



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 02:10 pm BST

PDB ID : 1W4C
Title : P4 protein from Bacteriophage PHI12 apo state
Authors : Mancini, E.J.; Kainov, D.E.; Grimes, J.M.; Tuma, R.; Bamford, D.H.; Stuart, D.I.
Deposited on : 2004-07-22
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
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

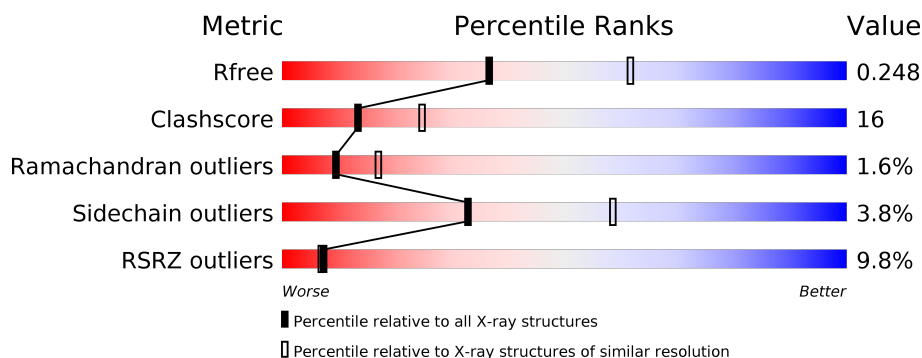
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



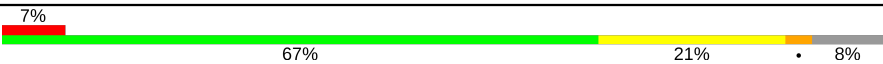

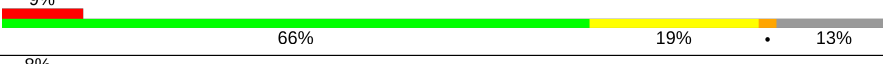

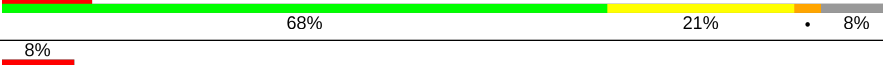

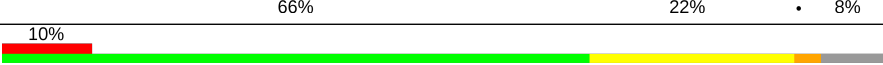



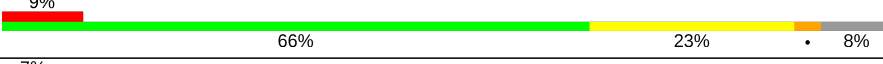







Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	331	
1	B	331	
1	C	331	
1	D	331	
1	E	331	
1	F	331	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	331	
1	H	331	
1	I	331	
1	J	331	
1	K	331	
1	L	331	
1	M	331	
1	N	331	
1	O	331	
1	P	331	
1	Q	331	
1	R	331	
1	S	331	
1	T	331	
1	U	331	
1	V	331	
1	W	331	
1	X	331	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 57270 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 NTPASE P4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			
1	B	304	Total	C	N	O	S	0	0	0
			2288	1434	399	448	7			
1	C	304	Total	C	N	O	S	0	0	0
			2288	1433	399	449	7			
1	D	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			
1	E	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	F	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	G	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	H	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			
1	I	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			
1	J	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	K	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	L	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			
1	M	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	N	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	O	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	P	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	R	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	S	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	T	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	U	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			
1	V	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	W	304	Total	C	N	O	S	0	0	0
			2289	1434	399	449	7			
1	X	289	Total	C	N	O	S	0	0	1
			2171	1361	379	424	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	110	Total	O	0	0
			110	110		
2	B	119	Total	O	0	0
			119	119		
2	C	129	Total	O	0	0
			129	129		
2	D	145	Total	O	0	0
			145	145		
2	E	143	Total	O	0	0
			143	143		
2	F	151	Total	O	0	0
			151	151		
2	G	101	Total	O	0	0
			101	101		
2	H	178	Total	O	0	0
			178	178		
2	I	193	Total	O	0	0
			193	193		
2	J	159	Total	O	0	0
			159	159		
2	K	122	Total	O	0	0
			122	122		

Continued on next page...

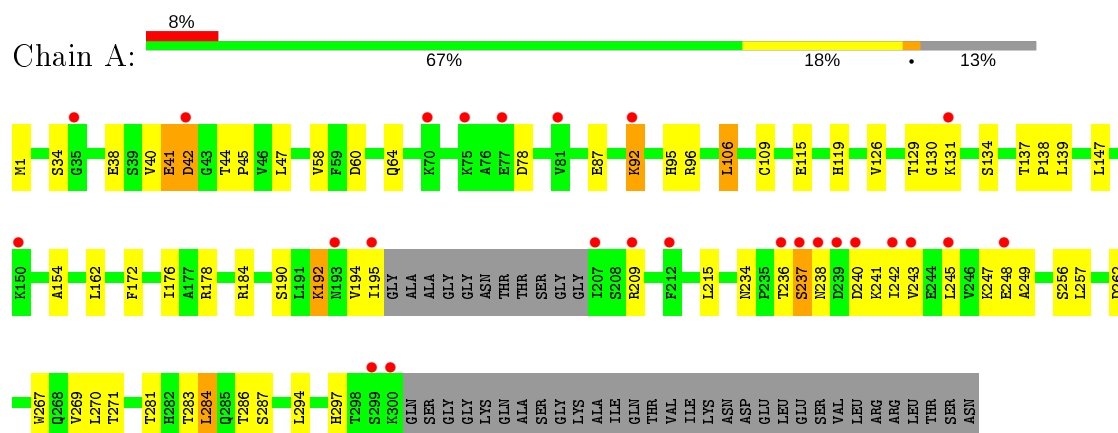
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	L	93	Total 93	O 93	0	0
2	M	169	Total 169	O 169	0	0
2	N	202	Total 202	O 202	0	0
2	O	144	Total 144	O 144	0	0
2	P	103	Total 103	O 103	0	0
2	Q	93	Total 93	O 93	0	0
2	R	110	Total 110	O 110	0	0
2	S	146	Total 146	O 146	0	0
2	T	88	Total 88	O 88	0	0
2	U	73	Total 73	O 73	0	0
2	V	118	Total 118	O 118	0	0
2	W	120	Total 120	O 120	0	0
2	X	153	Total 153	O 153	0	0

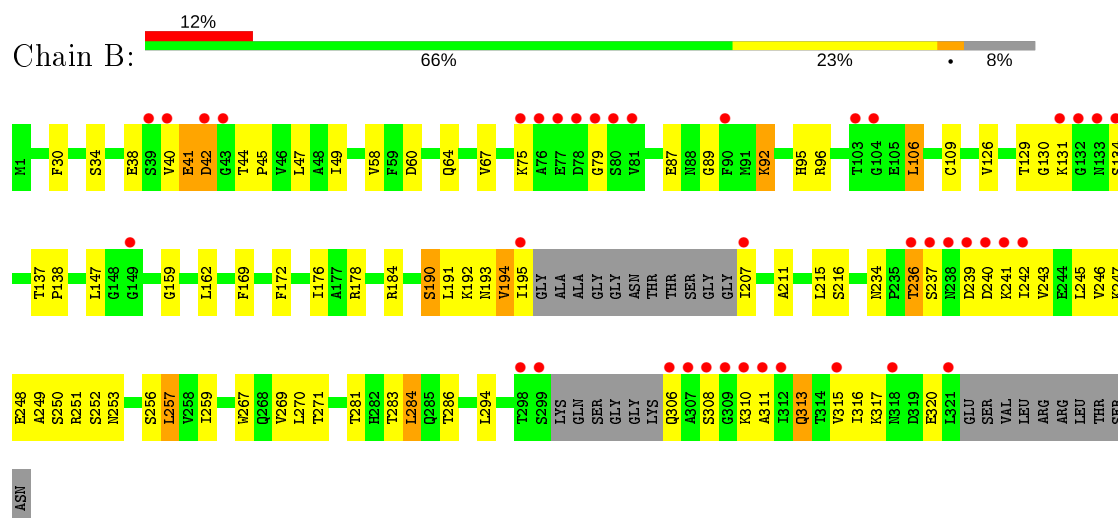
3 Residue-property plots [i](#)

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

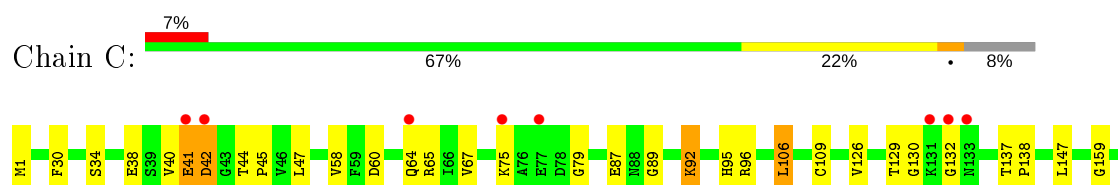
• Molecule 1: NTPASE P4

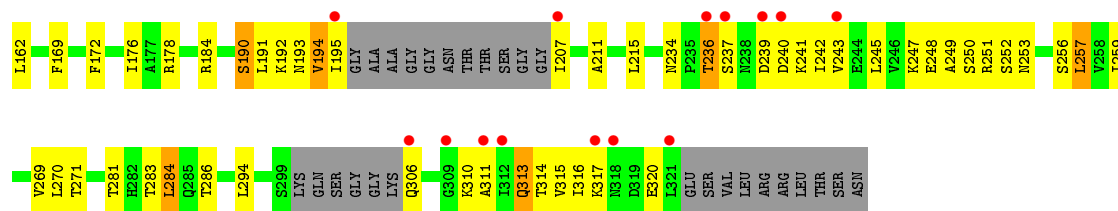


• Molecule 1: NTPASE P4

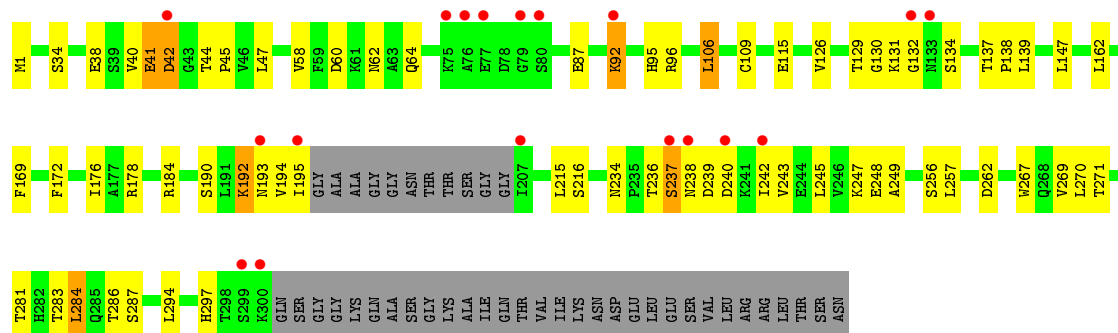


• Molecule 1: NTPASE P4

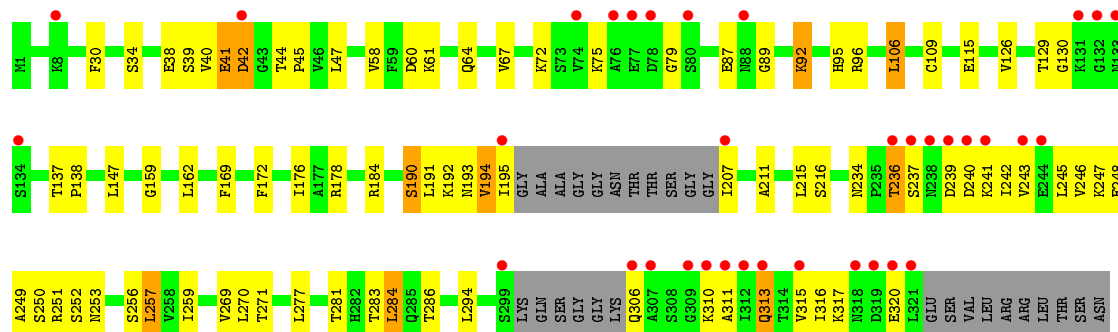




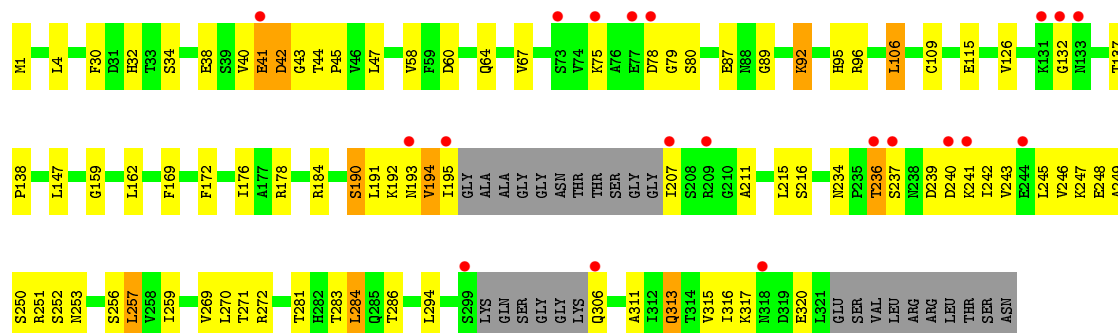
• Molecule 1: NTPASE P4



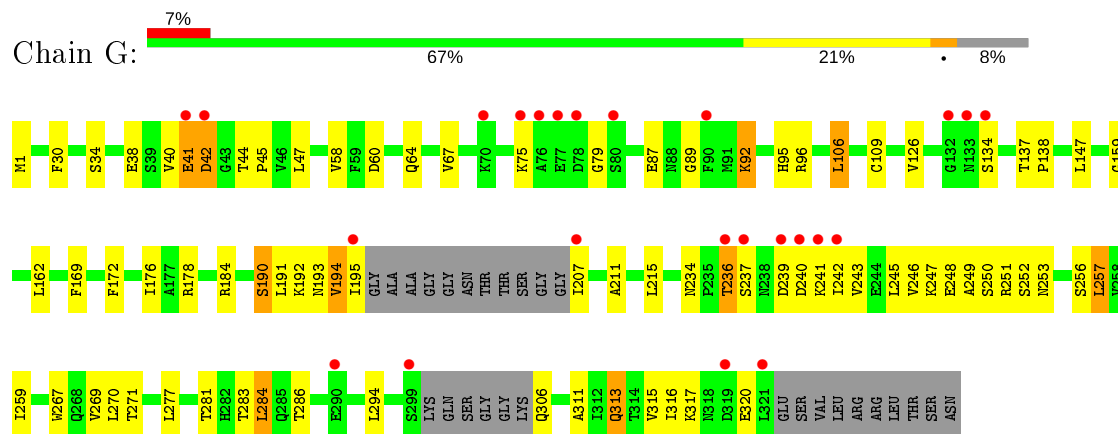
• Molecule 1: NTPASE P4



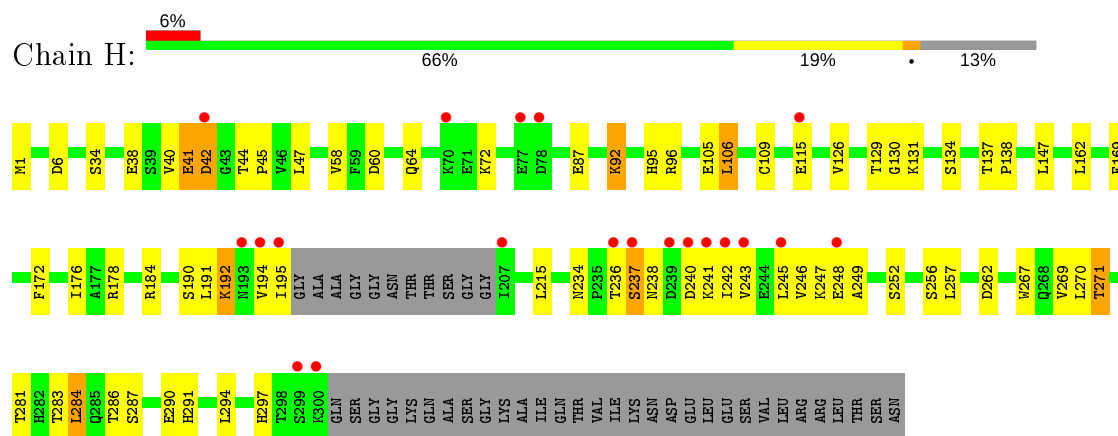
• Molecule 1: NTPASE P4



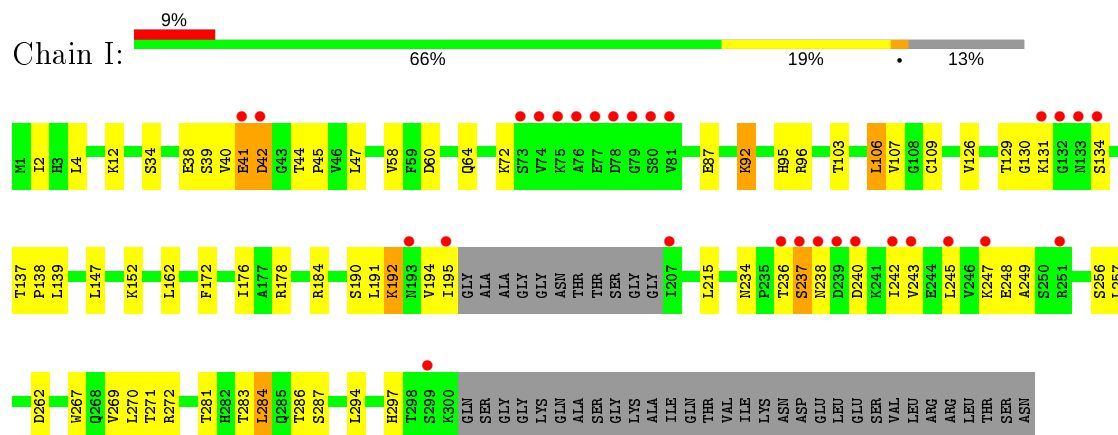
- Molecule 1: NTPASE P4



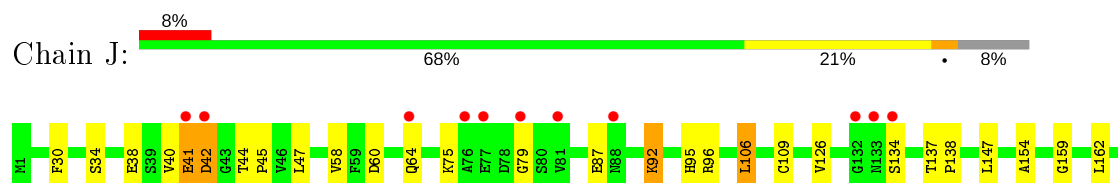
- Molecule 1: NTPASE P4

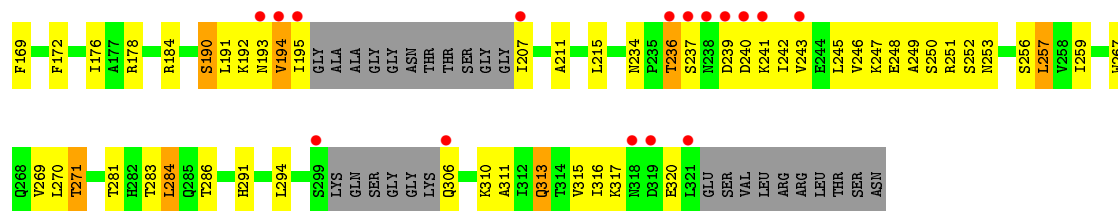


- Molecule 1: NTPASE P4

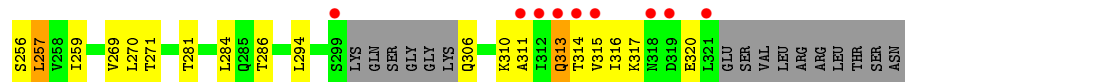
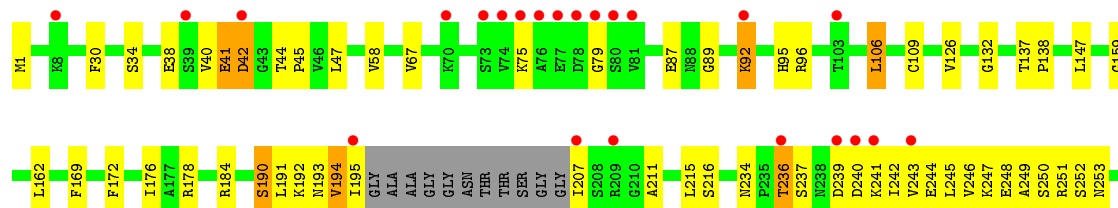


- Molecule 1: NTPASE P4

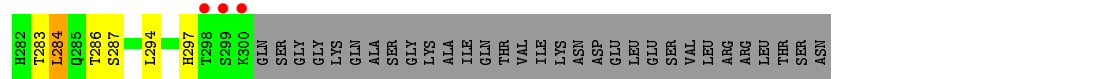
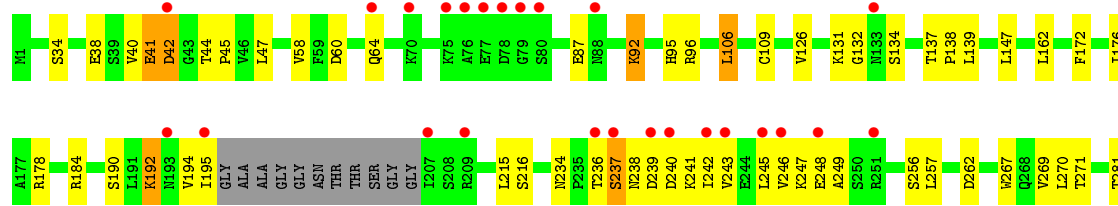




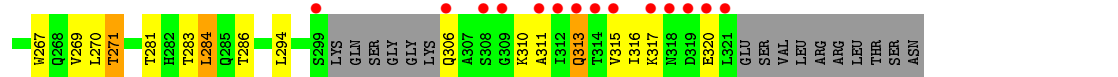
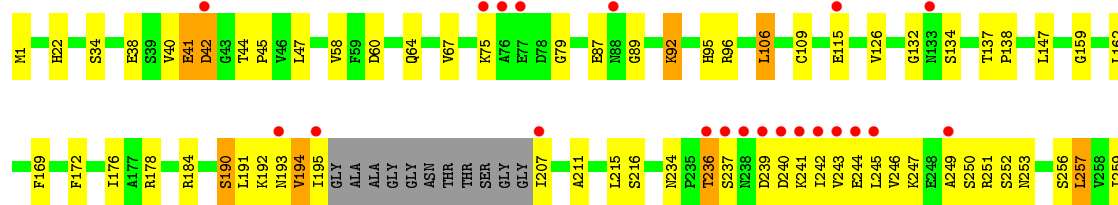
• Molecule 1: NTPASE P4



