1	F	166	ILE
1	G	166	ILE
1	G	189	THR
1	H	166	ILE
1	I	166	ILE
1	J	166	ILE
1	J	179	PRO
1	K	166	ILE
1	K	180	ARG
1	L	180	ARG
1	M	179	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	208	CYS
1	N	166	ILE
1	N	180	ARG
1	P	166	ILE
1	Q	180	ARG
1	R	166	ILE
1	T	166	ILE
1	V	166	ILE
1	A	100	ASN
1	A	166	ILE
1	B	166	ILE
1	C	100	ASN
1	D	100	ASN
1	D	183	PRO
1	E	166	ILE
1	E	183	PRO
1	E	208	CYS
1	F	100	ASN
1	F	179	PRO
1	I	100	ASN
1	J	100	ASN
1	K	100	ASN
1	L	100	ASN
1	L	166	ILE
1	M	100	ASN
1	M	166	ILE
1	N	100	ASN
1	O	100	ASN
1	O	166	ILE
1	P	100	ASN
1	Q	100	ASN
1	Q	166	ILE
1	R	100	ASN
1	S	100	ASN
1	S	166	ILE
1	T	180	ARG
1	U	166	ILE
1	V	100	ASN
1	B	100	ASN
1	D	180	ARG
1	E	100	ASN
1	E	180	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	188	LEU
1	F	189	THR
1	G	100	ASN
1	H	100	ASN
1	J	183	PRO
1	T	100	ASN
1	U	100	ASN
1	A	180	ARG
1	C	166	ILE
1	M	181	GLN
1	U	183	PRO
1	C	202	GLU
1	E	196	LEU
1	L	179	PRO
1	D	198	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	155/169 (92%)	139 (90%)	16 (10%)	7	16
1	B	155/169 (92%)	136 (88%)	19 (12%)	4	11
1	C	155/169 (92%)	138 (89%)	17 (11%)	6	14
1	D	155/169 (92%)	138 (89%)	17 (11%)	6	14
1	E	155/169 (92%)	136 (88%)	19 (12%)	4	11
1	F	155/169 (92%)	138 (89%)	17 (11%)	6	14
1	G	155/169 (92%)	137 (88%)	18 (12%)	5	12
1	H	155/169 (92%)	140 (90%)	15 (10%)	8	19
1	I	155/169 (92%)	138 (89%)	17 (11%)	6	14
1	J	155/169 (92%)	135 (87%)	20 (13%)	4	10
1	K	155/169 (92%)	136 (88%)	19 (12%)	4	11
1	L	155/169 (92%)	138 (89%)	17 (11%)	6	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	155/169 (92%)	140 (90%)	15 (10%)	8	19
1	N	155/169 (92%)	139 (90%)	16 (10%)	7	16
1	O	155/169 (92%)	138 (89%)	17 (11%)	6	14
1	P	155/169 (92%)	138 (89%)	17 (11%)	6	14
1	Q	155/169 (92%)	137 (88%)	18 (12%)	5	12
1	R	155/169 (92%)	138 (89%)	17 (11%)	6	14
1	S	155/169 (92%)	136 (88%)	19 (12%)	4	11
1	T	155/169 (92%)	137 (88%)	18 (12%)	5	12
1	U	155/169 (92%)	140 (90%)	15 (10%)	8	19
1	V	155/169 (92%)	138 (89%)	17 (11%)	6	14
All	All	3410/3718 (92%)	3030 (89%)	380 (11%)	6	14

All (380) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	40	GLN
1	A	47	LEU
1	A	70	ARG
1	A	82	ASN
1	A	100	ASN
1	A	115	LEU
1	A	124	VAL
1	A	139	LEU
1	A	155	LEU
1	A	166	ILE
1	A	167	LEU
1	A	174	SER
1	A	182	LEU
1	A	184	LEU
1	A	208	CYS
1	B	24	LEU
1	B	40	GLN
1	B	47	LEU
1	B	70	ARG
1	B	82	ASN
1	B	100	ASN
1	B	112	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	115	LEU
1	B	124	VAL
1	B	139	LEU
1	B	155	LEU
1	B	166	ILE
1	B	167	LEU
1	B	174	SER
1	B	175	LEU
1	B	182	LEU
1	B	189	THR
1	B	193	ARG
1	B	194	GLN
1	C	24	LEU
1	C	40	GLN
1	C	47	LEU
1	C	70	ARG
1	C	82	ASN
1	C	100	ASN
1	C	115	LEU
1	C	124	VAL
1	C	139	LEU
1	C	155	LEU
1	C	166	ILE
1	C	167	LEU
1	C	174	SER
1	C	180	ARG
1	C	182	LEU
1	C	184	LEU
1	C	196	LEU
1	D	24	LEU
1	D	40	GLN
1	D	47	LEU
1	D	70	ARG
1	D	82	ASN
1	D	100	ASN
1	D	112	ARG
1	D	115	LEU
1	D	124	VAL
1	D	139	LEU
1	D	155	LEU
1	D	166	ILE
1	D	167	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	174	SER
1	D	181	GLN
1	D	194	GLN
1	D	199	SER
1	E	24	LEU
1	E	40	GLN
1	E	47	LEU
1	E	70	ARG
1	E	82	ASN
1	E	100	ASN
1	E	112	ARG
1	E	115	LEU
1	E	124	VAL
1	E	139	LEU
1	E	155	LEU
1	E	166	ILE
1	E	167	LEU
1	E	174	SER
1	E	175	LEU
1	E	181	GLN
1	E	184	LEU
1	E	196	LEU
1	E	199	SER
1	F	24	LEU
1	F	40	GLN
1	F	47	LEU
1	F	70	ARG
1	F	82	ASN
1	F	100	ASN
1	F	115	LEU
1	F	124	VAL
1	F	139	LEU
1	F	155	LEU
1	F	166	ILE
1	F	167	LEU
1	F	174	SER
1	F	175	LEU
1	F	182	LEU
1	F	184	LEU
1	F	204	ARG
1	G	24	LEU
1	G	40	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	47	LEU
1	G	82	ASN
1	G	100	ASN
1	G	115	LEU
1	G	124	VAL
1	G	139	LEU
1	G	155	LEU
1	G	166	ILE
1	G	167	LEU
1	G	174	SER
1	G	175	LEU
1	G	180	ARG
1	G	182	LEU
1	G	194	GLN
1	G	196	LEU
1	G	204	ARG
1	H	24	LEU
1	H	40	GLN
1	H	47	LEU
1	H	82	ASN
1	H	100	ASN
1	H	115	LEU
1	H	124	VAL
1	H	139	LEU
1	H	155	LEU
1	H	166	ILE
1	H	167	LEU
1	H	174	SER
1	H	180	ARG
1	H	184	LEU
1	H	196	LEU
1	I	24	LEU
1	I	40	GLN
1	I	47	LEU
1	I	70	ARG
1	I	82	ASN
1	I	100	ASN
1	I	115	LEU
1	I	124	VAL
1	I	139	LEU
1	I	155	LEU
1	I	166	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	167	LEU
1	I	174	SER
1	I	175	LEU
1	I	182	LEU
1	I	184	LEU
1	I	196	LEU
1	J	24	LEU
1	J	40	GLN
1	J	47	LEU
1	J	70	ARG
1	J	82	ASN
1	J	100	ASN
1	J	115	LEU
1	J	124	VAL
1	J	139	LEU
1	J	155	LEU
1	J	166	ILE
1	J	167	LEU
1	J	174	SER
1	J	175	LEU
1	J	181	GLN
1	J	182	LEU
1	J	183	PRO
1	J	184	LEU
1	J	196	LEU
1	J	202	GLU
1	K	24	LEU