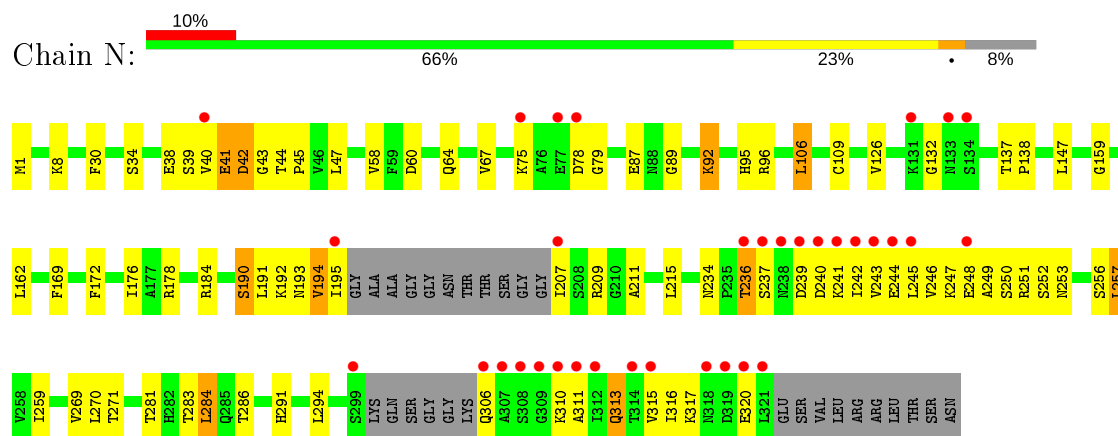
• Molecule 1: NTPASE P4



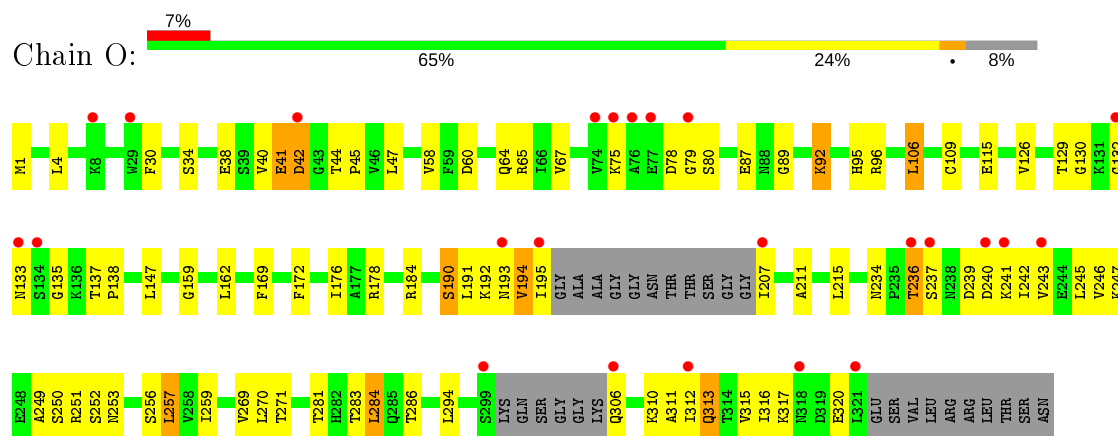
• Molecule 1: NTPASE P4



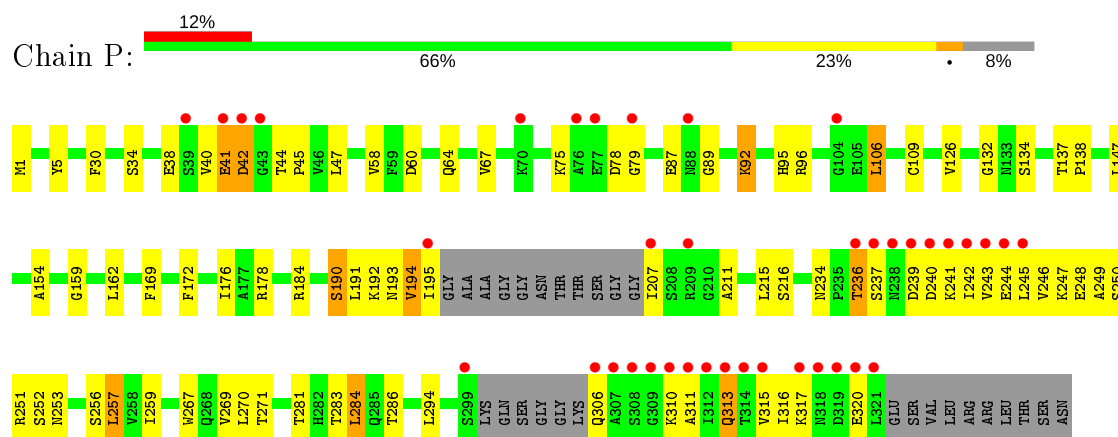
- Molecule 1: NTPASE P4



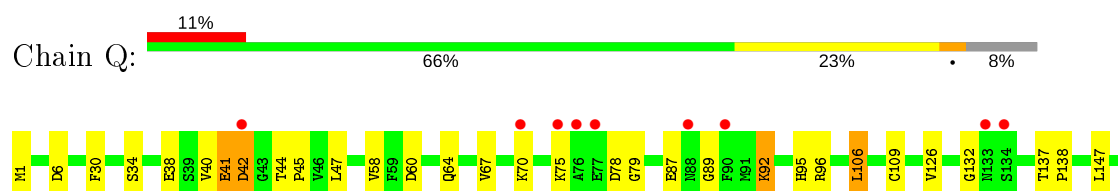
- Molecule 1: NTPASE P4

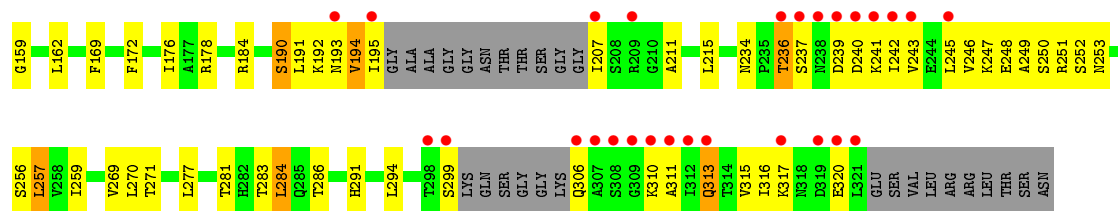


- Molecule 1: NTPASE P4

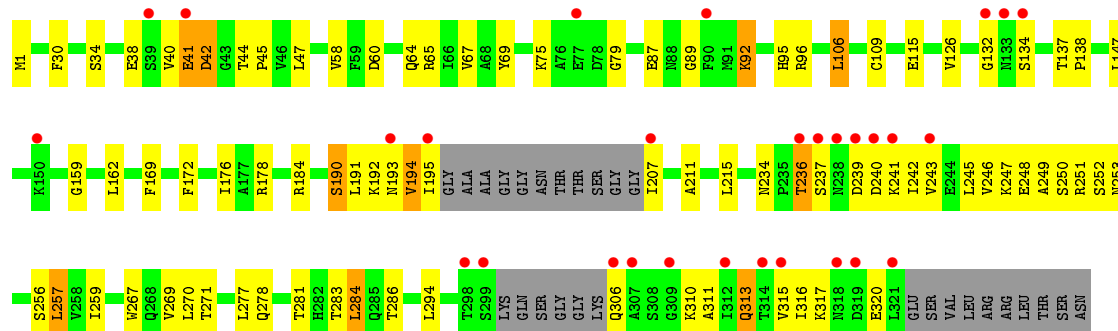


- Molecule 1: NTPASE P4

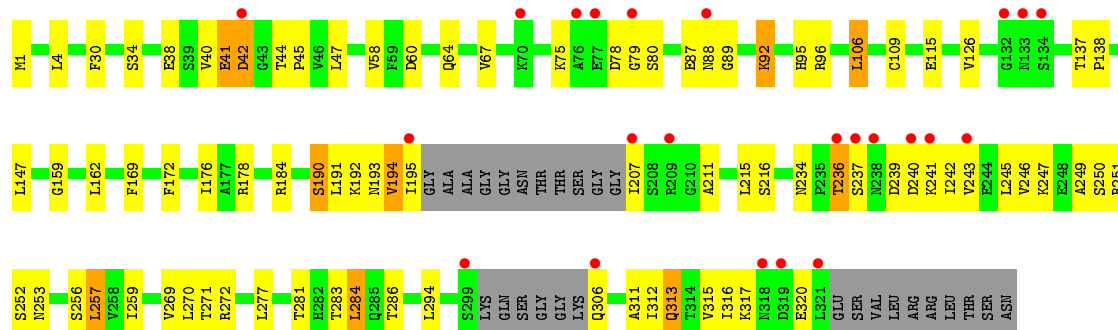




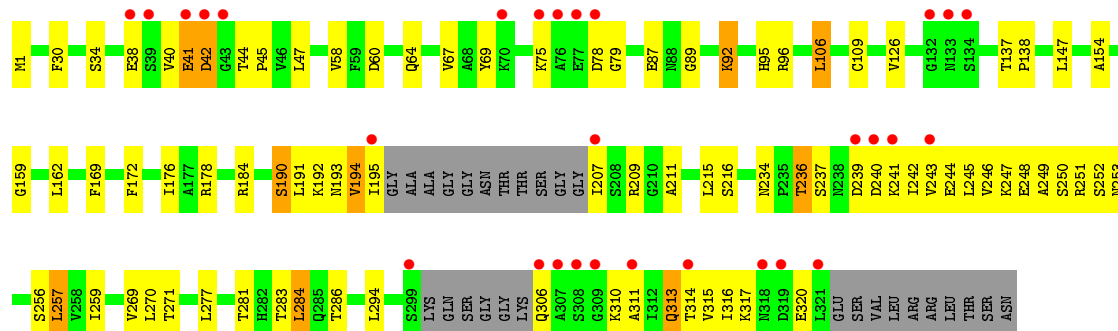
● Molecule 1: NTPASE P4



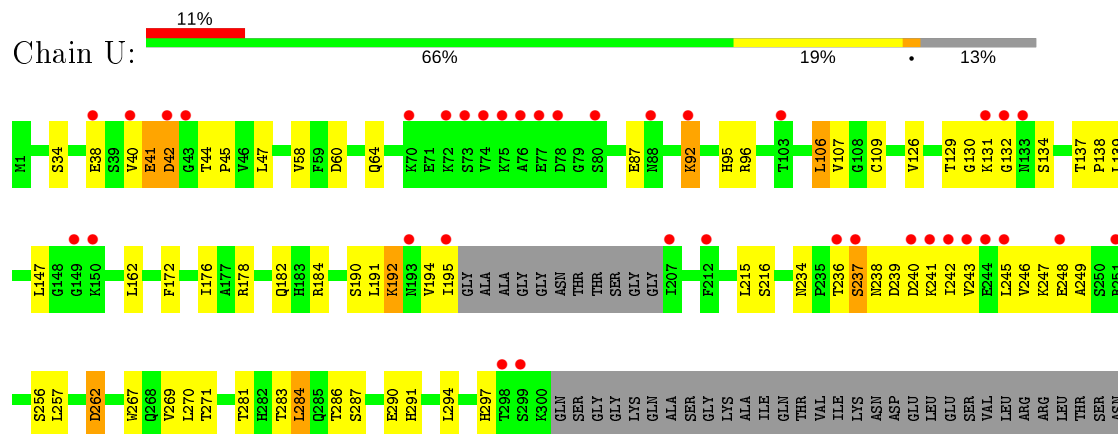
● Molecule 1: NTPASE P4



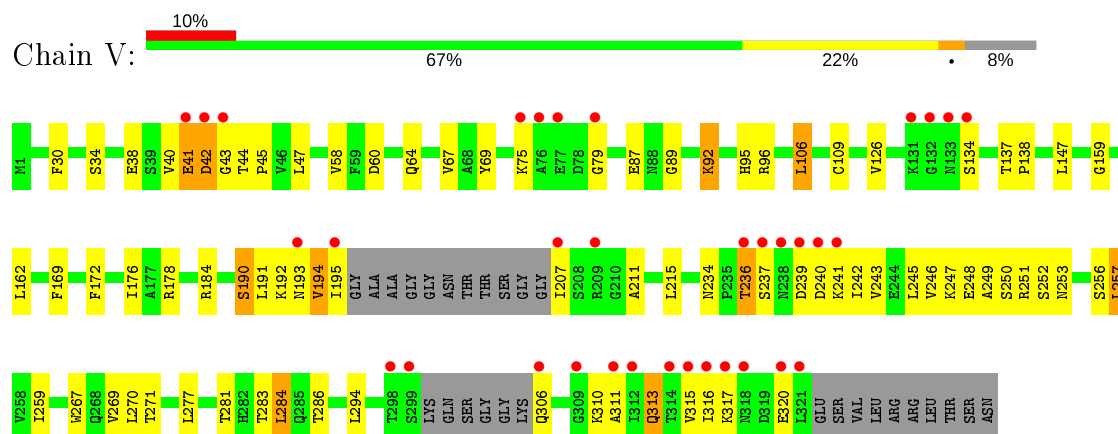
● Molecule 1: NTPASE P4



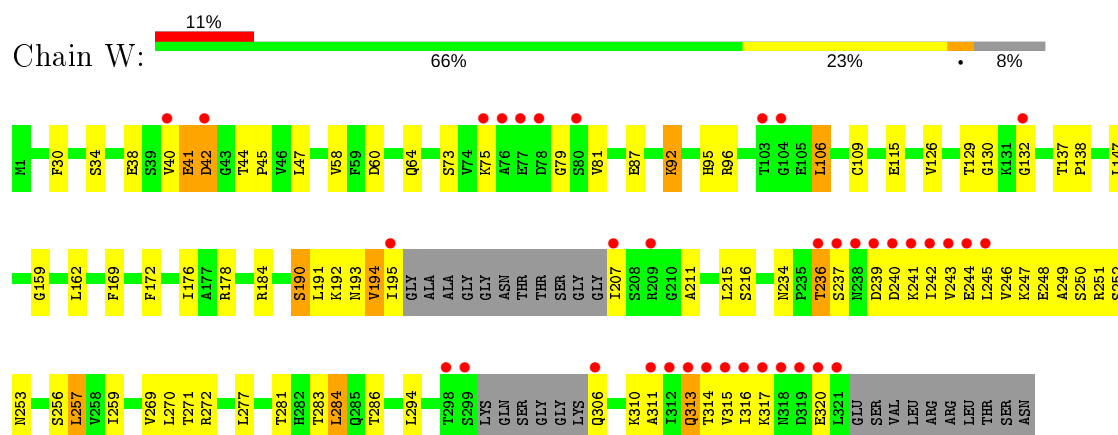
- Molecule 1: NTPASE P4



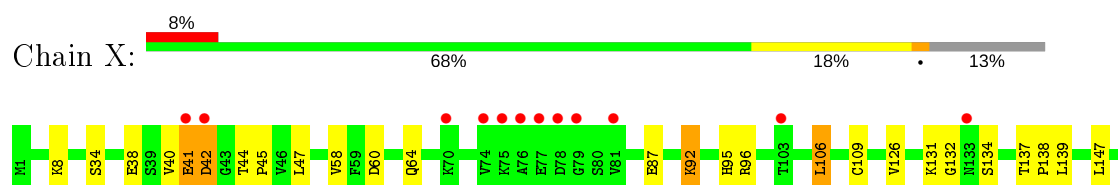
- Molecule 1: NTPASE P4

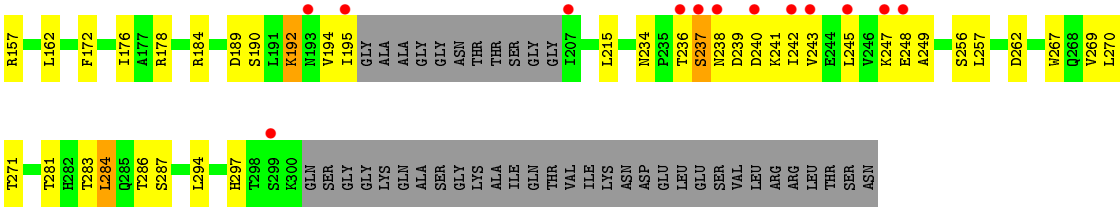


- Molecule 1: NTPASE P4



- Molecule 1: NTPASE P4





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	115.40Å 126.30Å 155.60Å 90.00° 91.60° 90.50°	Depositor
Resolution (Å)	20.00 – 2.50 20.01 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.0 (20.00-2.50) 95.9 (20.01-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 2.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.251 , 0.224 0.221 , 0.248	Depositor DCC
R_{free} test set	14484 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.004 for h,-k,-l 0.006 for -h,k,-l 0.001 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	57270	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.36	0/2208	0.66	0/2991
1	B	0.34	0/2324	0.65	0/3145
1	C	0.35	0/2323	0.64	0/3142
1	D	0.37	0/2208	0.65	0/2991
1	E	0.36	0/2325	0.65	0/3146
1	F	0.36	0/2325	0.65	0/3146
1	G	0.36	0/2325	0.64	0/3146
1	H	0.39	0/2208	0.66	0/2991
1	I	0.40	0/2208	0.67	0/2991
1	J	0.37	0/2325	0.65	0/3146
1	K	0.35	0/2325	0.65	0/3146
1	L	0.36	0/2208	0.66	0/2991
1	M	0.37	0/2325	0.65	0/3146
1	N	0.36	0/2325	0.65	0/3146
1	O	0.36	0/2325	0.64	0/3146
1	P	0.34	0/2325	0.65	0/3146
1	Q	0.35	0/2325	0.64	0/3146
1	R	0.35	0/2325	0.64	0/3146
1	S	0.36	0/2325	0.64	0/3146
1	T	0.35	0/2325	0.64	0/3146
1	U	0.36	0/2208	0.65	0/2991
1	V	0.35	0/2325	0.64	0/3146
1	W	0.35	0/2325	0.65	0/3146
1	X	0.38	0/2208	0.66	0/2991
All	All	0.36	0/54978	0.65	0/74414

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2171	0	2147	70	0
1	B	2288	0	2271	75	0
1	C	2288	0	2266	81	0
1	D	2171	0	2147	72	1
1	E	2289	0	2271	80	1
1	F	2289	0	2271	83	0
1	G	2289	0	2271	66	0
1	H	2171	0	2147	74	1
1	I	2171	0	2147	82	0
1	J	2289	0	2271	66	0
1	K	2289	0	2271	78	0
1	L	2171	0	2147	69	0
1	M	2289	0	2271	98	0
1	N	2289	0	2271	90	1
1	O	2289	0	2271	91	0
1	P	2289	0	2271	90	0
1	Q	2289	0	2271	88	0
1	R	2289	0	2271	86	0
1	S	2289	0	2271	78	0
1	T	2289	0	2271	82	0
1	U	2171	0	2147	80	0
1	V	2289	0	2271	76	0
1	W	2289	0	2271	89	1
1	X	2171	0	2147	76	1
2	A	110	0	0	6	0
2	B	119	0	0	5	0
2	C	129	0	0	3	0
2	D	145	0	0	4	0
2	E	143	0	0	11	0
2	F	151	0	0	9	0
2	G	101	0	0	1	0
2	H	178	0	0	9	0
2	I	193	0	0	11	0
2	J	159	0	0	2	0
2	K	122	0	0	2	0
2	L	93	0	0	4	0
2	M	169	0	0	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	202	0	0	5	0
2	O	144	0	0	6	0
2	P	103	0	0	8	0
2	Q	93	0	0	6	0
2	R	110	0	0	3	0
2	S	146	0	0	8	0
2	T	88	0	0	4	0
2	U	73	0	0	7	0
2	V	118	0	0	5	0
2	W	120	0	0	7	0
2	X	153	0	0	6	0
All	All	57270	0	53631	1731	3

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 16.