1	K	40	GLN
1	K	47	LEU
1	K	70	ARG
1	K	82	ASN
1	K	100	ASN
1	K	115	LEU
1	K	124	VAL
1	K	139	LEU
1	K	155	LEU
1	K	166	ILE
1	K	167	LEU
1	K	174	SER
1	K	175	LEU
1	K	180	ARG
1	K	182	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	184	LEU
1	K	189	THR
1	K	196	LEU
1	L	24	LEU
1	L	40	GLN
1	L	47	LEU
1	L	82	ASN
1	L	100	ASN
1	L	112	ARG
1	L	115	LEU
1	L	124	VAL
1	L	139	LEU
1	L	155	LEU
1	L	166	ILE
1	L	167	LEU
1	L	174	SER
1	L	175	LEU
1	L	196	LEU
1	L	199	SER
1	L	204	ARG
1	M	24	LEU
1	M	40	GLN
1	M	47	LEU
1	M	70	ARG
1	M	82	ASN
1	M	100	ASN
1	M	115	LEU
1	M	124	VAL
1	M	139	LEU
1	M	155	LEU
1	M	166	ILE
1	M	167	LEU
1	M	174	SER
1	M	182	LEU
1	M	196	LEU
1	N	24	LEU
1	N	40	GLN
1	N	47	LEU
1	N	70	ARG
1	N	82	ASN
1	N	100	ASN
1	N	115	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	124	VAL
1	N	139	LEU
1	N	155	LEU
1	N	166	ILE
1	N	167	LEU
1	N	174	SER
1	N	175	LEU
1	N	182	LEU
1	N	196	LEU
1	O	24	LEU
1	O	40	GLN
1	O	47	LEU
1	O	70	ARG
1	O	82	ASN
1	O	100	ASN
1	O	115	LEU
1	O	124	VAL
1	O	139	LEU
1	O	155	LEU
1	O	166	ILE
1	O	167	LEU
1	O	174	SER
1	O	179	PRO
1	O	181	GLN
1	O	182	LEU
1	O	196	LEU
1	P	24	LEU
1	P	40	GLN
1	P	47	LEU
1	P	70	ARG
1	P	82	ASN
1	P	100	ASN
1	P	112	ARG
1	P	115	LEU
1	P	124	VAL
1	P	139	LEU
1	P	155	LEU
1	P	166	ILE
1	P	167	LEU
1	P	174	SER
1	P	175	LEU
1	P	182	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	196	LEU
1	Q	24	LEU
1	Q	40	GLN
1	Q	47	LEU
1	Q	70	ARG
1	Q	82	ASN
1	Q	100	ASN
1	Q	115	LEU
1	Q	124	VAL
1	Q	139	LEU
1	Q	155	LEU
1	Q	166	ILE
1	Q	167	LEU
1	Q	174	SER
1	Q	182	LEU
1	Q	184	LEU
1	Q	193	ARG
1	Q	196	LEU
1	Q	208	CYS
1	R	24	LEU
1	R	40	GLN
1	R	47	LEU
1	R	70	ARG
1	R	82	ASN
1	R	100	ASN
1	R	115	LEU
1	R	124	VAL
1	R	139	LEU
1	R	155	LEU
1	R	166	ILE
1	R	167	LEU
1	R	174	SER
1	R	175	LEU
1	R	184	LEU
1	R	193	ARG
1	R	196	LEU
1	S	24	LEU
1	S	40	GLN
1	S	47	LEU
1	S	70	ARG
1	S	82	ASN
1	S	100	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	115	LEU
1	S	124	VAL
1	S	139	LEU
1	S	155	LEU
1	S	166	ILE
1	S	167	LEU
1	S	174	SER
1	S	175	LEU
1	S	180	ARG
1	S	181	GLN
1	S	184	LEU
1	S	196	LEU
1	S	199	SER
1	T	24	LEU
1	T	40	GLN
1	T	47	LEU
1	T	70	ARG
1	T	82	ASN
1	T	100	ASN
1	T	115	LEU
1	T	124	VAL
1	T	139	LEU
1	T	155	LEU
1	T	166	ILE
1	T	167	LEU
1	T	174	SER
1	T	175	LEU
1	T	179	PRO
1	T	181	GLN
1	T	184	LEU
1	T	196	LEU
1	U	24	LEU
1	U	40	GLN
1	U	47	LEU
1	U	70	ARG
1	U	82	ASN
1	U	100	ASN
1	U	115	LEU
1	U	124	VAL
1	U	139	LEU
1	U	155	LEU
1	U	166	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	U	167	LEU
1	U	174	SER
1	U	183	PRO
1	U	196	LEU
1	V	24	LEU
1	V	40	GLN
1	V	47	LEU
1	V	70	ARG
1	V	82	ASN
1	V	100	ASN
1	V	115	LEU
1	V	124	VAL
1	V	139	LEU
1	V	155	LEU
1	V	166	ILE
1	V	167	LEU
1	V	174	SER
1	V	175	LEU
1	V	184	LEU
1	V	196	LEU
1	V	202	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (285) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	30	GLN
1	A	37	GLN
1	A	40	GLN
1	A	45	GLN
1	A	61	GLN
1	A	82	ASN
1	A	99	ASN
1	A	100	ASN
1	A	121	HIS
1	A	164	ASN
1	A	194	GLN
1	B	28	GLN
1	B	30	GLN
1	B	37	GLN
1	B	40	GLN
1	B	45	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	61	GLN
1	B	82	ASN
1	B	90	GLN
1	B	99	ASN
1	B	100	ASN
1	B	121	HIS
1	B	164	ASN
1	C	28	GLN
1	C	30	GLN
1	C	40	GLN
1	C	45	GLN
1	C	61	GLN
1	C	82	ASN
1	C	90	GLN
1	C	99	ASN
1	C	100	ASN
1	C	121	HIS
1	C	164	ASN
1	C	181	GLN
1	C	194	GLN
1	D	28	GLN
1	D	30	GLN
1	D	37	GLN
1	D	40	GLN
1	D	45	GLN
1	D	61	GLN
1	D	82	ASN
1	D	90	GLN
1	D	99	ASN
1	D	100	ASN
1	D	121	HIS
1	D	164	ASN
1	D	194	GLN
1	E	28	GLN
1	E	30	GLN
1	E	37	GLN
1	E	40	GLN
1	E	45	GLN
1	E	61	GLN
1	E	82	ASN
1	E	90	GLN
1	E	99	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	100	ASN
1	E	121	HIS
1	E	164	ASN
1	E	194	GLN
1	E	206	ASN
1	F	28	GLN
1	F	30	GLN
1	F	37	GLN
1	F	40	GLN
1	F	45	GLN
1	F	61	GLN
1	F	82	ASN
1	F	90	GLN
1	F	99	ASN
1	F	100	ASN
1	F	121	HIS
1	F	164	ASN
1	F	181	GLN
1	F	194	GLN
1	G	28	GLN
1	G	30	GLN
1	G	40	GLN
1	G	45	GLN
1	G	61	GLN
1	G	82	ASN
1	G	90	GLN
1	G	99	ASN
1	G	100	ASN
1	G	121	HIS
1	G	164	ASN
1	G	181	GLN
1	G	194	GLN
1	H	28	GLN
1	H	30	GLN
1	H	37	GLN
1	H	40	GLN
1	H	45	GLN
1	H	61	GLN
1	H	82	ASN
1	H	90	GLN
1	H	99	ASN
1	H	100	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	121	HIS
1	H	164	ASN
1	H	194	GLN
1	I	28	GLN
1	I	30	GLN
1	I	37	GLN
1	I	40	GLN
1	I	45	GLN
1	I	61	GLN
1	I	82	ASN
1	I	90	GLN
1	I	99	ASN
1	I	100	ASN
1	I	121	HIS
1	I	164	ASN
1	I	181	GLN
1	I	194	GLN
1	J	28	GLN
1	J	30	GLN
1	J	37	GLN
1	J	40	GLN
1	J	45	GLN
1	J	61	GLN
1	J	82	ASN