All (1731) 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:I:39:SER:HA	1:M:115:GLU:OE2	1.15	1.28
1:I:39:SER:HA	1:M:115:GLU:CD	1.56	1.26
1:S:251:ARG:HD2	1:T:236:THR:HG23	1.27	1.15
1:T:251:ARG:HD2	1:U:236:THR:HG23	1.15	1.13
1:K:251:ARG:HD2	1:L:236:THR:HG23	1.14	1.13
1:G:251:ARG:HD2	1:H:236:THR:HG23	1.30	1.10
1:M:237:SER:HB3	1:M:242:ILE:HD11	1.34	1.09
1:O:237:SER:HB3	1:O:242:ILE:HD11	1.34	1.09
1:B:251:ARG:HD2	1:C:236:THR:HG23	1.26	1.09
1:M:236:THR:HG23	1:R:251:ARG:HD2	1.18	1.09
1:S:237:SER:HB3	1:S:242:ILE:HD11	1.33	1.09
1:K:237:SER:HB3	1:K:242:ILE:HD11	1.34	1.08
1:C:237:SER:HB3	1:C:242:ILE:HD11	1.35	1.08
1:J:251:ARG:HD2	1:K:236:THR:HG23	1.35	1.08
1:Q:237:SER:HB3	1:Q:242:ILE:HD11	1.34	1.08
1:W:237:SER:HB3	1:W:242:ILE:HD11	1.34	1.08
1:E:237:SER:HB3	1:E:242:ILE:HD11	1.35	1.08
1:V:251:ARG:HD2	1:W:236:THR:HG23	1.23	1.08
1:G:237:SER:HB3	1:G:242:ILE:HD11	1.35	1.07
1:B:237:SER:HB3	1:B:242:ILE:HD11	1.36	1.07
1:O:251:ARG:HD2	1:P:236:THR:HG23	1.30	1.07
1:J:237:SER:HB3	1:J:242:ILE:HD11	1.34	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:251:ARG:HD2	1:N:236:THR:CG2	1.84	1.06
1:C:251:ARG:HD2	1:D:236:THR:HG23	1.36	1.06
1:F:237:SER:HB3	1:F:242:ILE:HD11	1.33	1.06
1:W:251:ARG:HD2	1:X:236:THR:HG23	1.09	1.06
1:M:251:ARG:CD	1:N:236:THR:HG23	1.85	1.05
1:E:251:ARG:HD2	1:F:236:THR:HG23	1.10	1.05
1:V:237:SER:HB3	1:V:242:ILE:HD11	1.34	1.05
1:Q:251:ARG:HD2	1:R:236:THR:HG23	1.09	1.04
1:T:237:SER:HB3	1:T:242:ILE:HD11	1.34	1.04
1:N:237:SER:HB3	1:N:242:ILE:HD11	1.34	1.04
1:P:237:SER:HB3	1:P:242:ILE:HD11	1.34	1.04
1:M:115:GLU:HG2	2:M:2068:HOH:O	1.57	1.03
1:R:237:SER:HB3	1:R:242:ILE:HD11	1.34	1.03
1:I:39:SER:CA	1:M:115:GLU:OE2	2.09	1.00
1:A:236:THR:HG23	1:F:251:ARG:HD2	1.43	1.00
1:N:251:ARG:HD2	1:O:236:THR:HG23	1.02	0.99
1:P:247:LYS:HA	2:P:2103:HOH:O	1.62	0.99
1:P:251:ARG:HD2	1:Q:236:THR:CG2	1.92	0.99
1:P:251:ARG:HD2	1:Q:236:THR:HG23	1.00	0.99
1:P:251:ARG:CD	1:Q:236:THR:HG23	1.93	0.98
1:M:251:ARG:HD2	1:N:236:THR:HG23	0.96	0.95
1:N:251:ARG:HD2	1:O:236:THR:CG2	1.96	0.95
1:E:251:ARG:HD2	1:F:236:THR:CG2	1.98	0.94
1:E:251:ARG:CD	1:F:236:THR:HG23	1.98	0.93
1:N:251:ARG:CD	1:O:236:THR:HG23	1.97	0.92
1:W:251:ARG:HD2	1:X:236:THR:CG2	2.01	0.89
1:I:39:SER:CA	1:M:115:GLU:CD	2.41	0.89
1:W:251:ARG:CD	1:X:236:THR:HG23	2.01	0.89
1:P:250:SER:HB2	2:P:2103:HOH:O	1.73	0.88
1:O:195:ILE:HD11	1:O:215:LEU:HD13	1.57	0.87
1:Q:195:ILE:HD11	1:Q:215:LEU:HD13	1.57	0.86
1:I:39:SER:CA	1:M:115:GLU:OE1	2.23	0.86
1:J:195:ILE:HD11	1:J:215:LEU:HD13	1.58	0.86
1:I:41:GLU:HG2	2:M:2024:HOH:O	1.75	0.86
1:B:195:ILE:HD11	1:B:215:LEU:HD13	1.58	0.85
1:F:195:ILE:HD11	1:F:215:LEU:HD13	1.57	0.85
1:P:195:ILE:HD11	1:P:215:LEU:HD13	1.59	0.85
1:V:195:ILE:HD11	1:V:215:LEU:HD13	1.58	0.85
1:W:81:VAL:HB	2:W:2032:HOH:O	1.76	0.85
1:Q:251:ARG:HD2	1:R:236:THR:CG2	2.02	0.85
1:R:195:ILE:HD11	1:R:215:LEU:HD13	1.58	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:CA	1:C:1:MET:CG	2.55	0.84
1:N:310:LYS:HE3	2:O:2066:HOH:O	1.77	0.84
1:I:131:LYS:HB2	1:I:243:VAL:HG11	1.60	0.84
1:E:195:ILE:HD11	1:E:215:LEU:HD13	1.57	0.84
1:N:195:ILE:HD11	1:N:215:LEU:HD13	1.60	0.84
1:W:195:ILE:HD11	1:W:215:LEU:HD13	1.59	0.84
1:S:251:ARG:HD2	1:T:236:THR:CG2	2.07	0.83
1:K:251:ARG:HD2	1:L:236:THR:CG2	2.04	0.83
1:D:131:LYS:HB2	1:D:243:VAL:HG11	1.60	0.83
1:G:195:ILE:HD11	1:G:215:LEU:HD13	1.58	0.83
1:H:131:LYS:HB2	1:H:243:VAL:HG11	1.60	0.83
1:K:251:ARG:CD	1:L:236:THR:HG23	2.04	0.83
1:X:131:LYS:HB2	1:X:243:VAL:HG11	1.60	0.83
1:S:195:ILE:HD11	1:S:215:LEU:HD13	1.59	0.83
1:T:195:ILE:HD11	1:T:215:LEU:HD13	1.60	0.83
1:K:195:ILE:HD11	1:K:215:LEU:HD13	1.59	0.83
1:M:236:THR:CG2	1:R:251:ARG:HD2	2.07	0.83
1:I:39:SER:CB	1:M:115:GLU:OE1	2.28	0.82
1:L:131:LYS:HB2	1:L:243:VAL:HG11	1.60	0.82
1:A:194:VAL:HG22	1:A:195:ILE:HG13	1.61	0.82
1:C:195:ILE:HD11	1:C:215:LEU:HD13	1.58	0.82
1:M:195:ILE:HD11	1:M:215:LEU:HD13	1.60	0.82
1:D:194:VAL:HG22	1:D:195:ILE:HG13	1.62	0.81
1:S:251:ARG:CD	1:T:236:THR:HG23	2.08	0.81
1:X:194:VAL:HG22	1:X:195:ILE:HG13	1.62	0.81
1:A:131:LYS:HB2	1:A:243:VAL:HG11	1.60	0.81
1:H:194:VAL:HG22	1:H:195:ILE:HG13	1.62	0.80
1:T:251:ARG:CD	1:U:236:THR:HG23	2.05	0.80
1:U:131:LYS:HB2	1:U:243:VAL:HG11	1.60	0.80
1:I:194:VAL:HG22	1:I:195:ILE:HG13	1.63	0.80
1:C:194:VAL:HG22	1:C:195:ILE:HG13	1.64	0.80
1:J:92:LYS:HA	1:J:92:LYS:HE3	1.64	0.80
1:S:92:LYS:HE3	1:S:92:LYS:HA	1.64	0.80
1:I:39:SER:HA	1:M:115:GLU:OE1	1.82	0.80
1:U:194:VAL:HG22	1:U:195:ILE:HG13	1.62	0.79
1:N:92:LYS:HE3	1:N:92:LYS:HA	1.65	0.79
1:T:251:ARG:HD2	1:U:236:THR:CG2	2.05	0.79
1:F:194:VAL:HG22	1:F:195:ILE:HG13	1.65	0.79
1:M:194:VAL:HG22	1:M:195:ILE:HG13	1.64	0.79
1:N:194:VAL:HG22	1:N:195:ILE:HG13	1.65	0.79
1:T:92:LYS:HA	1:T:92:LYS:HE3	1.65	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:LYS:HE3	1:E:92:LYS:HA	1.65	0.79
1:W:92:LYS:HA	1:W:92:LYS:HE3	1.65	0.79
1:F:92:LYS:HE3	1:F:92:LYS:HA	1.65	0.78
1:O:92:LYS:HE3	1:O:92:LYS:HA	1.65	0.78
1:P:194:VAL:HG22	1:P:195:ILE:HG13	1.65	0.78
1:P:92:LYS:HE3	1:P:92:LYS:HA	1.65	0.78
1:M:92:LYS:HA	1:M:92:LYS:HE3	1.65	0.78
1:K:194:VAL:HG22	1:K:195:ILE:HG13	1.65	0.78
1:L:194:VAL:HG22	1:L:195:ILE:HG13	1.62	0.78
1:T:194:VAL:HG22	1:T:195:ILE:HG13	1.65	0.78
1:J:194:VAL:HG22	1:J:195:ILE:HG13	1.66	0.78
1:N:251:ARG:HH11	1:O:236:THR:HG22	1.48	0.78
1:V:194:VAL:HG22	1:V:195:ILE:HG13	1.66	0.78
1:G:92:LYS:HE3	1:G:92:LYS:HA	1.65	0.78
1:Q:251:ARG:CD	1:R:236:THR:HG23	2.02	0.78
1:W:194:VAL:HG22	1:W:195:ILE:HG13	1.65	0.78
1:Q:92:LYS:HE3	1:Q:92:LYS:HA	1.66	0.78
1:V:92:LYS:HE3	1:V:92:LYS:HA	1.66	0.78
1:B:194:VAL:HG22	1:B:195:ILE:HG13	1.66	0.78
1:C:92:LYS:HA	1:C:92:LYS:HE3	1.65	0.78
1:G:194:VAL:HG22	1:G:195:ILE:HG13	1.66	0.78
1:R:194:VAL:HG22	1:R:195:ILE:HG13	1.65	0.77
1:R:92:LYS:HE3	1:R:92:LYS:HA	1.66	0.77
1:O:194:VAL:HG22	1:O:195:ILE:HG13	1.65	0.77
1:Q:194:VAL:HG22	1:Q:195:ILE:HG13	1.65	0.77
1:X:157:ARG:HA	2:X:2102:HOH:O	1.82	0.77
1:B:92:LYS:HE3	1:B:92:LYS:HA	1.65	0.77
1:E:194:VAL:HG22	1:E:195:ILE:HG13	1.66	0.77
1:S:194:VAL:HG22	1:S:195:ILE:HG13	1.65	0.77
1:O:135:GLY:HA2	2:O:2066:HOH:O	1.85	0.77
1:N:251:ARG:HH11	1:O:236:THR:CG2	1.99	0.76
1:K:92:LYS:HA	1:K:92:LYS:HE3	1.66	0.76
1:M:236:THR:HG23	1:R:251:ARG:CD	2.08	0.75
1:R:191:LEU:O	1:R:194:VAL:HG13	1.85	0.75
1:I:39:SER:HB3	1:M:115:GLU:OE1	1.86	0.75
1:F:259:ILE:HD13	1:F:316:ILE:HG23	1.69	0.75
1:W:248:GLU:OE1	1:X:236:THR:HG22	1.88	0.74
1:P:251:ARG:HH11	1:Q:236:THR:HG22	1.53	0.74
1:K:259:ILE:HD13	1:K:316:ILE:HG23	1.70	0.74
1:B:259:ILE:HD13	1:B:316:ILE:HG23	1.70	0.74
1:E:259:ILE:HD13	1:E:316:ILE:HG23	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:191:LEU:O	1:P:194:VAL:HG13	1.88	0.74
1:G:259:ILE:HD13	1:G:316:ILE:HG23	1.69	0.74
1:N:310:LYS:HD2	1:O:132:GLY:O	1.86	0.74
1:S:259:ILE:HD13	1:S:316:ILE:HG23	1.69	0.74
1:F:191:LEU:O	1:F:194:VAL:HG13	1.88	0.73
1:N:259:ILE:HD13	1:N:316:ILE:HG23	1.70	0.73
1:C:259:ILE:HD13	1:C:316:ILE:HG23	1.70	0.73
1:G:191:LEU:O	1:G:194:VAL:HG13	1.89	0.73
1:R:259:ILE:HD13	1:R:316:ILE:HG23	1.70	0.73
1:M:251:ARG:HH11	1:N:236:THR:HG22	1.54	0.73
1:O:191:LEU:O	1:O:194:VAL:HG13	1.89	0.73
1:Q:259:ILE:HD13	1:Q:316:ILE:HG23	1.70	0.72
1:P:259:ILE:HD13	1:P:316:ILE:HG23	1.70	0.72
1:C:191:LEU:O	1:C:194:VAL:HG13	1.89	0.72
1:H:195:ILE:HA	2:H:2132:HOH:O	1.87	0.72
1:N:191:LEU:O	1:N:194:VAL:HG13	1.89	0.72
1:E:61:LYS:HE2	2:E:2030:HOH:O	1.89	0.72
1:J:259:ILE:HD13	1:J:316:ILE:HG23	1.69	0.72
1:Q:251:ARG:HH11	1:R:236:THR:CG2	2.03	0.72
1:V:191:LEU:O	1:V:194:VAL:HG13	1.90	0.72
1:V:259:ILE:HD13	1:V:316:ILE:HG23	1.71	0.72
1:W:259:ILE:HD13	1:W:316:ILE:HG23	1.70	0.72
1:R:34:SER:O	1:R:38:GLU:HG3	1.90	0.72
1:M:259:ILE:HD13	1:M:316:ILE:HG23	1.70	0.72
1:Q:191:LEU:O	1:Q:194:VAL:HG13	1.89	0.72
1:J:191:LEU:O	1:J:194:VAL:HG13	1.90	0.72
1:O:259:ILE:HD13	1:O:316:ILE:HG23	1.69	0.72
1:V:251:ARG:HD2	1:W:236:THR:CG2	2.11	0.72
1:X:189:ASP:HB3	2:X:2102:HOH:O	1.90	0.71
1:E:191:LEU:O	1:E:194:VAL:HG13	1.88	0.71
1:T:248:GLU:OE1	1:U:236:THR:HG22	1.89	0.71
1:T:259:ILE:HD13	1:T:316:ILE:HG23	1.71	0.71
1:W:191:LEU:O	1:W:194:VAL:HG13	1.90	0.71
1:G:251:ARG:CD	1:H:236:THR:HG23	2.15	0.71
1:Q:34:SER:O	1:Q:38:GLU:HG3	1.91	0.71
1:K:252:SER:OG	1:L:236:THR:HG21	1.89	0.70
1:U:34:SER:O	1:U:38:GLU:HG3	1.91	0.70
1:G:251:ARG:HD2	1:H:236:THR:CG2	2.15	0.70
1:N:8:LYS:HD2	2:N:2007:HOH:O	1.91	0.70
1:V:251:ARG:CD	1:W:236:THR:HG23	2.12	0.70
1:T:191:LEU:O	1:T:194:VAL:HG13	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:191:LEU:O	1:K:194:VAL:HG13	1.90	0.70
1:Q:251:ARG:HH11	1:R:236:THR:HG22	1.57	0.70
1:J:195:ILE:HG12	1:J:215:LEU:HD22	1.74	0.70
1:M:191:LEU:O	1:M:194:VAL:HG13	1.91	0.70
1:C:248:GLU:OE1	1:D:236:THR:HG22	1.92	0.69
1:I:192:LYS:HB3	1:I:192:LYS:NZ	2.07	0.69
1:G:34:SER:O	1:G:38:GLU:HG3	1.93	0.69
1:S:191:LEU:O	1:S:194:VAL:HG13	1.91	0.69
1:B:191:LEU:O	1:B:194:VAL:HG13	1.91	0.69
1:A:195:ILE:HA	2:A:2079:HOH:O	1.93	0.69
1:E:195:ILE:HG12	1:E:215:LEU:HD22	1.75	0.69
1:F:195:ILE:HG12	1:F:215:LEU:HD22	1.73	0.69
1:P:195:ILE:HG12	1:P:215:LEU:HD22	1.74	0.69
1:Q:195:ILE:HG12	1:Q:215:LEU:HD22	1.74	0.69
1:H:192:LYS:HB2	2:H:2127:HOH:O	1.90	0.69
1:I:192:LYS:HB2	2:I:2130:HOH:O	1.93	0.69
1:I:72:LYS:HE2	2:M:2021:HOH:O	1.92	0.69
1:K:248:GLU:OE1	1:L:236:THR:HG22	1.92	0.69
1:U:192:LYS:HB3	1:U:192:LYS:NZ	2.08	0.69
1:H:192:LYS:HB3	1:H:192:LYS:NZ	2.08	0.69
1:L:34:SER:O	1:L:38:GLU:HG3	1.92	0.69
1:P:251:ARG:HH11	1:Q:236:THR:CG2	2.06	0.69
1:X:34:SER:O	1:X:38:GLU:HG3	1.92	0.69
1:K:249:ALA:HA	1:K:253:ASN:HD22	1.58	0.69
1:O:195:ILE:HG12	1:O:215:LEU:HD22	1.74	0.69
1:T:34:SER:O	1:T:38:GLU:HG3	1.93	0.69
1:W:314:THR:HG21	1:X:239:ASP:CG	2.14	0.68
1:X:192:LYS:NZ	1:X:192:LYS:HB3	2.08	0.68
1:B:207:ILE:HD13	2:B:2079:HOH:O	1.91	0.68
1:E:34:SER:O	1:E:38:GLU:HG3	1.94	0.68
1:L:192:LYS:NZ	1:L:192:LYS:HB3	2.09	0.68
1:M:249:ALA:HA	1:M:253:ASN:HD22	1.59	0.68
1:P:184:ARG:HD3	2:P:2051:HOH:O	1.91	0.68
1:O:251:ARG:HD2	1:P:236:THR:CG2	2.14	0.68
1:D:192:LYS:NZ	1:D:192:LYS:HB3	2.08	0.68
1:J:251:ARG:HD2	1:K:236:THR:CG2	2.20	0.68
1:K:314:THR:HG21	1:L:239:ASP:CB	2.24	0.68
1:U:107:VAL:HA	2:U:2027:HOH:O	1.93	0.68
1:J:239:ASP:OD2	1:J:241:LYS:HG2	1.93	0.68
1:P:34:SER:O	1:P:38:GLU:HG3	1.93	0.68
1:C:249:ALA:HA	1:C:253:ASN:HD22	1.59	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:195:ILE:HG12	1:M:215:LEU:HD22	1.75	0.68
1:O:34:SER:O	1:O:38:GLU:HG3	1.94	0.68
1:B:195:ILE:HG12	1:B:215:LEU:HD22	1.76	0.68
1:E:251:ARG:HH11	1:F:236:THR:CG2	2.05	0.68
1:F:239:ASP:OD2	1:F:241:LYS:HG2	1.94	0.68
1:N:239:ASP:OD2	1:N:241:LYS:HG2	1.94	0.68
1:B:34:SER:O	1:B:38:GLU:HG3	1.93	0.68
1:I:195:ILE:HD11	1:I:215:LEU:HD13	1.75	0.68
1:K:195:ILE:HG12	1:K:215:LEU:HD22	1.75	0.68
1:O:251:ARG:CD	1:P:236:THR:HG23	2.15	0.68
1:V:239:ASP:OD2	1:V:241:LYS:HG2	1.94	0.68
1:W:239:ASP:OD2	1:W:241:LYS:HG2	1.94	0.68
1:B:239:ASP:OD2	1:B:241:LYS:HG2	1.94	0.68
1:F:249:ALA:HA	1:F:253:ASN:HD22	1.59	0.68
1:R:249:ALA:HA	1:R:253:ASN:HD22	1.59	0.68
1:S:239:ASP:OD2	1:S:241:LYS:HG2	1.93	0.67
1:F:34:SER:O	1:F:38:GLU:HG3	1.94	0.67
1:M:239:ASP:OD2	1:M:241:LYS:HG2	1.95	0.67
1:T:252:SER:OG	1:U:236:THR:HG21	1.95	0.67
1:W:195:ILE:HG12	1:W:215:LEU:HD22	1.75	0.67
1:C:34:SER:O	1:C:38:GLU:HG3	1.94	0.67
1:K:314:THR:HG21	1:L:239:ASP:CG	2.13	0.67
1:N:195:ILE:HG12	1:N:215:LEU:HD22	1.76	0.67
1:S:195:ILE:HG12	1:S:215:LEU:HD22	1.75	0.67
1:W:314:THR:HG21	1:X:239:ASP:CB	2.25	0.67
1:C:239:ASP:OD2	1:C:241:LYS:HG2	1.95	0.67
1:E:61:LYS:CE	2:E:2030:HOH:O	2.41	0.67
1:J:251:ARG:CD	1:K:236:THR:HG23	2.21	0.67
1:K:34:SER:O	1:K:38:GLU:HG3	1.94	0.67
1:Q:239:ASP:OD2	1:Q:241:LYS:HG2	1.94	0.67
1:S:249:ALA:HA	1:S:253:ASN:HD22	1.60	0.67
1:V:34:SER:O	1:V:38:GLU:HG3	1.93	0.67
1:W:252:SER:OG	1:X:236:THR:HG21	1.94	0.67
1:E:239:ASP:OD2	1:E:241:LYS:HG2	1.94	0.67
1:Q:249:ALA:HA	1:Q:253:ASN:HD22	1.60	0.67
1:T:239:ASP:OD2	1:T:241:LYS:HG2	1.94	0.67
1:I:34:SER:O	1:I:38:GLU:HG3	1.95	0.67
1:N:34:SER:O	1:N:38:GLU:HG3	1.94	0.67
1:R:239:ASP:OD2	1:R:241:LYS:HG2	1.94	0.67
1:G:195:ILE:HG12	1:G:215:LEU:HD22	1.75	0.67
1:R:195:ILE:HG12	1:R:215:LEU:HD22	1.74	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:ILE:HG12	1:C:215:LEU:HD22	1.76	0.67
1:K:239:ASP:OD2	1:K:241:LYS:HG2	1.95	0.66
1:M:34:SER:O	1:M:38:GLU:HG3	1.95	0.66
1:O:239:ASP:OD2	1:O:241:LYS:HG2	1.94	0.66
1:G:239:ASP:OD2	1:G:241:LYS:HG2	1.94	0.66
1:P:239:ASP:OD2	1:P:241:LYS:HG2	1.95	0.66
1:U:192:LYS:HB2	2:U:2045:HOH:O	1.94	0.66
1:W:34:SER:O	1:W:38:GLU:HG3	1.95	0.66
1:W:73:SER:HB3	2:W:2032:HOH:O	1.93	0.66
1:A:192:LYS:HB3	1:A:192:LYS:NZ	2.10	0.66
1:E:249:ALA:HA	1:E:253:ASN:HD22	1.59	0.66
1:P:249:ALA:HA	1:P:253:ASN:HD22	1.59	0.66
1:B:251:ARG:HD2	1:C:236:THR:CG2	2.15	0.66
1:L:195:ILE:HD11	1:L:215:LEU:HD13	1.76	0.66
1:V:195:ILE:HG12	1:V:215:LEU:HD22	1.75	0.66
1:A:195:ILE:HD11	1:A:215:LEU:HD13	1.77	0.66
1:D:195:ILE:HD11	1:D:215:LEU:HD13	1.76	0.66
1:H:34:SER:O	1:H:38:GLU:HG3	1.96	0.66
1:Q:310:LYS:HD2	1:R:132:GLY:O	1.96	0.66
1:T:195:ILE:HG12	1:T:215:LEU:HD22	1.76	0.66
1:A:34:SER:O	1:A:38:GLU:HG3	1.95	0.66
1:D:195:ILE:HB	2:D:2102:HOH:O	1.96	0.66
1:U:195:ILE:HD11	1:U:215:LEU:HD13	1.77	0.66
1:Q:40:VAL:CG1	1:Q:44:THR:HB	2.26	0.66
1:V:249:ALA:HA	1:V:253:ASN:HD22	1.61	0.66
1:W:40:VAL:CG1	1:W:44:THR:HB	2.26	0.66
1:E:115:GLU:HG2	2:E:2055:HOH:O	1.97	0.65
1:J:249:ALA:HA	1:J:253:ASN:HD22	1.60	0.65
1:J:34:SER:O	1:J:38:GLU:HG3	1.96	0.65
1:J:40:VAL:CG1	1:J:44:THR:HB	2.26	0.65
1:L:172:PHE:CZ	1:L:176:ILE:HD11	2.31	0.65
1:H:195:ILE:HD11	1:H:215:LEU:HD13	1.77	0.65
1:I:41:GLU:HG3	2:M:2023:HOH:O	1.95	0.65
1:U:240:ASP:C	1:U:242:ILE:H	2.00	0.65
1:D:172:PHE:CZ	1:D:176:ILE:HD11	2.31	0.65
1:D:240:ASP:C	1:D:242:ILE:H	2.00	0.65
1:D:247:LYS:NZ	1:D:247:LYS:HB2	2.12	0.65
1:D:34:SER:O	1:D:38:GLU:HG3	1.96	0.65
1:O:249:ALA:HA	1:O:253:ASN:HD22	1.61	0.65
1:T:40:VAL:CG1	1:T:44:THR:HB	2.26	0.65
1:X:195:ILE:HD11	1:X:215:LEU:HD13	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LYS:HA	1:A:92:LYS:HE3	1.79	0.65
1:D:92:LYS:HE3	1:D:92:LYS:HA	1.78	0.65
1:M:251:ARG:HH11	1:N:236:THR:CG2	2.09	0.65
1:N:249:ALA:HA	1:N:253:ASN:HD22	1.60	0.65
1:O:40:VAL:CG1	1:O:44:THR:HB	2.27	0.65
1:U:172:PHE:CZ	1:U:176:ILE:HD11	2.31	0.65
1:K:40:VAL:CG1	1:K:44:THR:HB	2.26	0.65
1:B:40:VAL:CG1	1:B:44:THR:HB	2.27	0.64
1:I:240:ASP:C	1:I:242:ILE:H	2.01	0.64
1:U:192:LYS:HA	2:U:2054:HOH:O	1.96	0.64
1:X:240:ASP:C	1:X:242:ILE:H	2.00	0.64
1:B:249:ALA:HA	1:B:253:ASN:HD22	1.62	0.64
1:E:40:VAL:CG1	1:E:44:THR:HB	2.27	0.64
1:E:252:SER:HB3	1:F:192:LYS:HE3	1.79	0.64
1:E:251:ARG:HH11	1:F:236:THR:HG22	1.61	0.64
1:N:251:ARG:HB2	1:N:317:LYS:HE2	1.79	0.64
1:P:40:VAL:CG1	1:P:44:THR:HB	2.27	0.64
1:C:252:SER:OG	1:D:236:THR:HG21	1.96	0.64
1:L:246:VAL:HA	2:L:2071:HOH:O	1.96	0.64
1:R:40:VAL:CG1	1:R:44:THR:HB	2.28	0.64
1:T:314:THR:HG21	1:U:239:ASP:CG	2.18	0.64
1:E:195:ILE:HG22	1:E:195:ILE:O	1.98	0.64
1:L:92:LYS:HA	1:L:92:LYS:HE3	1.79	0.64
1:O:251:ARG:HB2	1:O:317:LYS:HE2	1.79	0.64
1:R:195:ILE:HG22	1:R:195:ILE:O	1.98	0.64
1:V:251:ARG:HB2	1:V:317:LYS:HE2	1.80	0.64
1:W:249:ALA:HA	1:W:253:ASN:HD22	1.63	0.64
1:X:172:PHE:CZ	1:X:176:ILE:HD11	2.32	0.64
1:S:34:SER:O	1:S:38:GLU:HG3	1.98	0.64
1:T:67:VAL:HG12	2:T:2020:HOH:O	1.97	0.64
1:A:172:PHE:CZ	1:A:176:ILE:HD11	2.33	0.64
1:C:195:ILE:HG22	1:C:195:ILE:O	1.98	0.64
1:F:195:ILE:HG22	1:F:195:ILE:O	1.97	0.64
1:M:40:VAL:CG1	1:M:44:THR:HB	2.27	0.64
1:T:251:ARG:HB2	1:T:317:LYS:HE2	1.80	0.64
1:A:240:ASP:C	1:A:242:ILE:H	2.01	0.64
1:A:247:LYS:HB2	1:A:247:LYS:NZ	2.13	0.64
1:H:247:LYS:HB2	1:H:247:LYS:NZ	2.13	0.64
1:I:247:LYS:HB2	1:I:247:LYS:NZ	2.13	0.64
1:K:251:ARG:HB2	1:K:317:LYS:HE2	1.80	0.64
1:P:216:SER:HB2	2:P:2070:HOH:O	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:195:ILE:HG22	1:S:195:ILE:O	1.98	0.64
1:U:41:GLU:O	1:U:42:ASP:HB2	1.98	0.64
1:C:40:VAL:CG1	1:C:44:THR:HB	2.27	0.64
1:H:172:PHE:CZ	1:H:176:ILE:HD11	2.32	0.64
1:N:248:GLU:OE1	1:O:236:THR:HG22	1.98	0.64
1:U:92:LYS:HE3	1:U:92:LYS:HA	1.79	0.64
1:W:195:ILE:HG22	1:W:195:ILE:O	1.98	0.64
1:E:252:SER:HB3	1:F:192:LYS:CE	2.28	0.64
1:G:172:PHE:CZ	1:G:176:ILE:HD11	2.33	0.64
1:H:92:LYS:HE3	1:H:92:LYS:HA	1.80	0.64
1:K:195:ILE:HG22	1:K:195:ILE:O	1.98	0.64
1:L:41:GLU:O	1:L:42:ASP:HB2	1.98	0.64
1:O:195:ILE:O	1:O:195:ILE:HG22	1.97	0.64
1:H:192:LYS:HZ3	1:H:192:LYS:HB3	1.63	0.63
1:I:92:LYS:HA	1:I:92:LYS:HE3	1.79	0.63
1:M:195:ILE:O	1:M:195:ILE:HG22	1.98	0.63
1:A:41:GLU:O	1:A:42:ASP:HB2	1.98	0.63
1:H:240:ASP:C	1:H:242:ILE:H	2.00	0.63
1:L:240:ASP:C	1:L:242:ILE:H	2.00	0.63
1:P:310:LYS:HD2	1:Q:132:GLY:O	1.98	0.63
1:G:249:ALA:HA	1:G:253:ASN:HD22	1.62	0.63
1:I:192:LYS:O	1:I:194:VAL:N	2.30	0.63
1:L:192:LYS:HZ2	1:L:192:LYS:HB3	1.63	0.63
1:Q:195:ILE:HG22	1:Q:195:ILE:O	1.97	0.63
1:X:92:LYS:HA	1:X:92:LYS:HE3	1.79	0.63
1:B:251:ARG:CD	1:C:236:THR:HG23	2.16	0.63
1:G:40:VAL:CG1	1:G:44:THR:HB	2.28	0.63
1:P:172:PHE:CZ	1:P:176:ILE:HD11	2.33	0.63
1:N:195:ILE:HG22	1:N:195:ILE:O	1.98	0.63
1:V:195:ILE:HG22	1:V:195:ILE:O	1.98	0.63
1:F:43:GLY:HA2	2:F:2041:HOH:O	1.98	0.63
1:L:247:LYS:NZ	1:L:247:LYS:HB2	2.13	0.63
1:Q:251:ARG:HB2	1:Q:317:LYS:HE2	1.81	0.63
1:V:172:PHE:CZ	1:V:176:ILE:HD11	2.33	0.63
1:H:41:GLU:O	1:H:42:ASP:HB2	1.98	0.63
1:T:195:ILE:O	1:T:195:ILE:HG22	1.99	0.63
1:T:244:GLU:HG2	1:U:238:ASN:HD21	1.64	0.63
1:U:247:LYS:HB2	1:U:247:LYS:NZ	2.13	0.63
1:B:195:ILE:HG22	1:B:195:ILE:O	1.98	0.63
1:D:41:GLU:O	1:D:42:ASP:HB2	1.97	0.63
1:G:195:ILE:HG22	1:G:195:ILE:O	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:249:ALA:HA	1:T:253:ASN:HD22	1.62	0.63
1:G:251:ARG:HB2	1:G:317:LYS:HE2	1.80	0.62
1:U:192:LYS:O	1:U:194:VAL:N	2.32	0.62
1:W:251:ARG:HB2	1:W:317:LYS:HE2	1.80	0.62
1:E:251:ARG:HB2	1:E:317:LYS:HE2	1.81	0.62
1:M:251:ARG:HB2	1:M:317:LYS:HE2	1.81	0.62
1:P:195:ILE:HG22	1:P:195:ILE:O	1.99	0.62
1:R:172:PHE:CZ	1:R:176:ILE:HD11	2.34	0.62
1:V:40:VAL:CG1	1:V:44:THR:HB	2.29	0.62
1:X:192:LYS:O	1:X:194:VAL:N	2.31	0.62
1:C:251:ARG:HB2	1:C:317:LYS:HE2	1.81	0.62
1:R:251:ARG:HB2	1:R:317:LYS:HE2	1.81	0.62
1:S:40:VAL:CG1	1:S:44:THR:HB	2.29	0.62
1:X:41:GLU:O	1:X:42:ASP:HB2	1.99	0.62
1:I:41:GLU:CD	1:M:22:HIS:HB3	2.20	0.62
1:J:195:ILE:HG22	1:J:195:ILE:O	1.98	0.62
1:V:41:GLU:HB3	2:V:2022:HOH:O	1.99	0.62
1:P:251:ARG:HB2	1:P:317:LYS:HE2	1.80	0.62
1:Q:172:PHE:CZ	1:Q:176:ILE:HD11	2.33	0.62
1:F:251:ARG:HB2	1:F:317:LYS:HE2	1.80	0.62
1:H:192:LYS:O	1:H:194:VAL:N	2.32	0.62
1:K:172:PHE:CZ	1:K:176:ILE:HD11	2.35	0.62
1:L:178:ARG:NH1	1:L:178:ARG:HB2	2.15	0.62
1:M:271:THR:HG21	2:M:2073:HOH:O	2.00	0.62
1:T:286:THR:HB	1:T:294:LEU:HD11	1.81	0.62
1:X:247:LYS:NZ	1:X:247:LYS:HB2	2.13	0.62
1:C:172:PHE:CZ	1:C:176:ILE:HD11	2.33	0.62
1:J:251:ARG:HB2	1:J:317:LYS:HE2	1.80	0.62
1:S:1:MET:HA	2:T:2052:HOH:O	1.98	0.62
1:F:40:VAL:CG1	1:F:44:THR:HB	2.29	0.62
1:B:251:ARG:HB2	1:B:317:LYS:HE2	1.81	0.62
1:N:40:VAL:CG1	1:N:44:THR:HB	2.29	0.62
1:P:317:LYS:HE3	2:P:2103:HOH:O	1.99	0.62
1:S:251:ARG:HB2	1:S:317:LYS:HE2	1.80	0.62
1:I:240:ASP:HB3	1:I:242:ILE:HG12	1.82	0.61
1:I:41:GLU:O	1:I:42:ASP:HB2	1.99	0.61
1:H:192:LYS:HA	2:H:2129:HOH:O	1.99	0.61
1:D:192:LYS:O	1:D:194:VAL:N	2.33	0.61
1:T:172:PHE:CZ	1:T:176:ILE:HD11	2.36	0.61
1:A:240:ASP:HB3	1:A:242:ILE:HG12	1.82	0.61
1:U:240:ASP:HB3	1:U:242:ILE:HG12	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:PHE:CZ	1:B:176:ILE:HD11	2.35	0.61
1:D:41:GLU:HG3	2:D:2031:HOH:O	1.99	0.61
1:D:178:ARG:HB2	1:D:178:ARG:NH1	2.16	0.61
1:H:178:ARG:HB2	1:H:178:ARG:NH1	2.15	0.61
1:L:192:LYS:O	1:L:194:VAL:N	2.32	0.61
1:L:240:ASP:HB3	1:L:242:ILE:HG12	1.82	0.61
1:Q:286:THR:HB	1:Q:294:LEU:HD11	1.83	0.61
1:V:286:THR:HB	1:V:294:LEU:HD11	1.83	0.61
1:W:172:PHE:CZ	1:W:176:ILE:HD11	2.35	0.61
1:I:172:PHE:CZ	1:I:176:ILE:HD11	2.36	0.61
1:O:172:PHE:CZ	1:O:176:ILE:HD11	2.36	0.61
1:U:178:ARG:HB2	1:U:178:ARG:NH1	2.16	0.61
1:B:308:SER:HB2	2:B:2114:HOH:O	2.00	0.60
1:T:314:THR:HG21	1:U:239:ASP:CB	2.31	0.60
1:M:172:PHE:CZ	1:M:176:ILE:HD11	2.36	0.60
1:F:286:THR:HB	1:F:294:LEU:HD11	1.83	0.60
1:S:216:SER:HB2	2:S:2109:HOH:O	2.01	0.60
1:W:244:GLU:HG2	1:X:238:ASN:HD21	1.65	0.60
1:X:189:ASP:O	2:X:2102:HOH:O	2.16	0.60
1:X:178:ARG:NH1	1:X:178:ARG:HB2	2.16	0.60
1:N:43:GLY:HA2	2:N:2052:HOH:O	2.00	0.60
1:W:286:THR:HB	1:W:294:LEU:HD11	1.83	0.60
1:F:172:PHE:CZ	1:F:176:ILE:HD11	2.36	0.60
1:J:172:PHE:CZ	1:J:176:ILE:HD11	2.37	0.60
1:X:240:ASP:HB3	1:X:242:ILE:HG12	1.83	0.60
1:H:240:ASP:HB3	1:H:242:ILE:HG12	1.82	0.60
1:S:286:THR:HB	1:S:294:LEU:HD11	1.83	0.60
1:X:247:LYS:O	1:X:249:ALA:N	2.34	0.60
1:D:240:ASP:HB3	1:D:242:ILE:HG12	1.83	0.60
1:F:257:LEU:HD22	1:F:259:ILE:HG23	1.84	0.60
1:K:257:LEU:HD22	1:K:259:ILE:HG23	1.84	0.60
1:I:41:GLU:OE2	1:M:22:HIS:HB3	2.00	0.60
1:D:87:GLU:HB3	1:D:92:LYS:HD2	1.84	0.59
1:V:257:LEU:HD22	1:V:259:ILE:HG23	1.84	0.59
1:G:286:THR:HB	1:G:294:LEU:HD11	1.83	0.59
1:S:172:PHE:CZ	1:S:176:ILE:HD11	2.36	0.59
1:A:192:LYS:O	1:A:194:VAL:N	2.32	0.59
1:B:286:THR:HB	1:B:294:LEU:HD11	1.84	0.59
1:M:252:SER:HB3	1:N:192:LYS:CE	2.31	0.59
1:H:87:GLU:HB3	1:H:92:LYS:HD2	1.84	0.59
1:E:172:PHE:CZ	1:E:176:ILE:HD11	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:41:GLU:OE2	1:M:22:HIS:ND1	2.35	0.59
1:A:178:ARG:HB2	1:A:178:ARG:NH1	2.17	0.59
1:C:257:LEU:HD22	1:C:259:ILE:HG23	1.85	0.59
1:G:257:LEU:HD22	1:G:259:ILE:HG23	1.84	0.59
1:L:87:GLU:HB3	1:L:92:LYS:HD2	1.84	0.59
1:I:87:GLU:HB3	1:I:92:LYS:HD2	1.84	0.59
1:P:106:LEU:HD22	1:P:109:CYS:SG	2.42	0.59
1:Q:257:LEU:HD22	1:Q:259:ILE:HG23	1.85	0.59
1:X:87:GLU:HB3	1:X:92:LYS:HD2	1.85	0.59
1:H:195:ILE:HB	2:H:2131:HOH:O	2.02	0.59
1:J:286:THR:HB	1:J:294:LEU:HD11	1.85	0.59
1:M:257:LEU:HD22	1:M:259:ILE:HG23	1.85	0.59
1:R:286:THR:HB	1:R:294:LEU:HD11	1.85	0.59
1:C:251:ARG:HD2	1:D:236:THR:CG2	2.23	0.59
1:C:286:THR:HB	1:C:294:LEU:HD11	1.83	0.59
1:I:192:LYS:O	1:I:194:VAL:HG12	2.03	0.59
1:W:257:LEU:HD22	1:W:259:ILE:HG23	1.85	0.59
1:O:286:THR:HB	1:O:294:LEU:HD11	1.83	0.59
1:P:257:LEU:HD22	1:P:259:ILE:HG23	1.84	0.59
1:X:192:LYS:O	1:X:194:VAL:HG12	2.03	0.58
1:F:106:LEU:HD22	1:F:109:CYS:SG	2.43	0.58
1:M:236:THR:CG2	1:R:251:ARG:HH11	2.16	0.58
1:N:248:GLU:OE1	1:O:236:THR:CG2	2.52	0.58
1:U:87:GLU:HB3	1:U:92:LYS:HD2	1.84	0.58
1:X:192:LYS:HB3	1:X:192:LYS:HZ3	1.66	0.58
1:A:247:LYS:O	1:A:248:GLU:HB3	2.03	0.58
1:J:271:THR:HG21	2:J:2067:HOH:O	2.04	0.58
1:J:257:LEU:HD22	1:J:259:ILE:HG23	1.86	0.58
1:K:244:GLU:HG2	1:L:238:ASN:HD21	1.69	0.58
1:O:106:LEU:HD22	1:O:109:CYS:SG	2.44	0.58
1:U:216:SER:HB3	2:U:2055:HOH:O	2.04	0.58
1:D:247:LYS:O	1:D:248:GLU:HB3	2.04	0.58
1:I:178:ARG:NH1	1:I:178:ARG:HB2	2.18	0.58
1:K:286:THR:HB	1:K:294:LEU:HD11	1.85	0.58
1:N:286:THR:HB	1:N:294:LEU:HD11	1.85	0.58
1:Q:248:GLU:OE1	1:R:236:THR:HG22	2.03	0.58
1:A:87:GLU:HB3	1:A:92:LYS:HD2	1.84	0.58
1:M:236:THR:HG22	1:R:251:ARG:HH11	1.69	0.58
1:I:2:ILE:HD11	2:J:2108:HOH:O	2.02	0.58
1:N:172:PHE:CZ	1:N:176:ILE:HD11	2.39	0.58
1:V:310:LYS:HD2	1:W:132:GLY:O	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:115:GLU:HG2	2:R:2051:HOH:O	2.04	0.57
1:U:192:LYS:O	1:U:194:VAL:HG12	2.04	0.57
1:L:60:ASP:OD2	1:L:64:GLN:HB3	2.05	0.57
1:P:286:THR:HB	1:P:294:LEU:HD11	1.86	0.57
1:U:247:LYS:O	1:U:248:GLU:HB3	2.04	0.57
1:L:247:LYS:O	1:L:248:GLU:HB3	2.03	0.57
1:M:286:THR:HB	1:M:294:LEU:HD11	1.84	0.57
1:B:257:LEU:HD22	1:B:259:ILE:HG23	1.85	0.57
1:L:287:SER:OG	1:L:297:HIS:HE1	1.88	0.57
1:N:251:ARG:NH1	1:O:236:THR:HG22	2.18	0.57
1:R:106:LEU:HD22	1:R:109:CYS:SG	2.45	0.57
1:U:60:ASP:OD2	1:U:64:GLN:HB3	2.05	0.57
1:B:310:LYS:HD2	1:C:132:GLY:O	2.04	0.57
1:D:192:LYS:O	1:D:194:VAL:HG12	2.04	0.57
1:E:286:THR:HB	1:E:294:LEU:HD11	1.87	0.57
1:F:178:ARG:NH1	1:F:178:ARG:HB2	2.20	0.57
1:H:247:LYS:O	1:H:248:GLU:HB3	2.05	0.57
1:H:287:SER:OG	1:H:297:HIS:HE1	1.88	0.57
1:X:247:LYS:O	1:X:248:GLU:HB3	2.04	0.57
1:A:192:LYS:O	1:A:194:VAL:HG12	2.04	0.57
1:Q:178:ARG:HB2	1:Q:178:ARG:NH1	2.20	0.57
1:U:238:ASN:N	1:U:238:ASN:HD22	2.02	0.57
2:Q:2075:HOH:O	1:U:262:ASP:HB2	2.05	0.57
1:B:251:ARG:HH11	1:C:236:THR:CG2	2.18	0.56
1:A:236:THR:HG21	1:F:252:SER:OG	2.05	0.56
1:A:236:THR:HG22	1:F:248:GLU:OE1	2.04	0.56
1:L:192:LYS:O	1:L:194:VAL:HG12	2.04	0.56
1:S:257:LEU:HD22	1:S:259:ILE:HG23	1.85	0.56
1:V:106:LEU:HD22	1:V:109:CYS:SG	2.45	0.56
1:H:192:LYS:O	1:H:194:VAL:HG12	2.04	0.56
1:L:238:ASN:N	1:L:238:ASN:HD22	2.03	0.56
1:H:238:ASN:HD22	1:H:238:ASN:N	2.04	0.56
1:I:245:LEU:O	1:I:247:LYS:O	2.24	0.56
1:V:178:ARG:HB2	1:V:178:ARG:NH1	2.20	0.56
1:T:257:LEU:HD22	1:T:259:ILE:HG23	1.86	0.56
1:M:132:GLY:O	1:R:310:LYS:HD2	2.05	0.56
1:O:257:LEU:HD22	1:O:259:ILE:HG23	1.87	0.56
1:T:106:LEU:HD22	1:T:109:CYS:SG	2.46	0.56
1:W:310:LYS:HD2	1:X:132:GLY:O	2.05	0.56
1:E:216:SER:HB2	2:F:2113:HOH:O	2.06	0.56
1:E:257:LEU:HD22	1:E:259:ILE:HG23	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:247:LYS:O	1:I:248:GLU:HB3	2.05	0.56
1:Q:248:GLU:OE1	1:R:236:THR:CG2	2.53	0.56
1:E:251:ARG:NH1	1:F:236:THR:HG22	2.21	0.56
1:A:236:THR:CG2	1:F:251:ARG:HD2	2.27	0.56
1:G:42:ASP:HB3	2:G:2025:HOH:O	2.04	0.56
1:L:245:LEU:O	1:L:247:LYS:O	2.24	0.56
1:C:251:ARG:CD	1:D:236:THR:HG23	2.23	0.56
1:I:41:GLU:OE2	1:M:22:HIS:CG	2.58	0.56
1:S:106:LEU:HD22	1:S:109:CYS:SG	2.46	0.56
1:W:106:LEU:HD22	1:W:109:CYS:SG	2.46	0.56
1:X:238:ASN:N	1:X:238:ASN:HD22	2.03	0.56
1:D:238:ASN:HD22	1:D:238:ASN:N	2.04	0.56
1:H:245:LEU:O	1:H:247:LYS:O	2.24	0.56
1:H:247:LYS:O	1:H:249:ALA:N	2.36	0.56
1:D:192:LYS:HB3	1:D:192:LYS:HZ3	1.69	0.56
1:N:92:LYS:HE3	1:N:92:LYS:CA	2.36	0.56
1:A:192:LYS:HB3	1:A:192:LYS:HZ3	1.71	0.55
1:C:106:LEU:HD22	1:C:109:CYS:SG	2.46	0.55
1:D:60:ASP:OD2	1:D:64:GLN:HB3	2.06	0.55
1:N:178:ARG:HB2	1:N:178:ARG:NH1	2.21	0.55
1:S:207:ILE:HD13	2:S:2104:HOH:O	2.06	0.55
1:U:192:LYS:HB3	1:U:192:LYS:HZ3	1.69	0.55
1:I:72:LYS:HE3	2:I:2031:HOH:O	2.05	0.55
1:N:92:LYS:HA	1:N:92:LYS:CE	2.36	0.55
1:S:178:ARG:NH1	1:S:178:ARG:HB2	2.21	0.55
1:A:247:LYS:O	1:A:249:ALA:N	2.36	0.55
1:A:60:ASP:OD2	1:A:64:GLN:HB3	2.06	0.55
1:I:247:LYS:O	1:I:249:ALA:N	2.36	0.55
1:J:92:LYS:CA	1:J:92:LYS:HE3	2.36	0.55
1:U:247:LYS:O	1:U:249:ALA:N	2.37	0.55
1:D:247:LYS:O	1:D:249:ALA:N	2.37	0.55
1:I:238:ASN:N	1:I:238:ASN:HD22	2.04	0.55
1:R:257:LEU:HD22	1:R:259:ILE:HG23	1.87	0.55
1:U:184:ARG:HD3	2:U:2040:HOH:O	2.05	0.55
1:U:287:SER:OG	1:U:297:HIS:HE1	1.90	0.55
1:B:106:LEU:HD22	1:B:109:CYS:SG	2.46	0.55
1:D:245:LEU:O	1:D:247:LYS:O	2.25	0.55
1:E:72:LYS:HE3	2:E:2039:HOH:O	2.06	0.55
1:G:1:MET:HA	2:H:2118:HOH:O	2.07	0.55
1:X:60:ASP:OD2	1:X:64:GLN:HB3	2.06	0.55
1:A:238:ASN:N	1:A:238:ASN:HD22	2.04	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:106:LEU:HD22	1:U:109:CYS:SG	2.47	0.55
1:B:95:HIS:HD2	1:B:96:ARG:O	1.89	0.55
1:H:72:LYS:HE3	2:H:2018:HOH:O	2.06	0.55
1:M:106:LEU:HD22	1:M:109:CYS:SG	2.47	0.55
1:A:245:LEU:O	1:A:247:LYS:O	2.25	0.54
1:K:310:LYS:HD2	1:L:132:GLY:O	2.06	0.54
1:N:257:LEU:HD22	1:N:259:ILE:HG23	1.87	0.54
1:U:95:HIS:HD2	1:U:96:ARG:O	1.89	0.54
1:L:247:LYS:O	1:L:249:ALA:N	2.37	0.54
1:M:252:SER:HB3	1:N:192:LYS:HE3	1.89	0.54
1:U:245:LEU:O	1:U:247:LYS:O	2.23	0.54
1:X:245:LEU:O	1:X:247:LYS:O	2.25	0.54
1:E:106:LEU:HD22	1:E:109:CYS:SG	2.47	0.54
1:M:244:GLU:HG2	1:N:239:ASP:HB2	1.90	0.54
1:P:251:ARG:NH1	1:Q:236:THR:HG22	2.22	0.54
1:F:92:LYS:HE3	1:F:92:LYS:CA	2.36	0.54
1:M:178:ARG:NH1	1:M:178:ARG:HB2	2.23	0.54
1:B:178:ARG:NH1	1:B:178:ARG:HB2	2.23	0.54
1:D:287:SER:OG	1:D:297:HIS:HE1	1.90	0.54
1:K:259:ILE:CD1	1:K:316:ILE:HG23	2.37	0.54
1:Q:92:LYS:CE	1:Q:92:LYS:HA	2.38	0.54
1:Q:251:ARG:NH1	1:R:236:THR:HG22	2.21	0.54
1:U:40:VAL:CG1	1:U:44:THR:HB	2.38	0.54
1:V:313:GLN:HE22	1:V:317:LYS:HZ3	1.56	0.54
1:A:236:THR:HG23	1:F:251:ARG:CD	2.27	0.54
1:G:92:LYS:CA	1:G:92:LYS:HE3	2.36	0.54
1:S:92:LYS:HE3	1:S:92:LYS:CA	2.36	0.54
1:W:132:GLY:HA3	2:W:2049:HOH:O	2.07	0.54
1:C:92:LYS:HA	1:C:92:LYS:CE	2.37	0.54
1:E:40:VAL:O	2:E:2030:HOH:O	2.18	0.54
1:Q:106:LEU:HD22	1:Q:109:CYS:SG	2.48	0.54
1:R:178:ARG:NH1	1:R:178:ARG:HB2	2.23	0.54
1:F:313:GLN:HE22	1:F:317:LYS:HZ3	1.54	0.54
1:F:92:LYS:HA	1:F:92:LYS:CE	2.37	0.54
1:H:60:ASP:OD2	1:H:64:GLN:HB3	2.07	0.54
1:K:106:LEU:HD22	1:K:109:CYS:SG	2.48	0.54
1:O:178:ARG:NH1	1:O:178:ARG:HB2	2.23	0.54
1:P:178:ARG:NH1	1:P:178:ARG:HB2	2.23	0.54
1:P:259:ILE:CD1	1:P:316:ILE:HG23	2.38	0.54
1:T:259:ILE:CD1	1:T:316:ILE:HG23	2.38	0.54
1:U:134:SER:HB3	1:U:267:TRP:CZ2	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:ARG:NH1	1:C:178:ARG:HB2	2.23	0.53
1:D:195:ILE:HG12	1:D:215:LEU:HD22	1.90	0.53
1:L:40:VAL:CG1	1:L:44:THR:HB	2.38	0.53
1:W:259:ILE:CD1	1:W:316:ILE:HG23	2.38	0.53
1:H:95:HIS:HD2	1:H:96:ARG:O	1.91	0.53
1:I:134:SER:HB3	1:I:267:TRP:CZ2	2.43	0.53
1:K:92:LYS:HE3	1:K:92:LYS:CA	2.37	0.53
1:N:209:ARG:HD3	2:N:2158:HOH:O	2.07	0.53
1:N:311:ALA:O	1:N:315:VAL:HG23	2.09	0.53
1:T:178:ARG:NH1	1:T:178:ARG:HB2	2.22	0.53
1:W:92:LYS:CE	1:W:92:LYS:HA	2.37	0.53
1:A:40:VAL:CG1	1:A:44:THR:HB	2.39	0.53
1:L:134:SER:HB3	1:L:267:TRP:CZ2	2.43	0.53
1:W:192:LYS:O	1:W:193:ASN:HB2	2.09	0.53
1:A:106:LEU:HD22	1:A:109:CYS:SG	2.49	0.53
1:A:95:HIS:HD2	1:A:96:ARG:O	1.92	0.53
1:B:259:ILE:CD1	1:B:316:ILE:HG23	2.38	0.53
1:G:95:HIS:HD2	1:G:96:ARG:O	1.91	0.53
1:K:178:ARG:HB2	1:K:178:ARG:NH1	2.24	0.53
1:N:259:ILE:CD1	1:N:316:ILE:HG23	2.38	0.53
1:G:178:ARG:HB2	1:G:178:ARG:NH1	2.24	0.53
1:G:192:LYS:O	1:G:193:ASN:HB2	2.09	0.53
1:I:106:LEU:HD22	1:I:109:CYS:SG	2.48	0.53
1:M:92:LYS:HE3	1:M:92:LYS:CA	2.37	0.53
1:O:192:LYS:O	1:O:193:ASN:HB2	2.09	0.53
1:W:178:ARG:NH1	1:W:178:ARG:HB2	2.23	0.53
1:D:134:SER:HB3	1:D:267:TRP:CZ2	2.44	0.53
1:E:92:LYS:CA	1:E:92:LYS:HE3	2.37	0.53
1:I:287:SER:OG	1:I:297:HIS:HE1	1.92	0.53
1:T:310:LYS:HD2	1:U:132:GLY:O	2.09	0.53
1:U:131:LYS:HA	2:U:2032:HOH:O	2.07	0.53
1:W:92:LYS:CA	1:W:92:LYS:HE3	2.37	0.53
1:D:286:THR:HB	1:D:294:LEU:HD11	1.90	0.53
1:E:178:ARG:HB2	1:E:178:ARG:NH1	2.24	0.53
1:I:107:VAL:HA	2:I:2090:HOH:O	2.09	0.53
1:P:311:ALA:O	1:P:315:VAL:HG23	2.09	0.53
2:M:2109:HOH:O	1:R:1:MET:HA	2.08	0.53
1:S:92:LYS:HA	1:S:92:LYS:CE	2.36	0.53
1:C:195:ILE:HG23	1:C:245:LEU:HG	1.91	0.53
1:H:40:VAL:CG1	1:H:44:THR:HB	2.38	0.53
1:P:92:LYS:CA	1:P:92:LYS:HE3	2.37	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:259:ILE:CD1	1:Q:316:ILE:HG23	2.38	0.53
1:S:137:THR:HB	1:S:138:PRO:HD3	1.91	0.53
1:T:311:ALA:O	1:T:315:VAL:HG23	2.09	0.53
1:A:134:SER:HB3	1:A:267:TRP:CZ2	2.44	0.53
1:B:248:GLU:OE1	1:C:236:THR:HG22	2.08	0.53
1:G:106:LEU:HD22	1:G:109:CYS:SG	2.49	0.53
1:G:259:ILE:CD1	1:G:316:ILE:HG23	2.36	0.53
1:M:137:THR:HB	1:M:138:PRO:HD3	1.91	0.53
1:M:95:HIS:HD2	1:M:96:ARG:O	1.92	0.53
1:N:310:LYS:HB3	1:O:133:ASN:HA	1.91	0.53
1:Q:311:ALA:O	1:Q:315:VAL:HG23	2.08	0.53
1:X:95:HIS:HD2	1:X:96:ARG:O	1.92	0.53
1:T:92:LYS:HE3	1:T:92:LYS:CA	2.37	0.53
1:B:311:ALA:O	1:B:315:VAL:HG23	2.09	0.52
1:Q:237:SER:HB3	1:Q:242:ILE:CD1	2.25	0.52
1:T:92:LYS:CE	1:T:92:LYS:HA	2.37	0.52
1:X:134:SER:HB3	1:X:267:TRP:CZ2	2.44	0.52
1:C:192:LYS:O	1:C:193:ASN:HB2	2.09	0.52
1:F:192:LYS:O	1:F:193:ASN:HB2	2.09	0.52
1:F:259:ILE:CD1	1:F:316:ILE:HG23	2.37	0.52
1:K:311:ALA:O	1:K:315:VAL:HG23	2.09	0.52
1:L:95:HIS:HD2	1:L:96:ARG:O	1.92	0.52
1:M:251:ARG:NH1	1:N:236:THR:HG22	2.21	0.52
1:P:195:ILE:HG23	1:P:245:LEU:HG	1.90	0.52
1:R:195:ILE:HG23	1:R:245:LEU:HG	1.91	0.52
1:J:178:ARG:HB2	1:J:178:ARG:NH1	2.25	0.52
1:M:195:ILE:HG23	1:M:245:LEU:HG	1.91	0.52
1:V:195:ILE:HG23	1:V:245:LEU:HG	1.91	0.52
1:C:311:ALA:O	1:C:315:VAL:HG23	2.10	0.52
1:H:195:ILE:HG12	1:H:215:LEU:HD22	1.92	0.52
1:I:95:HIS:HD2	1:I:96:ARG:O	1.93	0.52
1:L:234:ASN:C	1:L:236:THR:H	2.13	0.52
1:M:192:LYS:O	1:M:193:ASN:HB2	2.09	0.52
1:O:259:ILE:CD1	1:O:316:ILE:HG23	2.37	0.52
1:V:311:ALA:O	1:V:315:VAL:HG23	2.09	0.52
1:V:92:LYS:CE	1:V:92:LYS:HA	2.38	0.52
1:D:40:VAL:CG1	1:D:44:THR:HB	2.39	0.52
1:F:95:HIS:HD2	1:F:96:ARG:O	1.92	0.52
1:H:252:SER:HB2	1:I:236:THR:HG21	1.90	0.52
1:L:195:ILE:HG12	1:L:215:LEU:HD22	1.92	0.52
1:M:259:ILE:CD1	1:M:316:ILE:HG23	2.38	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:106:LEU:HD22	1:N:109:CYS:SG	2.49	0.52
1:P:244:GLU:HG2	1:Q:239:ASP:HB2	1.91	0.52
1:Q:195:ILE:HG23	1:Q:245:LEU:HG	1.91	0.52
1:T:195:ILE:HG23	1:T:245:LEU:HG	1.91	0.52
1:X:242:ILE:HG22	1:X:242:ILE:O	2.10	0.52
1:B:248:GLU:OE1	1:C:236:THR:CG2	2.58	0.52
1:D:106:LEU:HD22	1:D:109:CYS:SG	2.49	0.52
1:G:311:ALA:O	1:G:315:VAL:HG23	2.10	0.52
1:I:242:ILE:O	1:I:242:ILE:HG22	2.09	0.52
1:M:311:ALA:O	1:M:315:VAL:HG23	2.10	0.52
1:O:92:LYS:CA	1:O:92:LYS:HE3	2.37	0.52
1:R:237:SER:HB3	1:R:242:ILE:CD1	2.24	0.52
1:B:195:ILE:HG23	1:B:245:LEU:HG	1.92	0.52
1:E:192:LYS:O	1:E:193:ASN:HB2	2.10	0.52
1:E:195:ILE:HG23	1:E:245:LEU:HG	1.91	0.52
1:E:42:ASP:N	2:E:2030:HOH:O	2.42	0.52
1:H:106:LEU:HD22	1:H:109:CYS:SG	2.50	0.52
1:R:259:ILE:CD1	1:R:316:ILE:HG23	2.39	0.52
1:S:88:ASN:HB2	2:S:2049:HOH:O	2.10	0.52
1:V:259:ILE:CD1	1:V:316:ILE:HG23	2.39	0.52
1:V:92:LYS:HE3	1:V:92:LYS:CA	2.37	0.52
1:W:311:ALA:O	1:W:315:VAL:HG23	2.09	0.52
1:B:92:LYS:CE	1:B:92:LYS:HA	2.37	0.52
1:L:286:THR:HB	1:L:294:LEU:HD11	1.91	0.52
1:M:92:LYS:HA	1:M:92:LYS:CE	2.37	0.52
1:N:195:ILE:HG23	1:N:245:LEU:HG	1.92	0.52
1:O:92:LYS:CE	1:O:92:LYS:HA	2.37	0.52
1:Q:313:GLN:HE22	1:Q:317:LYS:HZ3	1.58	0.52
1:R:311:ALA:O	1:R:315:VAL:HG23	2.10	0.52
1:S:259:ILE:CD1	1:S:316:ILE:HG23	2.38	0.52
1:X:40:VAL:CG1	1:X:44:THR:HB	2.40	0.52
1:F:195:ILE:HG23	1:F:245:LEU:HG	1.91	0.52
1:R:95:HIS:HD2	1:R:96:ARG:O	1.93	0.52
1:T:244:GLU:HG2	1:U:238:ASN:ND2	2.25	0.52
1:W:251:ARG:HH11	1:X:236:THR:HG22	1.75	0.52
2:I:2015:HOH:O	1:J:291:HIS:HD2	1.93	0.52
1:J:92:LYS:CE	1:J:92:LYS:HA	2.37	0.52
1:K:195:ILE:HG23	1:K:245:LEU:HG	1.91	0.52
1:O:311:ALA:O	1:O:315:VAL:HG23	2.10	0.52
1:Q:95:HIS:HD2	1:Q:96:ARG:O	1.92	0.52
1:R:92:LYS:CA	1:R:92:LYS:HE3	2.38	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:252:SER:HB3	1:T:192:LYS:CE	2.40	0.52
1:X:195:ILE:HG12	1:X:215:LEU:HD22	1.92	0.52
1:D:95:HIS:HD2	1:D:96:ARG:O	1.93	0.51
1:G:195:ILE:HG23	1:G:245:LEU:HG	1.91	0.51
1:J:259:ILE:CD1	1:J:316:ILE:HG23	2.37	0.51
1:M:313:GLN:HE22	1:M:317:LYS:HZ3	1.58	0.51
1:O:195:ILE:HG23	1:O:245:LEU:HG	1.92	0.51
1:Q:192:LYS:O	1:Q:193:ASN:HB2	2.10	0.51
1:S:252:SER:HB3	1:T:192:LYS:HE3	1.91	0.51
1:T:192:LYS:O	1:T:193:ASN:HB2	2.11	0.51
1:T:234:ASN:C	1:T:236:THR:H	2.14	0.51
1:W:195:ILE:HG23	1:W:245:LEU:HG	1.91	0.51
1:X:192:LYS:HA	2:X:2108:HOH:O	2.10	0.51
1:K:92:LYS:HA	1:K:92:LYS:CE	2.38	0.51
1:P:248:GLU:OE1	1:Q:236:THR:HG22	2.10	0.51
1:U:234:ASN:C	1:U:236:THR:H	2.14	0.51
1:A:147:LEU:O	1:A:184:ARG:NH2	2.44	0.51
1:B:192:LYS:O	1:B:193:ASN:HB2	2.10	0.51
1:D:1:MET:HA	2:E:2089:HOH:O	2.10	0.51
1:D:242:ILE:O	1:D:242:ILE:HG22	2.09	0.51
1:H:234:ASN:C	1:H:236:THR:H	2.13	0.51
1:H:286:THR:HB	1:H:294:LEU:HD11	1.91	0.51
1:M:236:THR:HG22	1:R:248:GLU:OE1	2.09	0.51
1:Q:137:THR:HB	1:Q:138:PRO:HD3	1.92	0.51
1:S:311:ALA:O	1:S:315:VAL:HG23	2.09	0.51
1:T:209:ARG:HD3	2:T:2059:HOH:O	2.10	0.51
1:E:259:ILE:CD1	1:E:316:ILE:HG23	2.38	0.51
1:F:311:ALA:O	1:F:315:VAL:HG23	2.10	0.51
1:G:234:ASN:C	1:G:236:THR:H	2.14	0.51
1:I:195:ILE:HG12	1:I:215:LEU:HD22	1.92	0.51
1:S:195:ILE:HG23	1:S:245:LEU:HG	1.92	0.51
1:A:287:SER:OG	1:A:297:HIS:HE1	1.94	0.51
1:B:234:ASN:C	1:B:236:THR:H	2.14	0.51
1:B:92:LYS:HE3	1:B:92:LYS:CA	2.37	0.51
1:C:234:ASN:C	1:C:236:THR:H	2.13	0.51
1:G:92:LYS:CE	1:G:92:LYS:HA	2.36	0.51
1:J:106:LEU:HD22	1:J:109:CYS:SG	2.50	0.51
1:K:192:LYS:O	1:K:193:ASN:HB2	2.11	0.51
1:O:259:ILE:HD13	1:O:316:ILE:CG2	2.41	0.51
1:P:192:LYS:O	1:P:193:ASN:HB2	2.11	0.51
1:Q:92:LYS:CA	1:Q:92:LYS:HE3	2.38	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:92:LYS:CE	1:R:92:LYS:HA	2.38	0.51
1:S:192:LYS:O	1:S:193:ASN:HB2	2.10	0.51
1:X:147:LEU:O	1:X:184:ARG:NH2	2.44	0.51
1:E:92:LYS:HA	1:E:92:LYS:CE	2.37	0.51
1:F:147:LEU:O	1:F:184:ARG:NH2	2.44	0.51
1:H:105:GLU:HB3	2:H:2062:HOH:O	2.10	0.51
1:I:234:ASN:C	1:I:236:THR:H	2.13	0.51
1:L:147:LEU:O	1:L:184:ARG:NH2	2.44	0.51
1:P:190:SER:OG	1:P:192:LYS:HB3	2.10	0.51
1:U:195:ILE:HG12	1:U:215:LEU:HD22	1.93	0.51
1:X:286:THR:HB	1:X:294:LEU:HD11	1.93	0.51
1:C:92:LYS:CA	1:C:92:LYS:HE3	2.37	0.51
1:F:115:GLU:HG2	2:F:2070:HOH:O	2.11	0.51
1:H:242:ILE:HG22	1:H:242:ILE:O	2.10	0.51
1:I:192:LYS:HA	2:I:2153:HOH:O	2.11	0.51
1:R:234:ASN:C	1:R:236:THR:H	2.14	0.51
1:B:251:ARG:HH11	1:C:236:THR:HG22	1.75	0.51
1:A:154:ALA:HA	1:F:4:LEU:HD23	1.93	0.51
1:G:313:GLN:HE22	1:G:317:LYS:NZ	2.09	0.51
1:I:272:ARG:NH1	2:I:2169:HOH:O	2.42	0.51
1:M:190:SER:OG	1:M:192:LYS:HB3	2.10	0.51
1:N:234:ASN:C	1:N:236:THR:H	2.14	0.51
1:Q:234:ASN:C	1:Q:236:THR:H	2.14	0.51
1:V:95:HIS:HD2	1:V:96:ARG:O	1.94	0.51
1:W:250:SER:HB2	1:W:317:LYS:HE3	1.93	0.51
1:X:234:ASN:C	1:X:236:THR:H	2.14	0.51
1:C:313:GLN:HE22	1:C:317:LYS:HZ3	1.59	0.51
1:F:313:GLN:HE22	1:F:317:LYS:NZ	2.08	0.51
1:G:137:THR:HB	1:G:138:PRO:HD3	1.93	0.51
1:K:234:ASN:C	1:K:236:THR:H	2.14	0.51
1:S:250:SER:HB2	1:S:317:LYS:HE3	1.92	0.51
1:U:242:ILE:O	1:U:242:ILE:HG22	2.10	0.51
1:W:234:ASN:C	1:W:236:THR:H	2.13	0.51
1:G:248:GLU:OE1	1:H:236:THR:HG22	2.11	0.51
1:I:60:ASP:OD2	1:I:64:GLN:HB3	2.11	0.51
1:J:207:ILE:HG23	1:J:211:ALA:HB3	1.93	0.51
1:J:311:ALA:O	1:J:315:VAL:HG23	2.10	0.51
1:S:234:ASN:C	1:S:236:THR:H	2.15	0.51
1:O:234:ASN:C	1:O:236:THR:H	2.14	0.50
1:P:92:LYS:CE	1:P:92:LYS:HA	2.37	0.50
1:Q:70:LYS:HG2	2:Q:2022:HOH:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:190:SER:OG	1:R:192:LYS:HB3	2.12	0.50
2:M:2130:HOH:O	1:S:312:ILE:HD13	2.11	0.50
1:X:287:SER:OG	1:X:297:HIS:HE1	1.93	0.50
1:E:313:GLN:HE22	1:E:317:LYS:NZ	2.09	0.50
1:H:1:MET:HA	2:I:2142:HOH:O	2.11	0.50
1:K:95:HIS:HD2	1:K:96:ARG:O	1.94	0.50
1:P:234:ASN:C	1:P:236:THR:H	2.13	0.50
1:P:313:GLN:HE22	1:P:317:LYS:HZ3	1.58	0.50
1:A:195:ILE:HG12	1:A:215:LEU:HD22	1.91	0.50
1:C:137:THR:HB	1:C:138:PRO:HD3	1.93	0.50
1:H:134:SER:HB3	1:H:267:TRP:CZ2	2.47	0.50
1:I:40:VAL:CG1	1:I:44:THR:HB	2.40	0.50
1:J:192:LYS:O	1:J:193:ASN:HB2	2.11	0.50
1:J:234:ASN:C	1:J:236:THR:H	2.15	0.50
1:N:313:GLN:HE22	1:N:317:LYS:HZ3	1.57	0.50
1:R:313:GLN:HE22	1:R:317:LYS:HZ3	1.58	0.50
1:V:251:ARG:HH11	1:W:236:THR:CG2	2.24	0.50
1:A:234:ASN:C	1:A:236:THR:H	2.14	0.50
1:D:216:SER:HB2	2:E:2096:HOH:O	2.11	0.50
1:D:234:ASN:C	1:D:236:THR:H	2.14	0.50
1:J:195:ILE:HG23	1:J:245:LEU:HG	1.93	0.50
1:J:313:GLN:HE22	1:J:317:LYS:NZ	2.10	0.50
1:O:252:SER:HB3	1:P:192:LYS:HE3	1.92	0.50
1:V:234:ASN:C	1:V:236:THR:H	2.14	0.50
1:W:244:GLU:HG2	1:X:238:ASN:ND2	2.26	0.50
1:E:234:ASN:C	1:E:236:THR:H	2.14	0.50
1:K:216:SER:HB2	2:L:2059:HOH:O	2.11	0.50
1:L:242:ILE:O	1:L:242:ILE:HG22	2.11	0.50
1:R:65:ARG:HD2	2:R:2032:HOH:O	2.11	0.50
1:B:313:GLN:HE22	1:B:317:LYS:HZ3	1.59	0.50
1:G:250:SER:HB2	1:G:317:LYS:HE3	1.93	0.50
1:N:95:HIS:HD2	1:N:96:ARG:O	1.94	0.50
2:P:2005:HOH:O	1:Q:291:HIS:HD2	1.94	0.50
1:W:137:THR:HB	1:W:138:PRO:HD3	1.93	0.50
1:A:286:THR:HB	1:A:294:LEU:HD11	1.93	0.50
1:C:313:GLN:HE22	1:C:317:LYS:NZ	2.09	0.50
1:S:159:GLY:HA3	1:S:193:ASN:ND2	2.26	0.50
1:S:313:GLN:HE22	1:S:317:LYS:NZ	2.10	0.50
1:U:182:GLN:NE2	2:U:2051:HOH:O	2.45	0.50
1:B:159:GLY:HA3	1:B:193:ASN:ND2	2.27	0.50
1:D:147:LEU:O	1:D:184:ARG:NH2	2.44	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:HIS:HD2	1:E:96:ARG:O	1.95	0.50
1:N:244:GLU:HG2	1:O:239:ASP:HB2	1.93	0.50
1:S:115:GLU:HG2	2:S:2062:HOH:O	2.10	0.50
1:E:252:SER:HA	2:F:2093:HOH:O	2.12	0.50
1:F:234:ASN:C	1:F:236:THR:H	2.14	0.50
1:H:41:GLU:OE2	1:X:8:LYS:NZ	2.40	0.50
1:I:286:THR:HB	1:I:294:LEU:HD11	1.92	0.50
1:J:159:GLY:HA3	1:J:193:ASN:ND2	2.27	0.50
1:K:313:GLN:HE22	1:K:317:LYS:NZ	2.09	0.50
1:L:106:LEU:HD22	1:L:109:CYS:SG	2.51	0.50
1:M:234:ASN:C	1:M:236:THR:H	2.14	0.50
1:M:313:GLN:HE22	1:M:317:LYS:NZ	2.10	0.50
1:M:310:LYS:HD2	1:N:132:GLY:O	2.12	0.50
1:R:313:GLN:HE22	1:R:317:LYS:NZ	2.10	0.50
1:V:134:SER:HA	2:V:2104:HOH:O	2.11	0.50
1:B:313:GLN:HE22	1:B:317:LYS:NZ	2.09	0.49
1:F:250:SER:HB2	1:F:317:LYS:HE3	1.93	0.49
1:O:313:GLN:HE22	1:O:317:LYS:NZ	2.10	0.49
1:Q:252:SER:HB3	1:R:192:LYS:HE3	1.94	0.49
1:R:192:LYS:O	1:R:193:ASN:HB2	2.12	0.49
1:V:190:SER:OG	1:V:192:LYS:HB3	2.12	0.49
1:V:313:GLN:HE22	1:V:317:LYS:NZ	2.10	0.49
1:W:313:GLN:HE22	1:W:317:LYS:NZ	2.10	0.49
1:B:259:ILE:HD13	1:B:316:ILE:CG2	2.41	0.49
1:C:147:LEU:O	1:C:184:ARG:NH2	2.45	0.49
1:C:259:ILE:CD1	1:C:316:ILE:HG23	2.38	0.49
1:E:159:GLY:HA3	1:E:193:ASN:ND2	2.27	0.49
1:G:147:LEU:O	1:G:184:ARG:NH2	2.45	0.49
1:N:237:SER:HB3	1:N:242:ILE:CD1	2.25	0.49
1:N:313:GLN:HE22	1:N:317:LYS:NZ	2.10	0.49
1:O:250:SER:HB2	1:O:317:LYS:HE3	1.94	0.49
1:P:259:ILE:HD13	1:P:316:ILE:CG2	2.41	0.49
1:T:313:GLN:HE22	1:T:317:LYS:NZ	2.10	0.49
1:W:313:GLN:HE22	1:W:317:LYS:HZ3	1.60	0.49
1:G:259:ILE:HD13	1:G:316:ILE:CG2	2.39	0.49
1:L:126:VAL:HG22	1:L:256:SER:HB2	1.94	0.49
1:M:259:ILE:HD13	1:M:316:ILE:CG2	2.41	0.49
1:N:193:ASN:N	2:N:2154:HOH:O	2.45	0.49
1:O:95:HIS:HD2	1:O:96:ARG:O	1.95	0.49
1:V:42:ASP:HB3	2:V:2024:HOH:O	2.12	0.49
1:X:126:VAL:HG22	1:X:256:SER:HB2	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:SER:HB2	1:B:317:LYS:HE3	1.95	0.49
1:C:250:SER:HB2	1:C:317:LYS:HE3	1.93	0.49
1:G:159:GLY:HA3	1:G:193:ASN:ND2	2.27	0.49
1:H:147:LEU:O	1:H:184:ARG:NH2	2.46	0.49
1:O:159:GLY:HA3	1:O:193:ASN:ND2	2.28	0.49
1:B:257:LEU:HD22	1:B:259:ILE:CG2	2.43	0.49
1:C:184:ARG:HD3	2:C:2067:HOH:O	2.12	0.49
1:E:311:ALA:O	1:E:315:VAL:HG23	2.10	0.49
1:H:271:THR:HG21	2:H:2085:HOH:O	2.11	0.49
1:J:137:THR:HB	1:J:138:PRO:HD3	1.93	0.49
1:K:137:THR:HB	1:K:138:PRO:HD3	1.95	0.49
1:M:60:ASP:HB2	2:M:2045:HOH:O	2.11	0.49
1:P:313:GLN:HE22	1:P:317:LYS:NZ	2.10	0.49
1:R:137:THR:HB	1:R:138:PRO:HD3	1.93	0.49
1:R:259:ILE:HD13	1:R:316:ILE:CG2	2.41	0.49
1:S:45:PRO:HB3	1:S:58:VAL:HG11	1.94	0.49
1:V:159:GLY:HA3	1:V:193:ASN:ND2	2.28	0.49
1:A:242:ILE:O	1:A:242:ILE:HG22	2.11	0.49
1:C:95:HIS:HD2	1:C:96:ARG:O	1.95	0.49
1:N:207:ILE:HG23	1:N:211:ALA:HB3	1.94	0.49
1:O:147:LEU:O	1:O:184:ARG:NH2	2.46	0.49
1:P:159:GLY:HA3	1:P:193:ASN:ND2	2.28	0.49
1:Q:313:GLN:HE22	1:Q:317:LYS:NZ	2.10	0.49
1:S:147:LEU:O	1:S:184:ARG:NH2	2.46	0.49
1:S:190:SER:OG	1:S:192:LYS:HB3	2.13	0.49
1:V:250:SER:HB2	1:V:317:LYS:HE3	1.94	0.49
1:A:236:THR:HB	2:A:2086:HOH:O	2.12	0.49
1:D:126:VAL:HG22	1:D:256:SER:HB2	1.94	0.49
1:E:207:ILE:HG23	1:E:211:ALA:HB3	1.94	0.49
1:J:250:SER:HB2	1:J:317:LYS:HE3	1.94	0.49
1:J:310:LYS:HD2	1:K:132:GLY:O	2.12	0.49
1:M:216:SER:HB2	2:M:2119:HOH:O	2.11	0.49
1:M:250:SER:HB2	1:M:317:LYS:HE3	1.94	0.49
1:P:95:HIS:HD2	1:P:96:ARG:O	1.95	0.49
1:U:147:LEU:O	1:U:184:ARG:NH2	2.45	0.49
1:U:286:THR:HB	1:U:294:LEU:HD11	1.93	0.49
1:C:190:SER:OG	1:C:192:LYS:HB3	2.13	0.49
1:K:147:LEU:O	1:K:184:ARG:NH2	2.46	0.49
1:N:192:LYS:O	1:N:193:ASN:HB2	2.12	0.49
1:O:193:ASN:HA	2:O:2106:HOH:O	2.12	0.49
1:T:95:HIS:HD2	1:T:96:ARG:O	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:192:LYS:O	1:V:193:ASN:HB2	2.12	0.49
1:B:137:THR:HB	1:B:138:PRO:HD3	1.95	0.49
1:F:32:HIS:HD2	2:F:2030:HOH:O	1.95	0.49
1:N:41:GLU:O	1:N:42:ASP:HB2	2.13	0.49
1:O:41:GLU:O	1:O:42:ASP:HB2	2.13	0.49
1:Q:252:SER:HB3	1:R:192:LYS:CE	2.43	0.49
1:R:45:PRO:HB3	1:R:58:VAL:HG11	1.94	0.49
1:W:190:SER:OG	1:W:192:LYS:HB3	2.12	0.49
1:E:147:LEU:O	1:E:184:ARG:NH2	2.46	0.49
1:K:159:GLY:HA3	1:K:193:ASN:ND2	2.28	0.49
1:M:64:GLN:HG3	2:M:2048:HOH:O	2.13	0.49
1:P:137:THR:HB	1:P:138:PRO:HD3	1.93	0.49
1:R:147:LEU:O	1:R:184:ARG:NH2	2.46	0.49
1:V:137:THR:HB	1:V:138:PRO:HD3	1.94	0.49
1:V:147:LEU:O	1:V:184:ARG:NH2	2.46	0.49
1:W:95:HIS:HD2	1:W:96:ARG:O	1.95	0.49
1:B:75:LYS:HE3	1:B:79:GLY:O	2.13	0.48
1:E:259:ILE:HD13	1:E:316:ILE:CG2	2.41	0.48
1:J:190:SER:OG	1:J:192:LYS:HB3	2.13	0.48
1:O:207:ILE:HG23	1:O:211:ALA:HB3	1.95	0.48
1:Q:147:LEU:O	1:Q:184:ARG:NH2	2.45	0.48
1:Q:159:GLY:HA3	1:Q:193:ASN:ND2	2.28	0.48
1:P:252:SER:HB3	1:Q:192:LYS:CE	2.42	0.48
1:T:137:THR:HB	1:T:138:PRO:HD3	1.94	0.48
1:T:207:ILE:HG23	1:T:211:ALA:HB3	1.95	0.48
1:W:192:LYS:HA	2:W:2080:HOH:O	2.12	0.48
1:G:207:ILE:HG23	1:G:211:ALA:HB3	1.94	0.48
1:Q:45:PRO:HB3	1:Q:58:VAL:HG11	1.94	0.48
1:T:216:SER:HB2	2:T:2060:HOH:O	2.13	0.48
1:T:250:SER:HB2	1:T:317:LYS:HE3	1.94	0.48
1:V:257:LEU:HD22	1:V:259:ILE:CG2	2.43	0.48
1:I:192:LYS:HZ3	1:I:192:LYS:HB3	1.74	0.48
1:J:313:GLN:HE22	1:J:317:LYS:HZ3	1.59	0.48
1:K:313:GLN:HE22	1:K:317:LYS:HZ3	1.61	0.48
2:M:2130:HOH:O	1:S:312:ILE:HG21	2.13	0.48
1:X:195:ILE:HA	2:X:2110:HOH:O	2.12	0.48
1:E:137:THR:HB	1:E:138:PRO:HD3	1.94	0.48
1:F:259:ILE:HD13	1:F:316:ILE:CG2	2.41	0.48
1:J:41:GLU:O	1:J:42:ASP:HB2	2.12	0.48
1:N:190:SER:OG	1:N:192:LYS:HB3	2.13	0.48
1:S:193:ASN:HA	2:S:2105:HOH:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:137:THR:HB	1:F:138:PRO:HD3	1.94	0.48
1:J:147:LEU:O	1:J:184:ARG:NH2	2.47	0.48
1:K:259:ILE:HD13	1:K:316:ILE:CG2	2.40	0.48
1:K:75:LYS:HE3	1:K:79:GLY:O	2.14	0.48
1:O:190:SER:OG	1:O:192:LYS:HB3	2.13	0.48
1:Q:207:ILE:HG23	1:Q:211:ALA:HB3	1.95	0.48
1:U:238:ASN:ND2	1:U:238:ASN:N	2.61	0.48
1:V:251:ARG:HH11	1:W:236:THR:HG22	1.78	0.48
1:B:192:LYS:O	1:B:194:VAL:N	2.47	0.48
1:C:159:GLY:HA3	1:C:193:ASN:ND2	2.29	0.48
1:F:159:GLY:HA3	1:F:193:ASN:ND2	2.29	0.48
1:N:250:SER:HB2	1:N:317:LYS:HE3	1.96	0.48
1:T:190:SER:OG	1:T:192:LYS:HB3	2.13	0.48
1:W:159:GLY:HA3	1:W:193:ASN:ND2	2.29	0.48
1:D:92:LYS:HE3	1:D:92:LYS:CA	2.44	0.48
1:E:75:LYS:HE3	1:E:79:GLY:O	2.14	0.48
1:M:41:GLU:O	1:M:42:ASP:HB2	2.14	0.48
1:N:236:THR:HG22	1:N:237:SER:N	2.28	0.48
1:N:270:LEU:N	1:N:270:LEU:HD22	2.29	0.48
1:V:75:LYS:HE3	1:V:79:GLY:O	2.14	0.48
1:X:106:LEU:HD22	1:X:109:CYS:SG	2.54	0.48
1:A:38:GLU:HB3	2:A:2020:HOH:O	2.14	0.48
1:G:190:SER:OG	1:G:192:LYS:HB3	2.14	0.48
1:P:250:SER:HB2	1:P:317:LYS:HE3	1.95	0.48
1:V:248:GLU:OE1	1:W:236:THR:HG22	2.13	0.48
1:D:137:THR:HB	1:D:138:PRO:HD3	1.96	0.48
1:E:190:SER:OG	1:E:192:LYS:HB3	2.13	0.48
1:E:250:SER:HB2	1:E:317:LYS:HE3	1.94	0.48
1:K:250:SER:HB2	1:K:317:LYS:HE3	1.95	0.48
1:L:238:ASN:N	1:L:238:ASN:ND2	2.62	0.48
1:V:169:PHE:O	1:V:172:PHE:HB3	2.13	0.48
1:A:283:THR:HG22	1:A:284:LEU:N	2.29	0.48
1:E:41:GLU:O	1:E:42:ASP:HB2	2.14	0.48
1:I:147:LEU:O	1:I:184:ARG:NH2	2.47	0.48
1:J:259:ILE:HD13	1:J:316:ILE:CG2	2.40	0.48
1:K:190:SER:OG	1:K:192:LYS:HB3	2.14	0.48
1:L:240:ASP:C	1:L:242:ILE:N	2.67	0.48
1:S:95:HIS:HD2	1:S:96:ARG:O	1.95	0.48
1:F:257:LEU:HD22	1:F:259:ILE:CG2	2.44	0.47
1:J:95:HIS:HD2	1:J:96:ARG:O	1.97	0.47
1:Q:190:SER:OG	1:Q:192:LYS:HB3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:250:SER:HB2	1:Q:317:LYS:HE3	1.96	0.47
1:C:310:LYS:HD2	1:D:132:GLY:O	2.14	0.47
1:F:192:LYS:O	1:F:194:VAL:N	2.47	0.47
1:O:75:LYS:HE3	1:O:79:GLY:O	2.14	0.47
1:P:147:LEU:O	1:P:184:ARG:NH2	2.47	0.47
1:T:159:GLY:HA3	1:T:193:ASN:ND2	2.28	0.47
1:T:169:PHE:O	1:T:172:PHE:HB3	2.14	0.47
1:B:147:LEU:O	1:B:184:ARG:NH2	2.48	0.47
1:B:41:GLU:O	1:B:42:ASP:HB2	2.14	0.47
1:F:190:SER:OG	1:F:192:LYS:HB3	2.14	0.47
1:F:41:GLU:O	1:F:42:ASP:HB2	2.14	0.47
1:F:45:PRO:HB3	1:F:58:VAL:HG11	1.96	0.47
1:H:6:ASP:HB3	1:I:152:LYS:HG2	1.96	0.47
1:K:1:MET:HA	2:L:2055:HOH:O	2.14	0.47
1:K:45:PRO:HB3	1:K:58:VAL:HG11	1.96	0.47
1:M:236:THR:CG2	1:R:248:GLU:OE1	2.62	0.47
1:O:137:THR:HB	1:O:138:PRO:HD3	1.96	0.47
1:R:250:SER:HB2	1:R:317:LYS:HE3	1.96	0.47
1:U:92:LYS:CA	1:U:92:LYS:HE3	2.45	0.47
1:X:238:ASN:N	1:X:238:ASN:ND2	2.62	0.47
1:E:169:PHE:O	1:E:172:PHE:HB3	2.14	0.47
1:F:207:ILE:HG23	1:F:211:ALA:HB3	1.95	0.47
1:G:257:LEU:HD22	1:G:259:ILE:CG2	2.44	0.47
1:H:234:ASN:HB3	2:H:2139:HOH:O	2.13	0.47
1:K:257:LEU:HD22	1:K:259:ILE:CG2	2.44	0.47
1:L:270:LEU:N	1:L:270:LEU:HD22	2.29	0.47
1:M:159:GLY:HA3	1:M:193:ASN:ND2	2.28	0.47
1:N:147:LEU:O	1:N:184:ARG:NH2	2.47	0.47
1:R:159:GLY:HA3	1:R:193:ASN:ND2	2.29	0.47
1:S:207:ILE:HG23	1:S:211:ALA:HB3	1.95	0.47
1:U:283:THR:HG22	1:U:284:LEU:N	2.29	0.47
1:V:207:ILE:HG23	1:V:211:ALA:HB3	1.96	0.47
1:V:259:ILE:HD13	1:V:316:ILE:CG2	2.43	0.47
1:C:257:LEU:HD22	1:C:259:ILE:CG2	2.43	0.47
1:C:45:PRO:HB3	1:C:58:VAL:HG11	1.96	0.47
1:H:92:LYS:HE3	1:H:92:LYS:CA	2.45	0.47
1:I:247:LYS:HZ2	1:I:247:LYS:HB2	1.78	0.47
1:M:75:LYS:HE3	1:M:79:GLY:O	2.14	0.47
1:N:75:LYS:HE3	1:N:79:GLY:O	2.13	0.47
1:P:257:LEU:HD22	1:P:259:ILE:CG2	2.45	0.47
1:T:45:PRO:HB3	1:T:58:VAL:HG11	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:PRO:HB3	1:E:58:VAL:HG11	1.96	0.47
1:G:313:GLN:HE22	1:G:317:LYS:HZ3	1.60	0.47
1:J:257:LEU:HD22	1:J:259:ILE:CG2	2.45	0.47
1:Q:75:LYS:HE3	1:Q:79:GLY:O	2.15	0.47
1:S:257:LEU:HD22	1:S:259:ILE:CG2	2.45	0.47
1:W:257:LEU:HD22	1:W:259:ILE:CG2	2.45	0.47
1:W:45:PRO:HB3	1:W:58:VAL:HG11	1.95	0.47
1:G:45:PRO:HB3	1:G:58:VAL:HG11	1.95	0.47
1:G:75:LYS:HE3	1:G:79:GLY:O	2.14	0.47
1:I:126:VAL:HG22	1:I:256:SER:HB2	1.97	0.47
1:S:41:GLU:O	1:S:42:ASP:HB2	2.15	0.47
1:T:147:LEU:O	1:T:184:ARG:NH2	2.48	0.47
1:T:313:GLN:HE22	1:T:317:LYS:HZ3	1.62	0.47
1:N:259:ILE:HD13	1:N:316:ILE:CG2	2.42	0.47
1:P:169:PHE:O	1:P:172:PHE:HB3	2.15	0.47
1:W:207:ILE:HG23	1:W:211:ALA:HB3	1.96	0.47
1:W:243:VAL:O	1:W:247:LYS:HG3	2.15	0.47
1:B:252:SER:HB3	1:C:192:LYS:HE3	1.97	0.47
1:G:237:SER:HB3	1:G:242:ILE:CD1	2.26	0.47
1:L:137:THR:HB	1:L:138:PRO:HD3	1.97	0.47
1:M:45:PRO:HB3	1:M:58:VAL:HG11	1.96	0.47
1:R:169:PHE:O	1:R:172:PHE:HB3	2.14	0.47
1:A:126:VAL:HG22	1:A:256:SER:HB2	1.97	0.47
1:C:41:GLU:O	1:C:42:ASP:HB2	2.15	0.47
1:E:310:LYS:HD2	1:F:132:GLY:O	2.14	0.47
1:G:41:GLU:O	1:G:42:ASP:HB2	2.15	0.47
1:H:238:ASN:ND2	1:H:238:ASN:N	2.62	0.47
1:R:281:THR:HG22	1:R:306:GLN:O	2.15	0.47
1:V:45:PRO:HB3	1:V:58:VAL:HG11	1.96	0.47
1:N:137:THR:HB	1:N:138:PRO:HD3	1.96	0.47
1:Q:243:VAL:O	1:Q:247:LYS:HG3	2.15	0.47
1:R:207:ILE:HG23	1:R:211:ALA:HB3	1.97	0.47
1:R:41:GLU:O	1:R:42:ASP:HB2	2.14	0.47
1:T:41:GLU:O	1:T:42:ASP:HB2	2.15	0.47
1:B:45:PRO:HB3	1:B:58:VAL:HG11	1.96	0.46
1:F:75:LYS:HE3	1:F:79:GLY:O	2.15	0.46
1:G:169:PHE:O	1:G:172:PHE:HB3	2.14	0.46
1:O:252:SER:HB3	1:P:192:LYS:CE	2.45	0.46
1:O:257:LEU:HD22	1:O:259:ILE:CG2	2.45	0.46
1:P:45:PRO:HB3	1:P:58:VAL:HG11	1.97	0.46
1:Q:236:THR:HG22	1:Q:237:SER:N	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:257:LEU:HD22	1:Q:259:ILE:CG2	2.44	0.46
1:T:75:LYS:HE3	1:T:79:GLY:O	2.15	0.46
1:W:41:GLU:O	1:W:42:ASP:HB2	2.15	0.46
1:C:259:ILE:HD13	1:C:316:ILE:CG2	2.41	0.46
1:F:272:ARG:HA	2:F:2131:HOH:O	2.15	0.46
1:G:236:THR:HG22	1:G:237:SER:N	2.31	0.46
1:I:238:ASN:N	1:I:238:ASN:ND2	2.63	0.46
1:J:45:PRO:HB3	1:J:58:VAL:HG11	1.97	0.46
1:J:75:LYS:HE3	1:J:79:GLY:O	2.16	0.46
1:K:192:LYS:O	1:K:194:VAL:N	2.47	0.46
1:N:192:LYS:O	1:N:194:VAL:N	2.48	0.46
1:N:243:VAL:O	1:N:247:LYS:HG3	2.15	0.46
1:O:310:LYS:HD2	1:P:132:GLY:O	2.15	0.46
1:S:259:ILE:HD13	1:S:316:ILE:CG2	2.41	0.46
1:V:281:THR:HG22	1:V:306:GLN:O	2.16	0.46
1:C:126:VAL:HG22	1:C:256:SER:HB2	1.97	0.46
1:F:236:THR:HG22	1:F:237:SER:N	2.30	0.46
1:N:252:SER:HB3	1:O:192:LYS:CE	2.45	0.46
1:R:278:GLN:HB2	2:R:2095:HOH:O	2.14	0.46
1:T:236:THR:HG22	1:T:237:SER:N	2.29	0.46
1:T:251:ARG:HH11	1:U:236:THR:HG22	1.80	0.46
1:U:240:ASP:C	1:U:242:ILE:N	2.67	0.46
1:A:92:LYS:HE3	1:A:92:LYS:CA	2.45	0.46
1:B:190:SER:OG	1:B:192:LYS:HB3	2.15	0.46
1:M:147:LEU:O	1:M:184:ARG:NH2	2.48	0.46
1:M:192:LYS:HE3	1:R:252:SER:HB3	1.98	0.46
1:M:236:THR:HB	2:M:2125:HOH:O	2.15	0.46
1:O:192:LYS:O	1:O:194:VAL:N	2.47	0.46
1:T:243:VAL:O	1:T:247:LYS:HG3	2.16	0.46
1:T:257:LEU:HD22	1:T:259:ILE:CG2	2.46	0.46
1:U:126:VAL:HG22	1:U:256:SER:HB2	1.96	0.46
1:V:192:LYS:O	1:V:194:VAL:N	2.48	0.46
1:A:247:LYS:HB2	1:A:247:LYS:HZ2	1.79	0.46
1:D:247:LYS:HZ3	1:D:247:LYS:HB2	1.80	0.46
1:D:92:LYS:HA	1:D:92:LYS:CE	2.45	0.46
2:I:2073:HOH:O	1:N:291:HIS:HE1	1.99	0.46
1:O:237:SER:HB3	1:O:242:ILE:CD1	2.25	0.46
1:P:207:ILE:HG23	1:P:211:ALA:HB3	1.96	0.46
1:W:75:LYS:HE3	1:W:79:GLY:O	2.15	0.46
1:B:236:THR:HG22	1:B:237:SER:N	2.31	0.46
1:C:169:PHE:O	1:C:172:PHE:HB3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:THR:HG22	1:C:306:GLN:O	2.16	0.46
1:E:126:VAL:HG22	1:E:256:SER:HB2	1.98	0.46
1:E:313:GLN:HE22	1:E:317:LYS:HZ3	1.62	0.46
1:H:45:PRO:HB3	1:H:58:VAL:HG11	1.98	0.46
1:I:12:LYS:HG3	2:I:2013:HOH:O	2.16	0.46
1:I:283:THR:HG22	1:I:284:LEU:N	2.31	0.46
1:K:87:GLU:HB3	1:K:92:LYS:HD2	1.98	0.46
1:L:283:THR:HG22	1:L:284:LEU:N	2.31	0.46
1:W:169:PHE:O	1:W:172:PHE:HB3	2.15	0.46
1:A:240:ASP:C	1:A:242:ILE:N	2.68	0.46
1:D:240:ASP:C	1:D:242:ILE:N	2.68	0.46
1:H:126:VAL:HG22	1:H:256:SER:HB2	1.97	0.46
1:K:41:GLU:O	1:K:42:ASP:HB2	2.15	0.46
1:Q:281:THR:HG22	1:Q:306:GLN:O	2.16	0.46
1:S:75:LYS:HE3	1:S:79:GLY:O	2.14	0.46
1:U:92:LYS:CE	1:U:92:LYS:HA	2.46	0.46
1:M:192:LYS:O	1:M:194:VAL:N	2.48	0.46
1:O:45:PRO:HB3	1:O:58:VAL:HG11	1.97	0.46
1:P:191:LEU:HD23	1:P:191:LEU:HA	1.81	0.46
1:P:41:GLU:O	1:P:42:ASP:HB2	2.16	0.46
1:S:281:THR:HG22	1:S:306:GLN:O	2.16	0.46
1:S:30:PHE:CG	1:S:184:ARG:HG3	2.51	0.46
1:X:92:LYS:HE3	1:X:92:LYS:CA	2.45	0.46
1:B:87:GLU:HB3	1:B:92:LYS:HD2	1.97	0.46
1:D:193:ASN:HA	2:D:2101:HOH:O	2.15	0.46
1:E:87:GLU:HB3	1:E:92:LYS:HD2	1.98	0.46
1:K:40:VAL:HA	2:K:2016:HOH:O	2.15	0.46
1:P:236:THR:HG22	1:P:237:SER:N	2.31	0.46
1:R:192:LYS:O	1:R:194:VAL:N	2.49	0.46
1:V:126:VAL:HG22	1:V:256:SER:HB2	1.97	0.46
1:X:137:THR:HB	1:X:138:PRO:HD3	1.98	0.46
1:A:238:ASN:N	1:A:238:ASN:ND2	2.63	0.46
1:E:192:LYS:O	1:E:194:VAL:N	2.49	0.46
1:J:236:THR:HG22	1:J:237:SER:N	2.31	0.46
1:L:216:SER:HB3	2:L:2062:HOH:O	2.15	0.46
1:K:244:GLU:HG2	1:L:238:ASN:ND2	2.30	0.46
1:L:287:SER:OG	1:L:297:HIS:CE1	2.67	0.46
1:M:281:THR:HG22	1:M:306:GLN:O	2.16	0.46
1:O:126:VAL:HG22	1:O:256:SER:HB2	1.97	0.46
1:Q:270:LEU:HD22	1:Q:270:LEU:N	2.31	0.46
1:R:243:VAL:O	1:R:247:LYS:HG3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:V:286:THR:HB	1:V:294:LEU:CD1	2.46	0.46
1:W:236:THR:HG22	1:W:237:SER:N	2.31	0.46
1:C:243:VAL:O	1:C:247:LYS:HG3	2.16	0.45
1:H:240:ASP:O	1:H:242:ILE:N	2.48	0.45
1:K:169:PHE:O	1:K:172:PHE:HB3	2.16	0.45
1:K:243:VAL:O	1:K:247:LYS:HG3	2.16	0.45
1:K:251:ARG:HH11	1:L:236:THR:HG22	1.81	0.45
1:N:159:GLY:HA3	1:N:193:ASN:ND2	2.31	0.45
1:W:270:LEU:HD22	1:W:270:LEU:N	2.31	0.45
1:M:87:GLU:HB3	1:M:92:LYS:HD2	1.99	0.45
1:N:126:VAL:HG22	1:N:256:SER:HB2	1.98	0.45
1:N:281:THR:HG22	1:N:306:GLN:O	2.17	0.45
1:P:126:VAL:HG22	1:P:256:SER:HB2	1.97	0.45
1:T:192:LYS:O	1:T:194:VAL:N	2.48	0.45
1:V:270:LEU:HD22	1:V:270:LEU:N	2.31	0.45
1:C:207:ILE:HG23	1:C:211:ALA:HB3	1.98	0.45
1:C:248:GLU:OE2	1:D:236:THR:HG21	2.17	0.45
1:C:60:ASP:OD2	1:C:64:GLN:HB3	2.17	0.45
1:E:283:THR:HG22	1:E:284:LEU:N	2.31	0.45
1:I:240:ASP:C	1:I:242:ILE:N	2.68	0.45
1:L:178:ARG:HB2	1:L:178:ARG:HH11	1.81	0.45
1:P:243:VAL:O	1:P:247:LYS:HG3	2.15	0.45
1:S:192:LYS:O	1:S:194:VAL:N	2.49	0.45
1:S:286:THR:HB	1:S:294:LEU:CD1	2.46	0.45
1:U:240:ASP:O	1:U:242:ILE:N	2.48	0.45
1:B:281:THR:HG22	1:B:306:GLN:O	2.17	0.45
1:E:243:VAL:O	1:E:247:LYS:HG3	2.15	0.45
1:A:178:ARG:NH2	1:F:80:SER:HA	2.32	0.45
1:I:192:LYS:HZ2	1:I:192:LYS:HB3	1.81	0.45
1:J:243:VAL:O	1:J:247:LYS:HG3	2.17	0.45
1:M:207:ILE:HG23	1:M:211:ALA:HB3	1.98	0.45
1:M:243:VAL:O	1:M:247:LYS:HG3	2.16	0.45
1:O:236:THR:HG22	1:O:237:SER:N	2.32	0.45
1:Q:41:GLU:O	1:Q:42:ASP:HB2	2.15	0.45
1:C:191:LEU:HD23	1:C:191:LEU:HA	1.80	0.45
1:E:236:THR:HG22	1:E:237:SER:N	2.30	0.45
1:G:281:THR:HG22	1:G:306:GLN:O	2.17	0.45
1:K:126:VAL:HG22	1:K:256:SER:HB2	1.99	0.45
1:M:236:THR:HG22	1:M:237:SER:N	2.31	0.45
1:O:243:VAL:O	1:O:247:LYS:HG3	2.16	0.45
1:O:313:GLN:HE22	1:O:317:LYS:HZ3	1.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:192:LYS:O	1:P:194:VAL:N	2.49	0.45
1:S:87:GLU:HB3	1:S:92:LYS:HD2	1.98	0.45
1:U:270:LEU:N	1:U:270:LEU:HD22	2.31	0.45
1:V:207:ILE:HD13	2:V:2083:HOH:O	2.16	0.45
1:V:236:THR:HG22	1:V:237:SER:N	2.31	0.45
1:V:87:GLU:HB3	1:V:92:LYS:HD2	1.98	0.45
1:B:169:PHE:O	1:B:172:PHE:HB3	2.17	0.45
1:C:286:THR:HB	1:C:294:LEU:CD1	2.47	0.45
1:C:87:GLU:HB3	1:C:92:LYS:HD2	1.98	0.45
1:F:126:VAL:HG22	1:F:256:SER:HB2	1.99	0.45
1:H:270:LEU:N	1:H:270:LEU:HD22	2.31	0.45
1:Q:87:GLU:HB3	1:Q:92:LYS:HD2	1.99	0.45
1:W:87:GLU:HB3	1:W:92:LYS:HD2	1.99	0.45
1:X:45:PRO:HB3	1:X:58:VAL:HG11	1.98	0.45
1:A:137:THR:HB	1:A:138:PRO:HD3	1.99	0.45
1:A:240:ASP:O	1:A:242:ILE:N	2.49	0.45
1:D:283:THR:HG22	1:D:284:LEU:N	2.32	0.45
1:H:92:LYS:CE	1:H:92:LYS:HA	2.47	0.45
1:J:192:LYS:O	1:J:194:VAL:N	2.49	0.45
1:K:184:ARG:HD3	2:K:2063:HOH:O	2.15	0.45
1:N:169:PHE:O	1:N:172:PHE:HB3	2.17	0.45
1:G:243:VAL:O	1:G:247:LYS:HG3	2.17	0.45
1:K:236:THR:HG22	1:K:237:SER:N	2.31	0.45
1:O:169:PHE:O	1:O:172:PHE:HB3	2.16	0.45
1:P:269:VAL:O	1:P:281:THR:HA	2.17	0.45
1:P:87:GLU:HB3	1:P:92:LYS:HD2	1.99	0.45
1:Q:259:ILE:HD13	1:Q:316:ILE:CG2	2.41	0.45
1:T:270:LEU:N	1:T:270:LEU:HD22	2.32	0.45
1:V:41:GLU:O	1:V:42:ASP:HB2	2.16	0.45
1:W:259:ILE:HD13	1:W:316:ILE:CG2	2.41	0.45
1:W:281:THR:HG22	1:W:306:GLN:O	2.17	0.45
1:C:75:LYS:HE3	1:C:79:GLY:O	2.16	0.45
1:F:30:PHE:CG	1:F:184:ARG:HG3	2.51	0.45
1:G:270:LEU:N	1:G:270:LEU:HD22	2.31	0.45
1:J:126:VAL:HG22	1:J:256:SER:HB2	1.99	0.45
1:P:30:PHE:CG	1:P:184:ARG:HG3	2.52	0.45
1:Q:283:THR:HG22	1:Q:284:LEU:N	2.32	0.45
1:R:236:THR:HG22	1:R:237:SER:N	2.32	0.45
1:B:207:ILE:HG23	1:B:211:ALA:HB3	1.98	0.45
1:B:283:THR:HG22	1:B:284:LEU:N	2.32	0.45
1:B:286:THR:HB	1:B:294:LEU:CD1	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:87:GLU:HB3	1:F:92:LYS:HD2	1.98	0.45
1:H:287:SER:OG	1:H:297:HIS:CE1	2.68	0.45
1:Q:169:PHE:O	1:Q:172:PHE:HB3	2.16	0.45
1:T:126:VAL:HG22	1:T:256:SER:HB2	1.97	0.45
1:T:259:ILE:HD13	1:T:316:ILE:CG2	2.42	0.45
1:U:195:ILE:HG22	1:U:195:ILE:O	2.17	0.45
1:C:192:LYS:O	1:C:194:VAL:N	2.48	0.44
1:D:287:SER:OG	1:D:297:HIS:CE1	2.70	0.44
1:G:87:GLU:HB3	1:G:92:LYS:HD2	1.99	0.44
1:H:137:THR:HB	1:H:138:PRO:HD3	1.98	0.44
1:H:283:THR:HG22	1:H:284:LEU:N	2.32	0.44
1:J:270:LEU:N	1:J:270:LEU:HD22	2.32	0.44
1:N:191:LEU:HD23	1:N:191:LEU:HA	1.83	0.44
1:O:30:PHE:CG	1:O:184:ARG:HG3	2.52	0.44
1:R:283:THR:HG22	1:R:284:LEU:N	2.32	0.44
1:V:243:VAL:O	1:V:247:LYS:HG3	2.17	0.44
1:X:195:ILE:HG22	1:X:195:ILE:O	2.17	0.44
1:D:270:LEU:HD22	1:D:270:LEU:N	2.32	0.44
1:P:248:GLU:OE1	1:Q:236:THR:CG2	2.65	0.44
1:U:269:VAL:O	1:U:281:THR:HA	2.18	0.44
1:V:191:LEU:HA	1:V:191:LEU:HD23	1.82	0.44
1:V:283:THR:HG22	1:V:284:LEU:N	2.32	0.44
1:E:270:LEU:HD22	1:E:270:LEU:N	2.32	0.44
1:I:92:LYS:HE3	1:I:92:LYS:CA	2.44	0.44
1:L:92:LYS:HA	1:L:92:LYS:CE	2.47	0.44
1:O:191:LEU:HD23	1:O:191:LEU:HA	1.83	0.44
1:O:87:GLU:HB3	1:O:92:LYS:HD2	1.99	0.44
1:Q:286:THR:HB	1:Q:294:LEU:CD1	2.47	0.44
1:R:257:LEU:HD22	1:R:259:ILE:CG2	2.47	0.44
1:R:317:LYS:HD3	1:R:320:GLU:OE2	2.18	0.44
1:S:169:PHE:O	1:S:172:PHE:HB3	2.17	0.44
1:W:147:LEU:O	1:W:184:ARG:NH2	2.50	0.44
1:A:270:LEU:N	1:A:270:LEU:HD22	2.32	0.44
1:B:131:LYS:HD3	2:B:2089:HOH:O	2.18	0.44
1:C:30:PHE:CG	1:C:184:ARG:HG3	2.52	0.44
1:D:195:ILE:O	1:D:195:ILE:HG22	2.18	0.44
1:F:169:PHE:O	1:F:172:PHE:HB3	2.17	0.44
1:F:283:THR:HG22	1:F:284:LEU:N	2.32	0.44
1:G:192:LYS:O	1:G:194:VAL:N	2.48	0.44
1:I:270:LEU:N	1:I:270:LEU:HD22	2.33	0.44
1:J:87:GLU:HB3	1:J:92:LYS:HD2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:207:ILE:HG23	1:K:211:ALA:HB3	1.98	0.44
1:K:30:PHE:CG	1:K:184:ARG:HG3	2.52	0.44
1:P:216:SER:HB3	2:Q:2054:HOH:O	2.17	0.44
1:Q:191:LEU:HA	1:Q:191:LEU:HD23	1.85	0.44
1:T:87:GLU:HB3	1:T:92:LYS:HD2	1.99	0.44
1:X:270:LEU:HD22	1:X:270:LEU:N	2.33	0.44
1:B:126:VAL:HG22	1:B:256:SER:HB2	2.00	0.44
1:C:237:SER:HB3	1:C:242:ILE:CD1	2.26	0.44
1:C:236:THR:HG22	1:C:237:SER:N	2.32	0.44
1:D:216:SER:HB3	2:E:2097:HOH:O	2.17	0.44
1:E:257:LEU:HD22	1:E:259:ILE:CG2	2.47	0.44
1:E:281:THR:HG22	1:E:306:GLN:O	2.17	0.44
1:I:195:ILE:HG22	1:I:195:ILE:O	2.18	0.44
1:J:169:PHE:O	1:J:172:PHE:HB3	2.18	0.44
1:Q:30:PHE:CG	1:Q:184:ARG:HG3	2.52	0.44
1:Q:299:SER:HA	2:Q:2091:HOH:O	2.18	0.44
1:Q:317:LYS:HD3	1:Q:320:GLU:OE2	2.18	0.44
1:W:216:SER:HB2	2:X:2105:HOH:O	2.15	0.44
1:W:126:VAL:HG22	1:W:256:SER:HB2	2.00	0.44
1:X:269:VAL:O	1:X:281:THR:HA	2.18	0.44
1:A:92:LYS:HA	1:A:92:LYS:CE	2.46	0.44
1:C:270:LEU:N	1:C:270:LEU:HD22	2.32	0.44
1:G:60:ASP:OD2	1:G:64:GLN:HB3	2.18	0.44
1:L:240:ASP:O	1:L:242:ILE:N	2.48	0.44
1:M:192:LYS:CE	1:R:252:SER:HB3	2.47	0.44
1:M:1:MET:HA	2:N:2145:HOH:O	2.17	0.44
1:M:257:LEU:HD22	1:M:259:ILE:CG2	2.46	0.44
1:U:137:THR:HB	1:U:138:PRO:HD3	1.99	0.44
1:U:247:LYS:HB2	1:U:247:LYS:HZ3	1.83	0.44
1:B:191:LEU:HA	1:B:191:LEU:HD23	1.80	0.44
1:F:281:THR:HG22	1:F:306:GLN:O	2.17	0.44
1:M:169:PHE:O	1:M:172:PHE:HB3	2.18	0.44
1:N:45:PRO:HB3	1:N:58:VAL:HG11	1.98	0.44
1:O:60:ASP:OD2	1:O:64:GLN:HB3	2.18	0.44
1:S:236:THR:HG22	1:S:237:SER:N	2.32	0.44
1:T:30:PHE:CG	1:T:184:ARG:HG3	2.53	0.44
1:T:281:THR:HG22	1:T:306:GLN:O	2.18	0.44
1:A:119:HIS:HA	2:A:2049:HOH:O	2.17	0.44
1:A:45:PRO:HB3	1:A:58:VAL:HG11	1.99	0.44
1:B:30:PHE:CG	1:B:184:ARG:HG3	2.52	0.44
1:D:242:ILE:O	1:D:245:LEU:HB3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:137:THR:HB	1:I:138:PRO:HD3	2.00	0.44
1:I:242:ILE:O	1:I:245:LEU:HB3	2.18	0.44
1:L:92:LYS:CA	1:L:92:LYS:HE3	2.45	0.44
1:M:270:LEU:HD22	1:M:270:LEU:N	2.33	0.44
1:N:192:LYS:HG2	1:N:193:ASN:N	2.33	0.44
1:N:87:GLU:HB3	1:N:92:LYS:HD2	1.99	0.44
1:P:281:THR:HG22	1:P:306:GLN:O	2.17	0.44
1:P:75:LYS:HE3	1:P:79:GLY:O	2.17	0.44
1:Q:192:LYS:HG2	1:Q:193:ASN:N	2.33	0.44
1:U:129:THR:OG1	1:U:130:GLY:N	2.50	0.44
1:V:192:LYS:HG2	1:V:193:ASN:N	2.33	0.44
1:A:240:ASP:OD2	1:A:241:LYS:N	2.51	0.44
1:K:242:ILE:O	1:K:246:VAL:HG23	2.18	0.44
1:N:317:LYS:HD3	1:N:320:GLU:OE2	2.18	0.44
1:O:192:LYS:HG2	1:O:193:ASN:N	2.33	0.44
1:S:270:LEU:HD22	1:S:270:LEU:N	2.33	0.44
1:S:272:ARG:NH1	2:S:2122:HOH:O	2.41	0.44
1:V:269:VAL:O	1:V:281:THR:HA	2.18	0.44
1:V:248:GLU:OE1	1:W:236:THR:CG2	2.66	0.44
1:W:251:ARG:HH11	1:X:236:THR:CG2	2.30	0.44
1:W:286:THR:HB	1:W:294:LEU:CD1	2.47	0.44
1:A:269:VAL:O	1:A:281:THR:HA	2.18	0.43
1:L:269:VAL:O	1:L:281:THR:HA	2.17	0.43
1:M:236:THR:HG22	1:R:251:ARG:NH1	2.33	0.43
1:O:286:THR:HB	1:O:294:LEU:CD1	2.47	0.43
1:R:270:LEU:N	1:R:270:LEU:HD22	2.33	0.43
1:R:75:LYS:HE3	1:R:79:GLY:O	2.18	0.43
1:S:126:VAL:HG22	1:S:256:SER:HB2	1.98	0.43
1:W:314:THR:HG21	1:X:239:ASP:HB2	2.00	0.43
1:B:317:LYS:HD3	1:B:320:GLU:OE2	2.18	0.43
1:D:269:VAL:O	1:D:281:THR:HA	2.18	0.43
1:G:283:THR:HG22	1:G:284:LEU:N	2.33	0.43
1:H:178:ARG:HB2	1:H:178:ARG:HH11	1.83	0.43
1:H:195:ILE:O	1:H:195:ILE:HG22	2.18	0.43
1:I:103:THR:HG21	2:I:2090:HOH:O	2.18	0.43
1:I:269:VAL:O	1:I:281:THR:HA	2.18	0.43
1:I:4:LEU:HD23	1:J:154:ALA:HA	1.99	0.43
1:M:126:VAL:HG22	1:M:256:SER:HB2	2.00	0.43
1:N:257:LEU:HD22	1:N:259:ILE:CG2	2.48	0.43
1:S:178:ARG:HD2	2:S:2096:HOH:O	2.18	0.43
1:S:313:GLN:HE22	1:S:317:LYS:HZ3	1.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:192:LYS:O	1:W:194:VAL:N	2.49	0.43
1:W:237:SER:HB3	1:W:242:ILE:CD1	2.25	0.43
1:X:240:ASP:C	1:X:242:ILE:N	2.68	0.43
1:X:283:THR:HG22	1:X:284:LEU:N	2.33	0.43
1:A:209:ARG:HD3	2:A:2080:HOH:O	2.18	0.43
1:D:238:ASN:N	1:D:238:ASN:ND2	2.63	0.43
1:E:30:PHE:CG	1:E:184:ARG:HG3	2.54	0.43
1:E:317:LYS:HD3	1:E:320:GLU:OE2	2.18	0.43
1:H:247:LYS:HZ2	1:H:247:LYS:HB2	1.84	0.43
1:J:281:THR:HG22	1:J:306:GLN:O	2.18	0.43
1:K:270:LEU:N	1:K:270:LEU:HD22	2.33	0.43
1:K:269:VAL:O	1:K:281:THR:HA	2.19	0.43
1:P:270:LEU:HD22	1:P:270:LEU:N	2.32	0.43
1:S:243:VAL:O	1:S:247:LYS:HG3	2.19	0.43
1:U:45:PRO:HB3	1:U:58:VAL:HG11	2.00	0.43
1:A:115:GLU:HG2	2:A:2048:HOH:O	2.18	0.43
1:F:243:VAL:O	1:F:247:LYS:HG3	2.18	0.43
1:I:40:VAL:HG12	1:I:44:THR:HB	2.00	0.43
1:I:92:LYS:HA	1:I:92:LYS:CE	2.46	0.43
1:L:139:LEU:HD13	1:L:139:LEU:C	2.39	0.43
1:P:192:LYS:HG2	1:P:193:ASN:N	2.33	0.43
1:S:237:SER:HB3	1:S:242:ILE:CD1	2.24	0.43
1:V:30:PHE:CG	1:V:184:ARG:HG3	2.54	0.43
1:C:269:VAL:O	1:C:281:THR:HA	2.18	0.43
1:F:216:SER:HB3	2:F:2120:HOH:O	2.18	0.43
1:G:192:LYS:HG2	1:G:193:ASN:N	2.34	0.43
1:L:40:VAL:HG12	1:L:44:THR:HB	2.01	0.43
1:M:317:LYS:HD3	1:M:320:GLU:OE2	2.18	0.43
1:Q:269:VAL:O	1:Q:281:THR:HA	2.19	0.43
1:Q:70:LYS:HA	2:Q:2022:HOH:O	2.18	0.43
1:W:242:ILE:O	1:W:246:VAL:HG23	2.18	0.43
1:B:192:LYS:HG2	1:B:193:ASN:N	2.34	0.43
1:C:192:LYS:HG2	1:C:193:ASN:N	2.33	0.43
1:G:252:SER:OG	1:H:236:THR:HG21	2.18	0.43
1:H:242:ILE:O	1:H:245:LEU:HB3	2.19	0.43
1:J:248:GLU:OE1	1:K:236:THR:HG22	2.19	0.43
1:K:281:THR:HG22	1:K:306:GLN:O	2.18	0.43
1:L:195:ILE:O	1:L:195:ILE:HG22	2.17	0.43
1:O:207:ILE:HA	1:O:207:ILE:HD13	1.92	0.43
1:S:192:LYS:HG2	1:S:193:ASN:N	2.34	0.43
1:B:243:VAL:O	1:B:247:LYS:HG3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:LYS:HG2	1:E:193:ASN:N	2.33	0.43
1:F:237:SER:HB3	1:F:242:ILE:CD1	2.24	0.43
1:F:270:LEU:N	1:F:270:LEU:HD22	2.34	0.43
1:G:317:LYS:HD3	1:G:320:GLU:OE2	2.19	0.43
1:L:41:GLU:HB2	1:L:44:THR:OG1	2.19	0.43
1:M:286:THR:HB	1:M:294:LEU:CD1	2.48	0.43
1:M:60:ASP:OD2	1:M:64:GLN:HB3	2.18	0.43
1:T:286:THR:HB	1:T:294:LEU:CD1	2.47	0.43
1:V:252:SER:HB3	1:W:192:LYS:HE3	1.99	0.43
1:A:195:ILE:HG22	1:A:195:ILE:O	2.18	0.43
1:B:60:ASP:OD2	1:B:64:GLN:HB3	2.18	0.43
1:G:126:VAL:HG22	1:G:256:SER:HB2	2.01	0.43
1:G:30:PHE:CG	1:G:184:ARG:HG3	2.54	0.43
1:R:192:LYS:HG2	1:R:193:ASN:N	2.34	0.43
1:R:269:VAL:O	1:R:281:THR:HA	2.18	0.43
1:T:269:VAL:O	1:T:281:THR:HA	2.18	0.43
1:V:317:LYS:HD3	1:V:320:GLU:OE2	2.19	0.43
1:X:247:LYS:HB2	1:X:247:LYS:HZ3	1.81	0.43
1:C:138:PRO:HD3	2:C:2060:HOH:O	2.19	0.43
1:C:283:THR:HG22	1:C:284:LEU:N	2.34	0.43
1:F:216:SER:HB2	2:F:2116:HOH:O	2.19	0.43
1:J:192:LYS:HG2	1:J:193:ASN:N	2.34	0.43
1:O:317:LYS:HD3	1:O:320:GLU:OE2	2.18	0.43
1:Q:242:ILE:O	1:Q:246:VAL:HG23	2.19	0.43
1:U:139:LEU:HD13	1:U:139:LEU:C	2.39	0.43
1:B:269:VAL:O	1:B:281:THR:HA	2.18	0.43
1:J:30:PHE:CG	1:J:184:ARG:HG3	2.54	0.43
1:K:286:THR:HB	1:K:294:LEU:CD1	2.48	0.43
1:M:237:SER:HB3	1:M:242:ILE:CD1	2.25	0.43
1:R:191:LEU:HA	1:R:191:LEU:HD23	1.81	0.43
1:T:192:LYS:HG2	1:T:193:ASN:N	2.34	0.43
1:T:283:THR:HG22	1:T:284:LEU:N	2.33	0.43
1:A:242:ILE:O	1:A:245:LEU:HB3	2.18	0.42
1:B:67:VAL:HA	1:B:89:GLY:HA2	2.01	0.42
1:E:269:VAL:O	1:E:281:THR:HA	2.19	0.42
1:E:61:LYS:NZ	2:E:2030:HOH:O	2.52	0.42
1:I:240:ASP:O	1:I:242:ILE:N	2.50	0.42
1:J:237:SER:HB3	1:J:242:ILE:CD1	2.25	0.42
1:J:60:ASP:OD2	1:J:64:GLN:HB3	2.19	0.42
1:Q:192:LYS:O	1:Q:194:VAL:N	2.50	0.42
1:R:87:GLU:HB3	1:R:92:LYS:HD2	1.99	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:VAL:HG12	1:A:44:THR:HB	2.00	0.42
1:B:270:LEU:HD22	1:B:270:LEU:N	2.34	0.42
1:C:317:LYS:HD3	1:C:320:GLU:OE2	2.19	0.42
1:E:60:ASP:OD2	1:E:64:GLN:HB3	2.19	0.42
1:F:317:LYS:HD3	1:F:320:GLU:OE2	2.19	0.42
1:H:41:GLU:HB2	1:H:44:THR:OG1	2.18	0.42
1:R:60:ASP:OD2	1:R:64:GLN:HB3	2.19	0.42
1:A:41:GLU:HB2	1:A:44:THR:OG1	2.19	0.42
1:F:192:LYS:HG2	1:F:193:ASN:N	2.34	0.42
1:J:242:ILE:O	1:J:246:VAL:HG23	2.19	0.42
1:K:192:LYS:HG2	1:K:193:ASN:N	2.34	0.42
1:R:67:VAL:HA	1:R:89:GLY:HA2	2.02	0.42
1:S:286:THR:CB	1:S:294:LEU:HD11	2.49	0.42
1:S:67:VAL:HA	1:S:89:GLY:HA2	2.02	0.42
1:U:242:ILE:O	1:U:245:LEU:HB3	2.19	0.42
1:W:192:LYS:HG2	1:W:193:ASN:N	2.34	0.42
1:X:40:VAL:HG12	1:X:44:THR:HB	2.01	0.42
1:X:92:LYS:HA	1:X:92:LYS:CE	2.46	0.42
1:A:41:GLU:O	1:A:42:ASP:CB	2.68	0.42
1:C:67:VAL:HA	1:C:89:GLY:HA2	2.02	0.42
1:E:237:SER:HB3	1:E:242:ILE:CD1	2.25	0.42
1:F:286:THR:HB	1:F:294:LEU:CD1	2.47	0.42
1:H:240:ASP:OD2	1:H:241:LYS:N	2.51	0.42
1:J:283:THR:HG22	1:J:284:LEU:N	2.34	0.42
1:L:242:ILE:O	1:L:245:LEU:HB3	2.20	0.42
1:M:242:ILE:O	1:M:246:VAL:HG23	2.18	0.42
1:U:41:GLU:HB2	1:U:44:THR:OG1	2.20	0.42
1:W:269:VAL:O	1:W:281:THR:HA	2.19	0.42
1:W:317:LYS:HD3	1:W:320:GLU:OE2	2.19	0.42
1:D:40:VAL:HG12	1:D:44:THR:HB	2.01	0.42
1:K:317:LYS:HD3	1:K:320:GLU:OE2	2.19	0.42
1:P:283:THR:HG22	1:P:284:LEU:N	2.33	0.42
1:P:75:LYS:HD3	2:P:2027:HOH:O	2.19	0.42
1:S:283:THR:HG22	1:S:284:LEU:N	2.34	0.42
1:T:244:GLU:CG	1:U:238:ASN:ND2	2.82	0.42
1:U:287:SER:OG	1:U:297:HIS:CE1	2.69	0.42
1:U:40:VAL:HG12	1:U:44:THR:HB	2.00	0.42
1:V:242:ILE:O	1:V:246:VAL:HG23	2.20	0.42
1:G:286:THR:HB	1:G:294:LEU:CD1	2.48	0.42
1:H:290:GLU:HG2	1:H:291:HIS:CD2	2.55	0.42
1:I:139:LEU:C	1:I:139:LEU:HD13	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:45:PRO:HB3	1:L:58:VAL:HG11	2.00	0.42
1:N:242:ILE:O	1:N:246:VAL:HG23	2.20	0.42
1:O:129:THR:OG1	1:O:130:GLY:N	2.52	0.42
1:O:251:ARG:HH11	1:P:236:THR:CG2	2.32	0.42
1:O:312:ILE:HG21	2:W:2092:HOH:O	2.20	0.42
1:O:65:ARG:HD2	2:O:2095:HOH:O	2.19	0.42
1:Q:6:ASP:HB2	2:Q:2004:HOH:O	2.20	0.42
1:A:236:THR:O	1:A:238:ASN:N	2.53	0.42
1:B:134:SER:HB3	1:B:267:TRP:CZ2	2.55	0.42
1:E:129:THR:OG1	1:E:130:GLY:N	2.51	0.42
1:N:207:ILE:HD13	1:N:207:ILE:HA	1.91	0.42
1:O:115:GLU:HG2	2:O:2061:HOH:O	2.18	0.42
1:T:317:LYS:HD3	1:T:320:GLU:OE2	2.20	0.42
1:V:60:ASP:OD2	1:V:64:GLN:HB3	2.20	0.42
2:W:2085:HOH:O	1:X:238:ASN:HA	2.19	0.42
1:B:49:ILE:HG13	2:B:2029:HOH:O	2.19	0.42
1:H:40:VAL:HG12	1:H:44:THR:HB	2.01	0.42
1:J:317:LYS:HD3	1:J:320:GLU:OE2	2.19	0.42
1:M:192:LYS:HG2	1:M:193:ASN:N	2.34	0.42
1:O:251:ARG:HH11	1:P:236:THR:HG22	1.85	0.42
1:P:317:LYS:HD3	1:P:320:GLU:OE2	2.20	0.42
1:Q:126:VAL:HG22	1:Q:256:SER:HB2	2.01	0.42
1:R:30:PHE:CG	1:R:184:ARG:HG3	2.54	0.42
1:B:216:SER:HB2	2:B:2084:HOH:O	2.19	0.42
1:D:41:GLU:HB2	1:D:44:THR:OG1	2.20	0.42
1:D:45:PRO:HB3	1:D:58:VAL:HG11	2.01	0.42
1:E:242:ILE:O	1:E:246:VAL:HG23	2.19	0.42
1:G:242:ILE:O	1:G:246:VAL:HG23	2.20	0.42
1:G:67:VAL:HA	1:G:89:GLY:HA2	2.01	0.42
1:N:286:THR:HB	1:N:294:LEU:CD1	2.50	0.42
1:O:270:LEU:N	1:O:270:LEU:HD22	2.34	0.42
1:P:252:SER:HB3	1:Q:192:LYS:HE3	2.01	0.42
1:W:30:PHE:CG	1:W:184:ARG:HG3	2.55	0.42
1:W:283:THR:HG22	1:W:284:LEU:N	2.35	0.42
1:A:129:THR:OG1	1:A:130:GLY:N	2.50	0.42
1:A:178:ARG:HB2	1:A:178:ARG:HH11	1.85	0.42
1:F:207:ILE:HD13	1:F:207:ILE:HA	1.92	0.42
1:H:169:PHE:O	1:H:172:PHE:HB3	2.20	0.42
1:N:283:THR:HG22	1:N:284:LEU:N	2.34	0.42
1:O:286:THR:CB	1:O:294:LEU:HD11	2.50	0.42
1:Q:60:ASP:OD2	1:Q:64:GLN:HB3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:126:VAL:HG22	1:R:256:SER:HB2	2.01	0.42
1:W:244:GLU:OE1	1:X:238:ASN:ND2	2.53	0.42
1:C:65:ARG:HD2	2:C:2032:HOH:O	2.19	0.41
1:F:1:MET:HB2	1:F:78:ASP:OD1	2.20	0.41
1:M:67:VAL:HA	1:M:89:GLY:HA2	2.02	0.41
1:P:286:THR:HB	1:P:294:LEU:CD1	2.48	0.41
1:S:60:ASP:OD2	1:S:64:GLN:HB3	2.20	0.41
1:T:248:GLU:OE2	1:U:236:THR:HG21	2.20	0.41
1:V:237:SER:HB3	1:V:242:ILE:CD1	2.25	0.41
1:X:236:THR:O	1:X:238:ASN:N	2.53	0.41
1:H:269:VAL:O	1:H:281:THR:HA	2.19	0.41
1:I:191:LEU:O	1:I:194:VAL:HG13	2.20	0.41
1:I:41:GLU:O	1:I:42:ASP:CB	2.68	0.41
1:L:247:LYS:HZ3	1:L:247:LYS:HB2	1.81	0.41
1:O:269:VAL:O	1:O:281:THR:HA	2.19	0.41
1:O:4:LEU:HD23	1:P:154:ALA:HA	2.01	0.41
1:O:67:VAL:HA	1:O:89:GLY:HA2	2.01	0.41
1:P:134:SER:HB3	1:P:267:TRP:CZ2	2.55	0.41
1:R:286:THR:HB	1:R:294:LEU:CD1	2.48	0.41
1:S:242:ILE:O	1:S:246:VAL:HG23	2.20	0.41
1:S:269:VAL:O	1:S:281:THR:HA	2.20	0.41
1:T:242:ILE:O	1:T:246:VAL:HG23	2.20	0.41
1:T:60:ASP:OD2	1:T:64:GLN:HB3	2.20	0.41
1:X:242:ILE:O	1:X:245:LEU:HB3	2.19	0.41
1:D:286:THR:HB	1:D:294:LEU:CD1	2.49	0.41
1:E:248:GLU:OE1	1:F:236:THR:CG2	2.68	0.41
1:G:269:VAL:O	1:G:281:THR:HA	2.20	0.41
1:H:191:LEU:O	1:H:194:VAL:HG13	2.21	0.41
1:I:45:PRO:HB3	1:I:58:VAL:HG11	2.03	0.41
1:L:240:ASP:OD2	1:L:241:LYS:N	2.51	0.41
2:I:2073:HOH:O	1:N:291:HIS:CE1	2.73	0.41
1:P:5:TYR:HA	2:P:2003:HOH:O	2.19	0.41
1:P:60:ASP:OD2	1:P:64:GLN:HB3	2.20	0.41
1:X:178:ARG:HH11	1:X:178:ARG:HB2	1.84	0.41
1:D:129:THR:OG1	1:D:130:GLY:N	2.50	0.41
1:L:236:THR:O	1:L:237:SER:C	2.59	0.41
1:Q:67:VAL:HA	1:Q:89:GLY:HA2	2.01	0.41
1:T:286:THR:CB	1:T:294:LEU:HD11	2.50	0.41
1:U:240:ASP:OD2	1:U:241:LYS:N	2.52	0.41
1:D:169:PHE:O	1:D:172:PHE:HB3	2.21	0.41
1:D:62:ASN:ND2	2:D:2039:HOH:O	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:252:SER:HB3	1:K:192:LYS:HE3	2.02	0.41
1:J:269:VAL:O	1:J:281:THR:HA	2.20	0.41
1:M:134:SER:HB3	1:M:267:TRP:CZ2	2.55	0.41
1:S:1:MET:HB2	1:S:78:ASP:OD1	2.21	0.41
1:U:191:LEU:O	1:U:194:VAL:HG13	2.20	0.41
1:V:207:ILE:HA	1:V:207:ILE:HD13	1.92	0.41
1:V:67:VAL:HA	1:V:89:GLY:HA2	2.03	0.41
1:W:244:GLU:CG	1:X:238:ASN:ND2	2.83	0.41
1:X:41:GLU:HB2	1:X:44:THR:OG1	2.20	0.41
1:A:237:SER:O	1:A:238:ASN:HB2	2.20	0.41
1:D:236:THR:O	1:D:237:SER:C	2.59	0.41
1:G:134:SER:HB3	1:G:267:TRP:CZ2	2.56	0.41
1:K:237:SER:HB3	1:K:242:ILE:CD1	2.25	0.41
1:O:242:ILE:O	1:O:246:VAL:HG23	2.21	0.41
1:Q:1:MET:HB2	1:Q:78:ASP:OD1	2.21	0.41
1:T:1:MET:HB2	1:T:78:ASP:OD1	2.20	0.41
1:T:67:VAL:HA	1:T:89:GLY:HA2	2.02	0.41
1:V:43:GLY:N	2:V:2024:HOH:O	2.52	0.41
1:A:139:LEU:C	1:A:139:LEU:HD13	2.40	0.41
1:B:242:ILE:O	1:B:246:VAL:HG23	2.19	0.41
1:F:242:ILE:O	1:F:246:VAL:HG23	2.21	0.41
1:J:286:THR:HB	1:J:294:LEU:CD1	2.48	0.41
1:M:283:THR:HG22	1:M:284:LEU:N	2.35	0.41
1:N:67:VAL:HA	1:N:89:GLY:HA2	2.03	0.41
1:O:281:THR:HG22	1:O:306:GLN:O	2.20	0.41
1:P:67:VAL:HA	1:P:89:GLY:HA2	2.02	0.41
1:R:242:ILE:O	1:R:246:VAL:HG23	2.19	0.41
1:U:247:LYS:HB2	1:U:247:LYS:HZ2	1.86	0.41
1:V:252:SER:HB3	1:W:192:LYS:CE	2.51	0.41
1:X:236:THR:O	1:X:237:SER:C	2.59	0.41
1:D:178:ARG:HB2	1:D:178:ARG:HH11	1.83	0.41
1:H:236:THR:O	1:H:238:ASN:N	2.53	0.41
1:I:41:GLU:OE2	1:M:22:HIS:CB	2.66	0.41
1:L:236:THR:O	1:L:238:ASN:N	2.54	0.41
1:N:269:VAL:O	1:N:281:THR:HA	2.20	0.41
1:N:60:ASP:OD2	1:N:64:GLN:HB3	2.20	0.41
1:O:283:THR:HG22	1:O:284:LEU:N	2.35	0.41
1:O:80:SER:HA	1:P:178:ARG:NH2	2.36	0.41
1:U:236:THR:O	1:U:238:ASN:N	2.54	0.41
1:B:129:THR:OG1	1:B:130:GLY:N	2.52	0.41
1:F:269:VAL:O	1:F:281:THR:HA	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:ASP:OD2	1:F:64:GLN:HB3	2.21	0.41
1:O:87:GLU:HB2	2:O:2043:HOH:O	2.21	0.41
1:R:134:SER:HB3	1:R:267:TRP:CZ2	2.56	0.41
1:U:236:THR:O	1:U:237:SER:C	2.59	0.41
1:U:237:SER:O	1:U:238:ASN:HB2	2.21	0.41
1:W:129:THR:OG1	1:W:130:GLY:N	2.51	0.41
1:X:139:LEU:C	1:X:139:LEU:HD13	2.41	0.41
1:A:236:THR:O	1:A:237:SER:C	2.59	0.41
1:I:129:THR:OG1	1:I:130:GLY:N	2.51	0.41
1:J:134:SER:HB3	1:J:267:TRP:CZ2	2.56	0.41
1:S:317:LYS:HD3	1:S:320:GLU:OE2	2.20	0.41
1:D:236:THR:O	1:D:238:ASN:N	2.53	0.41
1:D:248:GLU:OE1	1:E:236:THR:HG23	2.20	0.41
1:F:64:GLN:HG3	2:F:2043:HOH:O	2.20	0.41
1:I:131:LYS:HD3	1:I:243:VAL:HG11	2.03	0.41
1:I:236:THR:O	1:I:238:ASN:N	2.53	0.41
1:M:269:VAL:O	1:M:281:THR:HA	2.21	0.41
1:Q:286:THR:CB	1:Q:294:LEU:HD11	2.50	0.41
1:S:60:ASP:HB2	2:S:2037:HOH:O	2.21	0.41
1:W:248:GLU:OE2	1:X:236:THR:HG21	2.21	0.41
1:W:272:ARG:NH1	2:W:2097:HOH:O	2.44	0.41
1:X:240:ASP:O	1:X:242:ILE:N	2.48	0.41
1:B:286:THR:CB	1:B:294:LEU:HD11	2.51	0.40
1:D:237:SER:O	1:D:238:ASN:HB2	2.21	0.40
1:E:207:ILE:HD13	1:E:207:ILE:HA	1.92	0.40
1:E:236:THR:HB	2:E:2107:HOH:O	2.21	0.40
1:F:67:VAL:HA	1:F:89:GLY:HA2	2.03	0.40
1:H:246:VAL:HG23	1:H:247:LYS:N	2.37	0.40
1:K:191:LEU:HA	1:K:191:LEU:HD23	1.79	0.40
1:L:41:GLU:O	1:L:42:ASP:CB	2.67	0.40
1:N:30:PHE:CG	1:N:184:ARG:HG3	2.56	0.40
1:R:45:PRO:HD3	1:R:69:TYR:CE2	2.57	0.40
1:S:191:LEU:HD23	1:S:191:LEU:HA	1.82	0.40
1:U:178:ARG:HB2	1:U:178:ARG:HH11	1.85	0.40
1:U:290:GLU:HG2	1:U:291:HIS:CD2	2.56	0.40
1:W:60:ASP:OD2	1:W:64:GLN:HB3	2.20	0.40
1:A:287:SER:OG	1:A:297:HIS:CE1	2.75	0.40
1:D:240:ASP:O	1:D:242:ILE:N	2.48	0.40
1:G:286:THR:CB	1:G:294:LEU:HD11	2.51	0.40
1:H:129:THR:OG1	1:H:130:GLY:N	2.53	0.40
1:H:286:THR:HB	1:H:294:LEU:CD1	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:248:GLU:OE2	1:L:236:THR:HG21	2.21	0.40
1:V:134:SER:HB3	1:V:267:TRP:CZ2	2.56	0.40
1:A:1:MET:HB2	1:A:78:ASP:OD1	2.22	0.40
1:B:252:SER:HB3	1:C:192:LYS:CE	2.51	0.40
1:C:286:THR:CB	1:C:294:LEU:HD11	2.50	0.40
1:C:314:THR:HG21	1:D:239:ASP:CG	2.42	0.40
1:D:139:LEU:HD13	1:D:139:LEU:C	2.42	0.40
1:E:286:THR:HB	1:E:294:LEU:CD1	2.50	0.40
1:E:67:VAL:HA	1:E:89:GLY:HA2	2.02	0.40
1:H:237:SER:O	1:H:238:ASN:HB2	2.21	0.40
1:I:237:SER:O	1:I:238:ASN:HB2	2.22	0.40
1:K:67:VAL:HA	1:K:89:GLY:HA2	2.02	0.40
1:N:310:LYS:HB3	1:O:132:GLY:O	2.22	0.40
1:N:1:MET:HB2	1:N:78:ASP:OD1	2.21	0.40
1:O:1:MET:HB2	1:O:78:ASP:OD1	2.21	0.40
1:P:1:MET:HB2	1:P:78:ASP:OD1	2.21	0.40
1:P:207:ILE:HA	1:P:207:ILE:HD13	1.91	0.40
1:P:242:ILE:O	1:P:246:VAL:HG23	2.20	0.40
1:S:80:SER:HA	1:T:178:ARG:NH2	2.37	0.40
1:U:246:VAL:HG23	1:U:247:LYS:N	2.37	0.40
1:V:45:PRO:HD3	1:V:69:TYR:CE2	2.56	0.40
1:I:287:SER:OG	1:I:297:HIS:CE1	2.72	0.40
1:L:234:ASN:C	1:L:236:THR:N	2.75	0.40
1:T:45:PRO:HD3	1:T:69:TYR:CE2	2.57	0.40
1:X:240:ASP:OD2	1:X:241:LYS:N	2.52	0.40
1:C:129:THR:OG1	1:C:130:GLY:N	2.53	0.40
1:S:4:LEU:HD23	1:T:154:ALA:HA	2.03	0.40
1:X:241:LYS:N	1:X:241:LYS:HD2	2.37	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:115:GLU:OE2	1:N:39:SER:OG[1_655]	1.92	0.28
1:E:39:SER:CB	1:W:115:GLU:OE1[1_645]	2.04	0.16
1:D:115:GLU:OE2	1:X:38:GLU:O[1_545]	2.17	0.03