1	J	90	GLN
1	J	99	ASN
1	J	100	ASN
1	J	121	HIS
1	J	164	ASN
1	J	194	GLN
1	K	28	GLN
1	K	30	GLN
1	K	37	GLN
1	K	40	GLN
1	K	45	GLN
1	K	61	GLN
1	K	82	ASN
1	K	90	GLN
1	K	99	ASN
1	K	100	ASN
1	K	121	HIS
1	K	164	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	194	GLN
1	L	28	GLN
1	L	30	GLN
1	L	40	GLN
1	L	45	GLN
1	L	61	GLN
1	L	82	ASN
1	L	90	GLN
1	L	99	ASN
1	L	100	ASN
1	L	121	HIS
1	L	164	ASN
1	L	194	GLN
1	M	28	GLN
1	M	30	GLN
1	M	37	GLN
1	M	40	GLN
1	M	45	GLN
1	M	61	GLN
1	M	82	ASN
1	M	99	ASN
1	M	100	ASN
1	M	121	HIS
1	M	164	ASN
1	M	194	GLN
1	N	28	GLN
1	N	30	GLN
1	N	37	GLN
1	N	40	GLN
1	N	45	GLN
1	N	61	GLN
1	N	82	ASN
1	N	90	GLN
1	N	99	ASN
1	N	100	ASN
1	N	121	HIS
1	N	164	ASN
1	N	194	GLN
1	O	28	GLN
1	O	30	GLN
1	O	37	GLN
1	O	40	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	45	GLN
1	O	61	GLN
1	O	82	ASN
1	O	99	ASN
1	O	100	ASN
1	O	121	HIS
1	O	164	ASN
1	O	194	GLN
1	P	28	GLN
1	P	30	GLN
1	P	37	GLN
1	P	40	GLN
1	P	45	GLN
1	P	61	GLN
1	P	82	ASN
1	P	99	ASN
1	P	100	ASN
1	P	121	HIS
1	P	164	ASN
1	P	181	GLN
1	P	194	GLN
1	Q	28	GLN
1	Q	30	GLN
1	Q	37	GLN
1	Q	40	GLN
1	Q	45	GLN
1	Q	61	GLN
1	Q	82	ASN
1	Q	90	GLN
1	Q	99	ASN
1	Q	100	ASN
1	Q	121	HIS
1	Q	164	ASN
1	Q	194	GLN
1	R	28	GLN
1	R	30	GLN
1	R	37	GLN
1	R	40	GLN
1	R	45	GLN
1	R	61	GLN
1	R	82	ASN
1	R	90	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	99	ASN
1	R	100	ASN
1	R	121	HIS
1	R	164	ASN
1	R	194	GLN
1	S	28	GLN
1	S	30	GLN
1	S	37	GLN
1	S	40	GLN
1	S	45	GLN
1	S	61	GLN
1	S	82	ASN
1	S	90	GLN
1	S	99	ASN
1	S	100	ASN
1	S	121	HIS
1	S	164	ASN
1	S	194	GLN
1	T	28	GLN
1	T	30	GLN
1	T	37	GLN
1	T	40	GLN
1	T	45	GLN
1	T	61	GLN
1	T	82	ASN
1	T	99	ASN
1	T	100	ASN
1	T	121	HIS
1	T	164	ASN
1	T	181	GLN
1	T	194	GLN
1	U	28	GLN
1	U	30	GLN
1	U	37	GLN
1	U	40	GLN
1	U	45	GLN
1	U	61	GLN
1	U	82	ASN
1	U	90	GLN
1	U	99	ASN
1	U	100	ASN
1	U	121	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	U	164	ASN
1	U	181	GLN
1	U	194	GLN
1	V	28	GLN
1	V	30	GLN
1	V	37	GLN
1	V	40	GLN
1	V	45	GLN
1	V	61	GLN
1	V	82	ASN
1	V	90	GLN
1	V	99	ASN
1	V	100	ASN
1	V	121	HIS
1	V	164	ASN
1	V	194	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	186/209 (88%)	-0.16	7 (3%)	40	39	19, 37, 80, 95	0
1	B	186/209 (88%)	-0.16	13 (6%)	16	14	14, 32, 84, 98	0