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	285/331 (86%)	265 (93%)	16 (6%)	4 (1%)	11	20
1	B	298/331 (90%)	286 (96%)	7 (2%)	5 (2%)	9	16
1	C	298/331 (90%)	286 (96%)	7 (2%)	5 (2%)	9	16
1	D	285/331 (86%)	266 (93%)	15 (5%)	4 (1%)	11	20
1	E	298/331 (90%)	288 (97%)	5 (2%)	5 (2%)	9	16
1	F	298/331 (90%)	285 (96%)	8 (3%)	5 (2%)	9	16
1	G	298/331 (90%)	287 (96%)	6 (2%)	5 (2%)	9	16
1	H	285/331 (86%)	266 (93%)	15 (5%)	4 (1%)	11	20
1	I	285/331 (86%)	266 (93%)	15 (5%)	4 (1%)	11	20
1	J	298/331 (90%)	285 (96%)	8 (3%)	5 (2%)	9	16
1	K	298/331 (90%)	284 (95%)	9 (3%)	5 (2%)	9	16
1	L	285/331 (86%)	265 (93%)	16 (6%)	4 (1%)	11	20
1	M	298/331 (90%)	287 (96%)	6 (2%)	5 (2%)	9	16
1	N	298/331 (90%)	286 (96%)	7 (2%)	5 (2%)	9	16
1	O	298/331 (90%)	285 (96%)	8 (3%)	5 (2%)	9	16
1	P	298/331 (90%)	287 (96%)	6 (2%)	5 (2%)	9	16
1	Q	298/331 (90%)	287 (96%)	6 (2%)	5 (2%)	9	16
1	R	298/331 (90%)	286 (96%)	7 (2%)	5 (2%)	9	16
1	S	298/331 (90%)	288 (97%)	5 (2%)	5 (2%)	9	16
1	T	298/331 (90%)	286 (96%)	7 (2%)	5 (2%)	9	16
1	U	285/331 (86%)	266 (93%)	15 (5%)	4 (1%)	11	20
1	V	298/331 (90%)	285 (96%)	8 (3%)	5 (2%)	9	16
1	W	298/331 (90%)	286 (96%)	7 (2%)	5 (2%)	9	16
1	X	285/331 (86%)	265 (93%)	16 (6%)	4 (1%)	11	20
All	All	7061/7944 (89%)	6723 (95%)	225 (3%)	113 (2%)	9	17