1	C	186/209 (88%)	-0.15	9 (4%)	30	28	16, 35, 82, 101	0
1	D	186/209 (88%)	0.04	13 (6%)	16	14	22, 46, 91, 105	0
1	E	186/209 (88%)	0.28	13 (6%)	16	14	32, 58, 98, 108	0
1	F	186/209 (88%)	0.61	25 (13%)	3	2	39, 67, 102, 116	0
1	G	186/209 (88%)	0.55	20 (10%)	5	4	45, 73, 105, 118	0
1	H	186/209 (88%)	0.69	30 (16%)	1	1	42, 74, 103, 120	0
1	I	186/209 (88%)	0.51	21 (11%)	5	4	41, 69, 107, 116	0
1	J	186/209 (88%)	0.31	14 (7%)	14	12	33, 61, 101, 108	0
1	K	186/209 (88%)	0.14	13 (6%)	16	14	25, 48, 96, 105	0
1	L	186/209 (88%)	-0.18	9 (4%)	30	28	18, 37, 85, 97	0
1	M	186/209 (88%)	-0.10	9 (4%)	30	28	16, 35, 81, 94	0
1	N	186/209 (88%)	-0.14	10 (5%)	25	24	19, 36, 82, 104	0
1	O	186/209 (88%)	-0.06	15 (8%)	12	10	18, 38, 91, 100	0
1	P	186/209 (88%)	0.02	12 (6%)	18	17	21, 44, 91, 100	0
1	Q	186/209 (88%)	0.08	14 (7%)	14	12	23, 45, 95, 111	0
1	R	186/209 (88%)	0.01	14 (7%)	14	12	22, 43, 93, 100	0
1	S	186/209 (88%)	0.04	14 (7%)	14	12	21, 42, 91, 107	0
1	T	186/209 (88%)	0.07	13 (6%)	16	14	22, 46, 95, 109	0
1	U	186/209 (88%)	-0.07	9 (4%)	30	28	21, 46, 89, 106	0
1	V	186/209 (88%)	-0.08	12 (6%)	18	17	20, 42, 86, 98	0
All	All	4092/4598 (88%)	0.10	309 (7%)	13	12	14, 49, 95, 120	0

All (309) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	58	GLY	7.3
1	Q	209	ARG	6.7
1	I	209	ARG	6.6
1	H	208	CYS	6.4
1	M	58	GLY	6.2
1	C	57	ALA	6.1
1	N	58	GLY	6.1
1	E	180	ARG	6.0
1	F	209	ARG	5.5
1	I	60	GLY	5.5
1	L	209	ARG	5.3
1	T	180	ARG	5.3
1	C	61	GLN	5.2
1	F	60	GLY	5.2
1	F	56	MET	5.2
1	J	57	ALA	5.2
1	J	58	GLY	5.1
1	T	179	PRO	5.1
1	S	209	ARG	5.1
1	A	58	GLY	5.0
1	R	58	GLY	5.0
1	F	58	GLY	4.9
1	G	59	GLY	4.9
1	P	209	ARG	4.9
1	L	60	GLY	4.9
1	O	60	GLY	4.9
1	K	182	LEU	4.8
1	D	209	ARG	4.8
1	F	180	ARG	4.7
1	J	181	GLN	4.7
1	G	56	MET	4.7
1	B	209	ARG	4.7
1	B	180	ARG	4.6
1	Q	208	CYS	4.5
1	J	209	ARG	4.5
1	H	183	PRO	4.4
1	K	180	ARG	4.4
1	G	209	ARG	4.4
1	B	57	ALA	4.4
1	K	183	PRO	4.4
1	T	209	ARG	4.3
1	N	61	GLN	4.3
1	H	58	GLY	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	57	ALA	4.2
1	R	57	ALA	4.2
1	R	184	LEU	4.2
1	D	184	LEU	4.2
1	Q	61	GLN	4.1
1	Q	180	ARG	4.1
1	M	209	ARG	4.1
1	I	183	PRO	4.1
1	O	58	GLY	4.0
1	A	61	GLN	4.0
1	I	61	GLN	4.0
1	H	209	ARG	4.0
1	J	180	ARG	3.9
1	U	180	ARG	3.9
1	B	60	GLY	3.9
1	C	58	GLY	3.9
1	Q	57	ALA	3.9
1	J	56	MET	3.9
1	U	209	ARG	3.9
1	H	56	MET	3.9
1	M	57	ALA	3.8
1	H	207	SER	3.8
1	Q	58	GLY	3.8
1	K	61	GLN	3.8
1	S	61	GLN	3.8
1	V	208	CYS	3.8
1	M	180	ARG	3.8
1	O	185	GLU	3.8
1	C	60	GLY	3.7
1	I	59	GLY	3.7
1	K	58	GLY	3.7
1	S	58	GLY	3.7
1	I	56	MET	3.7
1	B	58	GLY	3.7
1	P	181	GLN	3.7
1	J	60	GLY	3.6
1	C	56	MET	3.6
1	O	100	ASN	3.6
1	H	60	GLY	3.6
1	G	58	GLY	3.6
1	G	184	LEU	3.6
1	I	64	CYS	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	59	GLY	3.5
1	T	184	LEU	3.5
1	I	180	ARG	3.5
1	C	59	GLY	3.5
1	P	59	GLY	3.5
1	Q	59	GLY	3.5
1	P	24	LEU	3.5
1	O	59	GLY	3.4
1	T	182	LEU	3.4
1	A	59	GLY	3.4
1	I	62	LYS	3.4
1	H	61	GLN	3.4
1	H	191	ALA	3.4
1	G	61	GLN	3.4
1	E	61	GLN	3.4
1	V	59	GLY	3.4
1	A	180	ARG	3.4
1	E	209	ARG	3.3
1	G	57	ALA	3.3
1	T	205	TYR	3.3
1	R	60	GLY	3.3
1	R	180	ARG	3.3
1	O	182	LEU	3.3
1	F	102	LYS	3.3
1	I	184	LEU	3.3
1	R	209	ARG	3.3
1	D	58	GLY	3.3
1	M	181	GLN	3.3
1	O	56	MET	3.3
1	G	182	LEU	3.2
1	Q	184	LEU	3.2
1	D	180	ARG	3.2
1	S	180	ARG	3.2
1	H	181	GLN	3.2
1	I	57	ALA	3.2
1	S	57	ALA	3.2
1	H	24	LEU	3.2
1	I	58	GLY	3.2
1	O	180	ARG	3.2
1	F	183	PRO	3.2
1	J	182	LEU	3.1
1	O	179	PRO	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	R	61	GLN	3.1
1	G	60	GLY	3.1
1	V	209	ARG	3.1
1	K	209	ARG	3.1
1	G	179	PRO	3.1
1	F	57	ALA	3.1
1	K	57	ALA	3.1
1	T	207	SER	3.1
1	E	181	GLN	3.0
1	R	183	PRO	3.0
1	T	183	PRO	3.0
1	G	99	ASN	3.0
1	R	179	PRO	3.0
1	G	205	TYR	3.0
1	H	182	LEU	3.0
1	E	179	PRO	3.0
1	N	60	GLY	3.0
1	B	99	ASN	3.0
1	C	62	LYS	3.0
1	Q	60	GLY	3.0
1	A	56	MET	3.0
1	F	188	LEU	3.0
1	A	209	ARG	3.0
1	F	208	CYS	3.0
1	U	181	GLN	2.9
1	O	184	LEU	2.9
1	K	56	MET	2.9
1	V	57	ALA	2.9
1	H	190	LYS	2.9
1	B	184	LEU	2.9
1	G	24	LEU	2.9
1	Q	181	GLN	2.9
1	P	184	LEU	2.9
1	U	184	LEU	2.9
1	P	60	GLY	2.9
1	V	58	GLY	2.9
1	F	62	LYS	2.9
1	F	99	ASN	2.9
1	J	183	PRO	2.9
1	E	56	MET	2.8
1	T	208	CYS	2.8
1	U	182	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	104	TYR	2.8
1	O	209	ARG	2.8
1	B	56	MET	2.8
1	F	59	GLY	2.8
1	J	61	GLN	2.8
1	I	189	THR	2.8
1	R	56	MET	2.8
1	E	205	TYR	2.8
1	H	64	CYS	2.8
1	V	60	GLY	2.8
1	S	60	GLY	2.8
1	O	61	GLN	2.8
1	H	205	TYR	2.8
1	M	182	LEU	2.8