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	236	THR
1	C	236	THR
1	E	236	THR
1	F	236	THR
1	G	236	THR
1	J	236	THR
1	K	236	THR
1	M	236	THR
1	N	236	THR
1	O	236	THR
1	P	236	THR
1	Q	236	THR
1	R	236	THR
1	S	236	THR
1	T	236	THR
1	V	236	THR
1	W	236	THR
1	B	41	GLU
1	B	240	ASP
1	C	41	GLU
1	C	240	ASP
1	E	41	GLU
1	E	240	ASP
1	F	41	GLU
1	F	240	ASP
1	G	41	GLU
1	G	240	ASP
1	J	41	GLU
1	J	240	ASP
1	K	41	GLU
1	K	240	ASP
1	M	41	GLU
1	M	240	ASP
1	N	41	GLU
1	N	240	ASP
1	O	41	GLU
1	O	240	ASP
1	P	41	GLU
1	P	240	ASP
1	Q	41	GLU
1	Q	240	ASP
1	R	41	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	240	ASP
1	S	41	GLU
1	S	240	ASP
1	T	41	GLU
1	T	240	ASP
1	V	41	GLU
1	V	240	ASP
1	W	41	GLU
1	W	240	ASP
1	B	42	ASP
1	B	190	SER
1	C	42	ASP
1	C	190	SER
1	E	42	ASP
1	E	190	SER
1	F	42	ASP
1	F	190	SER
1	G	42	ASP
1	G	190	SER
1	J	42	ASP
1	J	190	SER
1	K	42	ASP
1	K	190	SER
1	M	42	ASP
1	M	190	SER
1	N	42	ASP
1	N	190	SER
1	O	42	ASP
1	O	190	SER
1	P	42	ASP
1	P	190	SER
1	Q	42	ASP
1	Q	190	SER
1	R	42	ASP
1	R	190	SER
1	S	42	ASP
1	S	190	SER
1	T	42	ASP
1	T	190	SER
1	V	42	ASP
1	V	190	SER
1	W	42	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	W	190	SER
1	A	237	SER
1	D	237	SER
1	H	237	SER
1	I	41	GLU
1	I	237	SER
1	L	237	SER
1	U	41	GLU
1	U	237	SER
1	X	41	GLU
1	X	237	SER
1	A	190	SER
1	D	41	GLU
1	D	42	ASP
1	D	190	SER
1	H	190	SER
1	I	42	ASP
1	L	42	ASP
1	L	190	SER
1	X	42	ASP
1	X	190	SER
1	A	41	GLU
1	A	42	ASP
1	H	41	GLU
1	H	42	ASP
1	I	190	SER
1	L	41	GLU
1	U	42	ASP
1	U	190	SER

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	234/265 (88%)	225 (96%)	9 (4%)	33 58
1	B	247/265 (93%)	238 (96%)	9 (4%)	35 61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	246/265 (93%)	237 (96%)	9 (4%)	34	60
1	D	234/265 (88%)	225 (96%)	9 (4%)	33	58
1	E	247/265 (93%)	237 (96%)	10 (4%)	31	56
1	F	247/265 (93%)	238 (96%)	9 (4%)	35	61
1	G	247/265 (93%)	237 (96%)	10 (4%)	31	56
1	H	234/265 (88%)	225 (96%)	9 (4%)	33	58
1	I	234/265 (88%)	225 (96%)	9 (4%)	33	58
1	J	247/265 (93%)	238 (96%)	9 (4%)	35	61
1	K	247/265 (93%)	238 (96%)	9 (4%)	35	61
1	L	234/265 (88%)	225 (96%)	9 (4%)	33	58
1	M	247/265 (93%)	238 (96%)	9 (4%)	35	61
1	N	247/265 (93%)	238 (96%)	9 (4%)	35	61
1	O	247/265 (93%)	238 (96%)	9 (4%)	35	61
1	P	247/265 (93%)	238 (96%)	9 (4%)	35	61
1	Q	247/265 (93%)	237 (96%)	10 (4%)	31	56
1	R	247/265 (93%)	237 (96%)	10 (4%)	31	56
1	S	247/265 (93%)	237 (96%)	10 (4%)	31	56
1	T	247/265 (93%)	237 (96%)	10 (4%)	31	56
1	U	234/265 (88%)	225 (96%)	9 (4%)	33	58
1	V	247/265 (93%)	237 (96%)	10 (4%)	31	56
1	W	247/265 (93%)	237 (96%)	10 (4%)	31	56
1	X	234/265 (88%)	225 (96%)	9 (4%)	33	58
All	All	5836/6360 (92%)	5612 (96%)	224 (4%)	33	58