1	V	24	LEU	2.8
1	K	60	GLY	2.8
1	H	57	ALA	2.7
1	I	181	GLN	2.7
1	K	59	GLY	2.7
1	H	48	GLY	2.7
1	D	205	TYR	2.7
1	F	205	TYR	2.7
1	D	183	PRO	2.7
1	F	133	LYS	2.7
1	Q	207	SER	2.7
1	C	209	ARG	2.7
1	V	180	ARG	2.7
1	N	209	ARG	2.7
1	L	99	ASN	2.7
1	A	57	ALA	2.6
1	B	100	ASN	2.6
1	E	182	LEU	2.6
1	L	184	LEU	2.6
1	E	60	GLY	2.6
1	Q	205	TYR	2.6
1	F	179	PRO	2.6
1	G	181	GLN	2.6
1	N	57	ALA	2.6
1	Q	179	PRO	2.6
1	K	184	LEU	2.6
1	G	48	GLY	2.6
1	F	193	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	104	TYR	2.6
1	L	208	CYS	2.6
1	H	99	ASN	2.5
1	I	176	ASN	2.5
1	R	182	LEU	2.5
1	G	191	ALA	2.5
1	F	24	LEU	2.5
1	H	59	GLY	2.5
1	F	61	GLN	2.5
1	G	180	ARG	2.5
1	E	57	ALA	2.5
1	P	61	GLN	2.5
1	P	56	MET	2.5
1	N	99	ASN	2.5
1	F	181	GLN	2.5
1	E	177	LYS	2.5
1	S	24	LEU	2.5
1	H	179	PRO	2.4
1	B	182	LEU	2.4
1	D	99	ASN	2.4
1	I	99	ASN	2.4
1	B	59	GLY	2.4
1	H	175	LEU	2.4
1	P	182	LEU	2.4
1	P	99	ASN	2.4
1	H	55	ARG	2.4
1	B	61	GLN	2.4
1	H	184	LEU	2.4
1	L	57	ALA	2.3
1	U	58	GLY	2.3
1	S	56	MET	2.3
1	I	205	TYR	2.3
1	F	172	LEU	2.3
1	E	178	LEU	2.3
1	J	188	LEU	2.3
1	Q	24	LEU	2.3
1	F	189	THR	2.3
1	G	103	PHE	2.3
1	B	208	CYS	2.3
1	D	182	LEU	2.3
1	U	57	ALA	2.3
1	H	186	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	T	173	ARG	2.3
1	U	183	PRO	2.3
1	K	99	ASN	2.3
1	H	177	LYS	2.3
1	H	187	ASP	2.3
1	D	24	LEU	2.3
1	F	207	SER	2.3
1	I	182	LEU	2.3
1	N	185	GLU	2.3
1	G	131	GLY	2.2
1	S	179	PRO	2.2
1	L	180	ARG	2.2
1	V	61	GLN	2.2
1	I	175	LEU	2.2
1	O	183	PRO	2.2
1	V	184	LEU	2.2
1	M	99	ASN	2.2
1	S	208	CYS	2.2
1	C	24	LEU	2.2
1	S	178	LEU	2.2
1	L	56	MET	2.2
1	L	61	GLN	2.2
1	I	24	LEU	2.2
1	T	57	ALA	2.2
1	I	185	GLU	2.2
1	J	59	GLY	2.2
1	M	60	GLY	2.2
1	N	205	TYR	2.2
1	R	185	GLU	2.2
1	P	57	ALA	2.2
1	H	100	ASN	2.1
1	F	190	LYS	2.1
1	M	61	GLN	2.1
1	R	181	GLN	2.1
1	G	190	LYS	2.1
1	S	62	LYS	2.1
1	T	189	THR	2.1
1	H	133	LYS	2.1
1	J	186	VAL	2.1
1	D	177	LYS	2.1
1	S	205	TYR	2.1
1	D	57	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	S	59	GLY	2.1
1	N	62	LYS	2.0
1	O	181	GLN	2.0
1	D	207	SER	2.0
1	K	189	THR	2.0
1	T	56	MET	2.0
1	V	182	LEU	2.0
1	D	176	ASN	2.0
1	V	56	MET	2.0
1	R	24	LEU	2.0
1	J	49	PRO	2.0
1	U	208	CYS	2.0
1	P	185	GLU	2.0
1	H	62	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.