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	92	LYS
1	A	106	LEU
1	A	162	LEU
1	A	192	LYS
1	A	257	LEU
1	A	262	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	271	THR
1	A	284	LEU
1	B	47	LEU
1	B	92	LYS
1	B	106	LEU
1	B	162	LEU
1	B	194	VAL
1	B	257	LEU
1	B	271	THR
1	B	284	LEU
1	B	313	GLN
1	C	47	LEU
1	C	92	LYS
1	C	106	LEU
1	C	162	LEU
1	C	194	VAL
1	C	257	LEU
1	C	271	THR
1	C	284	LEU
1	C	313	GLN
1	D	47	LEU
1	D	92	LYS
1	D	106	LEU
1	D	162	LEU
1	D	192	LYS
1	D	257	LEU
1	D	262	ASP
1	D	271	THR
1	D	284	LEU
1	E	47	LEU
1	E	92	LYS
1	E	106	LEU
1	E	162	LEU
1	E	194	VAL
1	E	257	LEU
1	E	271	THR
1	E	277	LEU
1	E	284	LEU
1	E	313	GLN
1	F	47	LEU
1	F	92	LYS
1	F	106	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	162	LEU
1	F	194	VAL
1	F	257	LEU
1	F	271	THR
1	F	284	LEU
1	F	313	GLN
1	G	47	LEU
1	G	92	LYS
1	G	106	LEU
1	G	162	LEU
1	G	194	VAL
1	G	257	LEU
1	G	271	THR
1	G	277	LEU
1	G	284	LEU
1	G	313	GLN
1	H	47	LEU
1	H	92	LYS
1	H	106	LEU
1	H	162	LEU
1	H	192	LYS
1	H	257	LEU
1	H	262	ASP
1	H	271	THR
1	H	284	LEU
1	I	47	LEU
1	I	92	LYS
1	I	106	LEU
1	I	162	LEU
1	I	192	LYS
1	I	257	LEU
1	I	262	ASP
1	I	271	THR
1	I	284	LEU
1	J	47	LEU
1	J	92	LYS
1	J	106	LEU
1	J	162	LEU
1	J	194	VAL
1	J	257	LEU
1	J	271	THR
1	J	284	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	313	GLN
1	K	47	LEU
1	K	92	LYS
1	K	106	LEU
1	K	162	LEU
1	K	194	VAL
1	K	257	LEU
1	K	271	THR
1	K	284	LEU
1	K	313	GLN
1	L	47	LEU
1	L	92	LYS
1	L	106	LEU
1	L	162	LEU
1	L	192	LYS
1	L	257	LEU
1	L	262	ASP
1	L	271	THR
1	L	284	LEU
1	M	47	LEU
1	M	92	LYS
1	M	106	LEU
1	M	162	LEU
1	M	194	VAL
1	M	257	LEU
1	M	271	THR
1	M	284	LEU
1	M	313	GLN
1	N	47	LEU
1	N	92	LYS
1	N	106	LEU
1	N	162	LEU
1	N	194	VAL
1	N	257	LEU
1	N	271	THR
1	N	284	LEU
1	N	313	GLN
1	O	47	LEU
1	O	92	LYS
1	O	106	LEU
1	O	162	LEU
1	O	194	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	257	LEU
1	O	271	THR
1	O	284	LEU
1	O	313	GLN
1	P	47	LEU
1	P	92	LYS
1	P	106	LEU
1	P	162	LEU
1	P	194	VAL
1	P	257	LEU
1	P	271	THR
1	P	284	LEU
1	P	313	GLN
1	Q	47	LEU
1	Q	92	LYS
1	Q	106	LEU
1	Q	162	LEU
1	Q	194	VAL
1	Q	257	LEU
1	Q	271	THR
1	Q	277	LEU
1	Q	284	LEU
1	Q	313	GLN
1	R	47	LEU
1	R	92	LYS
1	R	106	LEU
1	R	162	LEU
1	R	194	VAL
1	R	257	LEU
1	R	271	THR
1	R	277	LEU
1	R	284	LEU
1	R	313	GLN
1	S	47	LEU
1	S	92	LYS
1	S	106	LEU
1	S	162	LEU
1	S	194	VAL
1	S	257	LEU
1	S	271	THR
1	S	277	LEU
1	S	284	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	313	GLN
1	T	47	LEU
1	T	92	LYS
1	T	106	LEU
1	T	162	LEU
1	T	194	VAL
1	T	257	LEU
1	T	271	THR
1	T	277	LEU
1	T	284	LEU
1	T	313	GLN
1	U	47	LEU
1	U	92	LYS
1	U	106	LEU
1	U	162	LEU
1	U	192	LYS
1	U	257	LEU
1	U	262	ASP
1	U	271	THR
1	U	284	LEU
1	V	47	LEU
1	V	92	LYS
1	V	106	LEU
1	V	162	LEU
1	V	194	VAL
1	V	257	LEU
1	V	271	THR
1	V	277	LEU
1	V	284	LEU
1	V	313	GLN
1	W	47	LEU
1	W	92	LYS
1	W	106	LEU
1	W	162	LEU
1	W	194	VAL
1	W	257	LEU
1	W	271	THR
1	W	277	LEU
1	W	284	LEU
1	W	313	GLN
1	X	47	LEU
1	X	92	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	106	LEU
1	X	162	LEU
1	X	192	LYS
1	X	257	LEU
1	X	262	ASP
1	X	271	THR
1	X	284	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (265) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	95	HIS
1	A	182	GLN
1	A	193	ASN
1	A	238	ASN
1	A	268	GLN
1	A	278	GLN
1	A	291	HIS
1	A	297	HIS
1	B	22	HIS
1	B	62	ASN
1	B	95	HIS
1	B	182	GLN
1	B	238	ASN
1	B	253	ASN
1	B	268	GLN
1	B	278	GLN
1	B	291	HIS
1	B	297	HIS
1	B	306	GLN
1	B	313	GLN
1	C	22	HIS
1	C	62	ASN
1	C	95	HIS
1	C	182	GLN
1	C	238	ASN
1	C	253	ASN
1	C	268	GLN
1	C	278	GLN
1	C	291	HIS
1	C	297	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	306	GLN
1	C	313	GLN
1	D	95	HIS
1	D	182	GLN
1	D	193	ASN
1	D	238	ASN
1	D	268	GLN
1	D	278	GLN
1	D	291	HIS
1	D	297	HIS
1	E	22	HIS
1	E	62	ASN
1	E	95	HIS
1	E	182	GLN
1	E	238	ASN
1	E	253	ASN
1	E	268	GLN
1	E	278	GLN
1	E	291	HIS
1	E	297	HIS
1	E	306	GLN
1	E	313	GLN
1	F	22	HIS
1	F	32	HIS
1	F	62	ASN
1	F	95	HIS
1	F	182	GLN
1	F	238	ASN
1	F	253	ASN
1	F	268	GLN
1	F	278	GLN
1	F	291	HIS
1	F	297	HIS
1	F	306	GLN
1	F	313	GLN
1	G	22	HIS
1	G	62	ASN
1	G	95	HIS
1	G	119	HIS
1	G	182	GLN
1	G	238	ASN
1	G	253	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	268	GLN
1	G	278	GLN
1	G	297	HIS
1	G	306	GLN
1	G	313	GLN
1	H	95	HIS
1	H	182	GLN
1	H	193	ASN
1	H	238	ASN
1	H	253	ASN
1	H	278	GLN
1	H	291	HIS
1	H	297	HIS
1	I	3	HIS
1	I	22	HIS
1	I	95	HIS
1	I	182	GLN
1	I	193	ASN
1	I	238	ASN
1	I	268	GLN
1	I	278	GLN
1	I	291	HIS
1	I	297	HIS
1	J	32	HIS
1	J	62	ASN
1	J	95	HIS
1	J	182	GLN
1	J	238	ASN
1	J	253	ASN
1	J	268	GLN
1	J	278	GLN
1	J	291	HIS
1	J	297	HIS
1	J	306	GLN
1	J	313	GLN
1	K	22	HIS
1	K	62	ASN
1	K	95	HIS
1	K	182	GLN
1	K	238	ASN
1	K	253	ASN
1	K	268	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	278	GLN
1	K	291	HIS
1	K	297	HIS
1	K	306	GLN
1	K	313	GLN
1	L	22	HIS
1	L	95	HIS
1	L	182	GLN
1	L	193	ASN
1	L	238	ASN
1	L	268	GLN
1	L	278	GLN
1	L	291	HIS
1	L	297	HIS
1	M	62	ASN
1	M	95	HIS
1	M	182	GLN
1	M	238	ASN
1	M	253	ASN
1	M	268	GLN
1	M	278	GLN
1	M	297	HIS
1	M	306	GLN
1	M	313	GLN
1	N	22	HIS
1	N	62	ASN
1	N	95	HIS
1	N	182	GLN
1	N	238	ASN
1	N	253	ASN
1	N	268	GLN
1	N	278	GLN
1	N	291	HIS
1	N	297	HIS
1	N	306	GLN
1	N	313	GLN
1	O	3	HIS
1	O	22	HIS
1	O	32	HIS
1	O	62	ASN
1	O	95	HIS
1	O	182	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	238	ASN
1	O	253	ASN
1	O	268	GLN
1	O	278	GLN
1	O	297	HIS
1	O	306	GLN
1	O	313	GLN
1	P	22	HIS
1	P	62	ASN
1	P	95	HIS
1	P	182	GLN
1	P	238	ASN
1	P	253	ASN
1	P	268	GLN
1	P	278	GLN
1	P	291	HIS
1	P	297	HIS
1	P	306	GLN
1	P	313	GLN
1	Q	22	HIS
1	Q	62	ASN
1	Q	95	HIS
1	Q	182	GLN
1	Q	238	ASN
1	Q	253	ASN
1	Q	268	GLN
1	Q	278	GLN
1	Q	297	HIS
1	Q	306	GLN
1	Q	313	GLN
1	R	22	HIS
1	R	62	ASN
1	R	95	HIS
1	R	182	GLN
1	R	238	ASN
1	R	253	ASN
1	R	268	GLN
1	R	278	GLN
1	R	297	HIS
1	R	306	GLN
1	R	313	GLN
1	S	22	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	62	ASN
1	S	95	HIS
1	S	182	GLN
1	S	238	ASN
1	S	253	ASN
1	S	268	GLN
1	S	278	GLN
1	S	291	HIS
1	S	297	HIS
1	S	306	GLN
1	S	313	GLN
1	T	22	HIS
1	T	62	ASN
1	T	95	HIS
1	T	182	GLN
1	T	238	ASN
1	T	253	ASN
1	T	268	GLN
1	T	278	GLN
1	T	291	HIS
1	T	297	HIS
1	T	306	GLN
1	T	313	GLN
1	U	22	HIS
1	U	95	HIS
1	U	182	GLN
1	U	193	ASN
1	U	238	ASN
1	U	268	GLN
1	U	278	GLN
1	U	291	HIS
1	U	297	HIS
1	V	3	HIS
1	V	22	HIS
1	V	62	ASN
1	V	95	HIS
1	V	182	GLN
1	V	238	ASN
1	V	253	ASN
1	V	268	GLN
1	V	278	GLN
1	V	297	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	V	306	GLN
1	V	313	GLN
1	W	22	HIS
1	W	62	ASN
1	W	95	HIS
1	W	182	GLN
1	W	238	ASN
1	W	253	ASN
1	W	268	GLN
1	W	278	GLN
1	W	291	HIS
1	W	297	HIS
1	W	306	GLN
1	W	313	GLN
1	X	22	HIS
1	X	95	HIS
1	X	182	GLN
1	X	193	ASN
1	X	238	ASN
1	X	253	ASN
1	X	268	GLN
1	X	278	GLN
1	X	291	HIS
1	X	297	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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	289/331 (87%)	0.22	25 (8%) 10 10	25, 38, 90, 114	0
1	B	304/331 (91%)	0.44	40 (13%) 3 3	26, 39, 89, 118	0
1	C	304/331 (91%)	0.20	22 (7%) 15 16	24, 37, 89, 119	0
1	D	289/331 (87%)	0.12	18 (6%) 20 21	22, 36, 90, 113	0
1	E	304/331 (91%)	0.32	35 (11%) 4 4	23, 37, 90, 119	0
1	F	304/331 (91%)	0.15	20 (6%) 18 19	23, 37, 89, 118	0
1	G	304/331 (91%)	0.29	24 (7%) 12 12	25, 38, 88, 119	0
1	H	289/331 (87%)	0.18	20 (6%) 16 17	20, 34, 90, 113	0
1	I	289/331 (87%)	0.40	29 (10%) 7 6	19, 33, 90, 113	0
1	J	304/331 (91%)	0.22	27 (8%) 9 9	20, 34, 88, 118	0
1	K	304/331 (91%)	0.30	32 (10%) 6 6	24, 38, 89, 119	0
1	L	289/331 (87%)	0.39	28 (9%) 7 7	25, 39, 91, 114	0
1	M	304/331 (91%)	0.42	35 (11%) 4 4	18, 34, 89, 119	0
1	N	304/331 (91%)	0.44	34 (11%) 5 4	19, 34, 90, 119	0
1	O	304/331 (91%)	0.20	24 (7%) 12 12	23, 36, 89, 119	0
1	P	304/331 (91%)	0.38	39 (12%) 3 3	26, 39, 90, 119	0
1	Q	304/331 (91%)	0.54	36 (11%) 4 4	27, 40, 90, 119	0
1	R	304/331 (91%)	0.35	29 (9%) 8 8	23, 37, 89, 119	0
1	S	304/331 (91%)	0.20	23 (7%) 13 14	22, 37, 89, 118	0
1	T	304/331 (91%)	0.33	29 (9%) 8 8	24, 40, 89, 118	0
1	U	289/331 (87%)	0.43	37 (12%) 3 3	27, 40, 91, 114	0
1	V	304/331 (91%)	0.30	34 (11%) 5 4	26, 39, 89, 119	0
1	W	304/331 (91%)	0.27	37 (12%) 4 3	25, 38, 90, 118	0
1	X	289/331 (87%)	0.24	25 (8%) 10 10	21, 36, 91, 114	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	7191/7944 (90%)	0.31	702 (9%) 7 7	18, 37, 91, 119	0

All (702) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	133	ASN	8.9
1	I	79	GLY	8.3
1	N	309	GLY	7.9
1	K	240	ASP	7.9
1	T	240	ASP	7.8
1	N	236	THR	7.4
1	E	312	ILE	7.3
1	I	76	ALA	7.3
1	S	133	ASN	7.3
1	L	195	ILE	7.2
1	M	318	ASN	7.2
1	M	241	LYS	7.2
1	W	240	ASP	7.1
1	U	195	ILE	7.1
1	X	195	ILE	7.1
1	A	300	LYS	7.1
1	R	240	ASP	7.0
1	T	76	ALA	7.0
1	P	311	ALA	6.8
1	E	133	ASN	6.7
1	D	299	SER	6.6
1	P	243	VAL	6.5
1	U	242	ILE	6.5
1	E	237	SER	6.5
1	E	240	ASP	6.4
1	N	240	ASP	6.4
1	P	240	ASP	6.4
1	O	237	SER	6.4
1	U	236	THR	6.3
1	I	236	THR	6.3
1	N	307	ALA	6.3
1	P	299	SER	6.3
1	R	133	ASN	6.2
1	X	76	ALA	6.2
1	K	76	ALA	6.2
1	C	321	LEU	6.2
1	Q	309	GLY	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	318	ASN	6.1
1	A	195	ILE	6.0
1	S	240	ASP	6.0
1	P	321	LEU	6.0
1	T	42	ASP	6.0
1	V	133	ASN	6.0
1	X	242	ILE	5.9
1	A	299	SER	5.9
1	V	240	ASP	5.9
1	O	79	GLY	5.9
1	J	240	ASP	5.9
1	B	240	ASP	5.8
1	G	237	SER	5.7
1	G	41	GLU	5.7
1	N	241	LYS	5.7
1	L	76	ALA	5.6
1	B	134	SER	5.6
1	B	238	ASN	5.6
1	K	321	LEU	5.6
1	G	195	ILE	5.6
1	J	207	ILE	5.6
1	O	195	ILE	5.5
1	L	236	THR	5.5
1	B	237	SER	5.5
1	H	77	GLU	5.5
1	S	237	SER	5.5
1	X	236	THR	5.5
1	I	132	GLY	5.5
1	E	236	THR	5.5
1	J	195	ILE	5.5
1	V	207	ILE	5.5
1	O	133	ASN	5.4
1	R	239	ASP	5.4
1	N	299	SER	5.4
1	R	309	GLY	5.4
1	S	132	GLY	5.4
1	Q	307	ALA	5.3
1	P	241	LYS	5.3
1	Q	299	SER	5.3
1	S	79	GLY	5.3
1	D	300	LYS	5.2
1	I	75	LYS	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	80	SER	5.1
1	K	78	ASP	5.1
1	Q	319	ASP	5.1
1	A	236	THR	5.1
1	U	207	ILE	5.1
1	V	132	GLY	5.1
1	R	236	THR	5.1
1	J	237	SER	5.1
1	T	241	LYS	5.0
1	G	133	ASN	5.0
1	F	207	ILE	5.0
1	Q	239	ASP	5.0
1	T	195	ILE	5.0
1	M	195	ILE	5.0
1	A	238	ASN	5.0
1	K	79	GLY	5.0
1	I	133	ASN	4.9
1	N	311	ALA	4.9
1	N	308	SER	4.9
1	V	237	SER	4.9
1	B	321	LEU	4.9
1	E	76	ALA	4.9
1	M	311	ALA	4.9
1	O	321	LEU	4.9
1	R	195	ILE	4.9
1	H	242	ILE	4.9
1	Q	133	ASN	4.8
1	G	207	ILE	4.8
1	N	321	LEU	4.8
1	X	245	LEU	4.8
1	W	195	ILE	4.8
1	R	321	LEU	4.8
1	J	236	THR	4.7
1	T	77	GLU	4.7
1	H	236	THR	4.7
1	F	195	ILE	4.7
1	F	240	ASP	4.7
1	M	239	ASP	4.7
1	X	41	GLU	4.7
1	U	40	VAL	4.7
1	M	312	ILE	4.7
1	N	207	ILE	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	315	VAL	4.6
1	Q	312	ILE	4.6
1	U	133	ASN	4.6
1	R	319	ASP	4.6
1	G	134	SER	4.6
1	I	242	ILE	4.6
1	B	241	LYS	4.6
1	L	75	LYS	4.6
1	E	299	SER	4.6
1	N	312	ILE	4.6
1	D	238	ASN	4.6
1	P	195	ILE	4.6
1	B	132	GLY	4.5
1	O	240	ASP	4.5
1	G	77	GLU	4.5
1	J	133	ASN	4.5
1	E	195	ILE	4.5
1	G	75	LYS	4.5
1	V	321	LEU	4.5
1	I	77	GLU	4.5
1	E	132	GLY	4.5
1	E	309	GLY	4.5
1	D	195	ILE	4.5
1	G	240	ASP	4.5
1	H	42	ASP	4.5
1	W	241	LYS	4.5
1	C	240	ASP	4.5
1	E	311	ALA	4.4
1	I	239	ASP	4.4
1	W	77	GLU	4.4
1	T	43	GLY	4.4
1	E	77	GLU	4.4
1	G	42	ASP	4.4
1	J	321	LEU	4.4
1	N	242	ILE	4.4
1	N	306	GLN	4.4
1	Q	241	LYS	4.3
1	T	306	GLN	4.3
1	L	240	ASP	4.3
1	J	241	LYS	4.3
1	N	244	GLU	4.3
1	I	78	ASP	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	193	ASN	4.3
1	L	243	VAL	4.3
1	Q	240	ASP	4.3
1	L	133	ASN	4.3
1	W	318	ASN	4.3
1	I	195	ILE	4.2
1	L	242	ILE	4.2
1	N	314	THR	4.2
1	Q	195	ILE	4.2
1	P	79	GLY	4.2
1	R	132	GLY	4.2
1	F	241	LYS	4.2
1	W	238	ASN	4.2
1	M	321	LEU	4.2
1	S	321	LEU	4.2
1	P	314	THR	4.2
1	N	238	ASN	4.2
1	N	195	ILE	4.2
1	U	245	LEU	4.2
1	V	76	ALA	4.2
1	N	243	VAL	4.2
1	R	237	SER	4.2
1	C	195	ILE	4.1
1	W	321	LEU	4.1
1	K	195	ILE	4.1
1	K	241	LYS	4.1
1	P	312	ILE	4.1
1	P	306	GLN	4.1
1	R	207	ILE	4.1
1	S	195	ILE	4.1
1	I	193	ASN	4.1
1	K	236	THR	4.1
1	M	240	ASP	4.1
1	U	77	GLU	4.1
1	W	76	ALA	4.1
1	X	79	GLY	4.1
1	U	193	ASN	4.1
1	Q	236	THR	4.0
1	M	306	GLN	4.0
1	M	299	SER	4.0
1	B	195	ILE	4.0
1	L	245	LEU	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	319	ASP	4.0
1	Q	207	ILE	4.0
1	R	306	GLN	4.0
1	D	237	SER	4.0
1	W	245	LEU	3.9
1	G	299	SER	3.9
1	N	237	SER	3.9
1	O	318	ASN	3.9
1	T	299	SER	3.9
1	U	76	ALA	3.9
1	U	248	GLU	3.9
1	I	74	VAL	3.9
1	P	308	SER	3.9
1	A	242	ILE	3.9
1	E	318	ASN	3.9
1	K	299	SER	3.9
1	O	299	SER	3.9
1	N	245	LEU	3.9
1	L	300	LYS	3.8
1	S	76	ALA	3.8
1	Q	321	LEU	3.8
1	S	241	LYS	3.8
1	R	243	VAL	3.8
1	B	307	ALA	3.8
1	V	134	SER	3.8
1	B	42	ASP	3.8
1	D	240	ASP	3.8
1	B	76	ALA	3.8
1	A	193	ASN	3.8
1	N	318	ASN	3.8
1	V	306	GLN	3.8
1	M	237	SER	3.8
1	M	320	GLU	3.7
1	V	236	THR	3.7
1	W	299	SER	3.7
1	Q	320	GLU	3.7
1	S	299	SER	3.7
1	U	299	SER	3.7
1	W	320	GLU	3.7
1	T	318	ASN	3.7
1	P	236	THR	3.7
1	X	299	SER	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	243	VAL	3.7
1	L	209	ARG	3.7
1	L	298	THR	3.7
1	A	77	GLU	3.7
1	I	41	GLU	3.6
1	B	239	ASP	3.6
1	W	319	ASP	3.6
1	A	207	ILE	3.6
1	V	312	ILE	3.6
1	X	207	ILE	3.6
1	C	42	ASP	3.6
1	L	80	SER	3.6
1	L	237	SER	3.6
1	W	243	VAL	3.6
1	E	319	ASP	3.6
1	I	299	SER	3.6
1	R	314	THR	3.6
1	P	77	GLU	3.6
1	V	318	ASN	3.6
1	R	241	LYS	3.6
1	R	134	SER	3.5
1	U	75	LYS	3.5
1	T	321	LEU	3.5
1	E	321	LEU	3.5
1	U	243	VAL	3.5
1	B	131	LYS	3.5
1	J	299	SER	3.5
1	H	240	ASP	3.5
1	T	75	LYS	3.5
1	W	242	ILE	3.5
1	Q	298	THR	3.5
1	R	312	ILE	3.4
1	P	76	ALA	3.4
1	U	78	ASP	3.4
1	A	237	SER	3.4
1	H	299	SER	3.4
1	M	315	VAL	3.4
1	B	299	SER	3.4
1	H	193	ASN	3.4
1	B	78	ASP	3.4
1	C	132	GLY	3.4
1	E	134	SER	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	243	VAL	3.4
1	W	312	ILE	3.4
1	F	133	ASN	3.4
1	S	236	THR	3.4
1	S	318	ASN	3.4
1	X	193	ASN	3.4
1	M	243	VAL	3.4
1	P	207	ILE	3.4
1	Q	313	GLN	3.3
1	T	133	ASN	3.3
1	U	42	ASP	3.3
1	M	314	THR	3.3
1	M	317	LYS	3.3
1	S	207	ILE	3.3
1	N	239	ASP	3.3
1	X	240	ASP	3.3
1	E	74	VAL	3.3
1	P	315	VAL	3.3
1	B	207	ILE	3.3
1	P	239	ASP	3.3
1	T	78	ASP	3.3
1	Q	311	ALA	3.3
1	M	133	ASN	3.2
1	L	64	GLN	3.2
1	S	134	SER	3.2
1	E	320	GLU	3.2
1	M	242	ILE	3.2
1	F	299	SER	3.2
1	H	237	SER	3.2
1	U	237	SER	3.2
1	P	319	ASP	3.2
1	K	207	ILE	3.2
1	O	207	ILE	3.2
1	O	193	ASN	3.2
1	N	320	GLU	3.2
1	Q	88	ASN	3.2
1	H	241	LYS	3.2
1	D	77	GLU	3.2
1	Q	308	SER	3.2
1	W	237	SER	3.2
1	C	309	GLY	3.2
1	O	236	THR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	V	195	ILE	3.1
1	X	238	ASN	3.1
1	C	243	VAL	3.1
1	Q	77	GLU	3.1
1	Q	76	ALA	3.1
1	C	131	LYS	3.1
1	U	88	ASN	3.1
1	V	77	GLU	3.1
1	X	77	GLU	3.1
1	H	239	ASP	3.1
1	K	42	ASP	3.1
1	W	239	ASP	3.1
1	X	103	THR	3.1
1	M	308	SER	3.1
1	R	318	ASN	3.1
1	Q	310	LYS	3.1
1	H	245	LEU	3.1
1	M	238	ASN	3.1
1	N	134	SER	3.1
1	K	75	LYS	3.1
1	L	77	GLU	3.1
1	E	306	GLN	3.1
1	S	306	GLN	3.1
1	Q	42	ASP	3.1
1	X	133	ASN	3.1
1	J	194	VAL	3.1
1	P	310	LYS	3.0
1	S	70	LYS	3.0
1	J	238	ASN	3.0
1	Q	238	ASN	3.0
1	V	311	ALA	3.0
1	S	243	VAL	3.0
1	U	131	LYS	3.0
1	B	242	ILE	3.0
1	G	78	ASP	3.0
1	G	241	LYS	3.0
1	M	88	ASN	3.0
1	X	248	GLU	3.0
1	R	299	SER	3.0
1	P	307	ALA	3.0
1	N	248	GLU	3.0
1	V	41	GLU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	T	207	ILE	3.0
1	V	75	LYS	3.0
1	B	80	SER	3.0
1	L	70	LYS	3.0
1	C	207	ILE	3.0
1	O	134	SER	3.0
1	U	73	SER	3.0
1	U	74	VAL	3.0
1	I	240	ASP	3.0
1	J	319	ASP	3.0
1	M	319	ASP	2.9
1	V	241	LYS	2.9
1	X	237	SER	2.9
1	B	311	ALA	2.9
1	U	149	GLY	2.9
1	V	238	ASN	2.9
1	R	41	GLU	2.9
1	F	131	LYS	2.9
1	Q	237	SER	2.9
1	L	88	ASN	2.9
1	T	309	GLY	2.9
1	T	243	VAL	2.9
1	N	133	ASN	2.9
1	I	131	LYS	2.9
1	S	209	ARG	2.9
1	A	42	ASP	2.9
1	B	298	THR	2.9
1	G	236	THR	2.9
1	B	312	ILE	2.9
1	L	207	ILE	2.9
1	P	238	ASN	2.9
1	I	251	ARG	2.9
1	K	70	LYS	2.9
1	Q	75	LYS	2.9
1	B	236	THR	2.9
1	P	70	LYS	2.9
1	B	318	ASN	2.8
1	H	243	VAL	2.8
1	X	78	ASP	2.8
1	E	241	LYS	2.8
1	H	195	ILE	2.8
1	O	241	LYS	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	U	150	LYS	2.8
1	B	103	THR	2.8
1	V	239	ASP	2.8
1	K	313	GLN	2.8
1	O	306	GLN	2.8
1	M	245	LEU	2.8
1	Q	245	LEU	2.8
1	K	239	ASP	2.8
1	L	42	ASP	2.8
1	B	309	GLY	2.8
1	F	75	LYS	2.8
1	D	207	ILE	2.8
1	I	207	ILE	2.8
1	K	311	ALA	2.8
1	P	245	LEU	2.8
1	U	70	LYS	2.8
1	E	88	ASN	2.8
1	L	79	GLY	2.8
1	E	78	ASP	2.8
1	W	207	ILE	2.8
1	D	76	ALA	2.8
1	B	306	GLN	2.7
1	W	315	VAL	2.7
1	B	75	LYS	2.7
1	I	237	SER	2.7
1	T	308	SER	2.7
1	C	77	GLU	2.7
1	D	242	ILE	2.7
1	E	207	ILE	2.7
1	W	236	THR	2.7
1	R	77	GLU	2.7
1	S	77	GLU	2.7
1	T	39	SER	2.7
1	Q	306	GLN	2.7
1	O	243	VAL	2.7
1	X	243	VAL	2.7
1	O	77	GLU	2.7
1	P	242	ILE	2.7
1	S	88	ASN	2.7
1	L	251	ARG	2.7
1	S	42	ASP	2.7
1	X	247	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	79	GLY	2.7
1	A	70	LYS	2.7
1	A	243	VAL	2.7
1	K	77	GLU	2.7
1	V	193	ASN	2.7
1	N	78	ASP	2.7
1	O	74	VAL	2.7
1	A	209	ARG	2.7
1	W	316	ILE	2.7
1	O	75	LYS	2.7
1	W	75	LYS	2.7
1	M	42	ASP	2.7
1	E	310	LYS	2.6
1	R	298	THR	2.6
1	U	241	LYS	2.6
1	D	75	LYS	2.6
1	J	243	VAL	2.6
1	C	306	GLN	2.6
1	E	244	GLU	2.6
1	H	115	GLU	2.6
1	F	209	ARG	2.6
1	L	299	SER	2.6
1	F	318	ASN	2.6
1	M	77	GLU	2.6
1	S	238	ASN	2.6
1	V	314	THR	2.6
1	J	239	ASP	2.6
1	P	41	GLU	2.6
1	G	132	GLY	2.6
1	O	8	LYS	2.6
1	B	40	VAL	2.6
1	K	81	VAL	2.6
1	W	78	ASP	2.6
1	I	238	ASN	2.6
1	K	39	SER	2.6
1	K	73	SER	2.6
1	D	42	ASP	2.6
1	W	42	ASP	2.6
1	L	246	VAL	2.6
1	M	236	THR	2.6
1	I	134	SER	2.6
1	O	132	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	41	GLU	2.6
1	G	321	LEU	2.5
1	N	131	LYS	2.5
1	P	317	LYS	2.5
1	Q	70	LYS	2.5
1	P	313	GLN	2.5
1	W	313	GLN	2.5
1	A	240	ASP	2.5
1	D	193	ASN	2.5
1	F	132	GLY	2.5
1	J	193	ASN	2.5
1	I	73	SER	2.5
1	O	42	ASP	2.5
1	O	76	ALA	2.5
1	X	75	LYS	2.5
1	K	74	VAL	2.5
1	B	104	GLY	2.5
1	U	38	GLU	2.5
1	V	320	GLU	2.5
1	P	39	SER	2.5
1	E	131	LYS	2.5
1	E	313	GLN	2.5
1	T	314	THR	2.5
1	B	90	PHE	2.5
1	T	70	LYS	2.5
1	X	70	LYS	2.5
1	H	248	GLU	2.5
1	L	239	ASP	2.5
1	Q	317	LYS	2.5
1	M	207	ILE	2.5
1	J	77	GLU	2.5
1	K	209	ARG	2.5
1	A	81	VAL	2.5
1	T	134	SER	2.5
1	W	80	SER	2.5
1	B	310	LYS	2.5
1	E	8	LYS	2.5
1	E	307	ALA	2.5
1	P	43	GLY	2.5
1	Q	193	ASN	2.5
1	D	80	SER	2.5
1	V	299	SER	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	70	LYS	2.5
1	Q	242	ILE	2.5
1	W	317	LYS	2.5
1	D	133	ASN	2.5
1	W	306	GLN	2.4
1	J	81	VAL	2.4
1	A	239	ASP	2.4
1	E	239	ASP	2.4
1	U	240	ASP	2.4
1	B	79	GLY	2.4
1	E	238	ASN	2.4
1	R	238	ASN	2.4
1	J	306	GLN	2.4
1	T	307	ALA	2.4
1	V	298	THR	2.4
1	Q	134	SER	2.4
1	C	239	ASP	2.4
1	H	300	LYS	2.4
1	U	43	GLY	2.4
1	C	311	ALA	2.4
1	W	314	THR	2.4
1	B	39	SER	2.4
1	B	315	VAL	2.4
1	H	194	VAL	2.4
1	G	239	ASP	2.4
1	U	72	LYS	2.4
1	A	35	GLY	2.4
1	R	193	ASN	2.4
1	P	320	GLU	2.4
1	I	81	VAL	2.4
1	N	75	LYS	2.4
1	M	309	GLY	2.4
1	X	42	ASP	2.4
1	J	88	ASN	2.4
1	J	132	GLY	2.4
1	V	43	GLY	2.4
1	W	244	GLU	2.4
1	M	75	LYS	2.4
1	V	131	LYS	2.4
1	B	81	VAL	2.4
1	J	41	GLU	2.4
1	I	247	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	319	ASP	2.4
1	S	319	ASP	2.4
1	C	133	ASN	2.3
1	P	309	GLY	2.3
1	V	315	VAL	2.3
1	X	74	VAL	2.3
1	U	251	ARG	2.3
1	M	244	GLU	2.3
1	U	298	THR	2.3
1	K	92	LYS	2.3
1	F	193	ASN	2.3
1	B	77	GLU	2.3
1	L	248	GLU	2.3
1	A	212	PHE	2.3
1	G	76	ALA	2.3
1	D	132	GLY	2.3
1	W	132	GLY	2.3
1	T	41	GLU	2.3
1	J	64	GLN	2.3
1	A	245	LEU	2.3
1	F	77	GLU	2.3
1	M	115	GLU	2.3
1	Q	209	ARG	2.3
1	F	236	THR	2.3
1	A	92	LYS	2.3
1	L	78	ASP	2.3
1	O	29	TRP	2.3
1	P	318	ASN	2.3
1	W	209	ARG	2.3
1	C	317	LYS	2.3
1	J	134	SER	2.3
1	T	311	ALA	2.3
1	F	78	ASP	2.3
1	A	150	LYS	2.3
1	V	309	GLY	2.3
1	U	212	PHE	2.3
1	W	311	ALA	2.3
1	V	317	LYS	2.2
1	V	42	ASP	2.2
1	H	70	LYS	2.2
1	E	315	VAL	2.2
1	X	81	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	237	SER	2.2
1	Q	90	PHE	2.2
1	J	318	ASN	2.2
1	G	80	SER	2.2
1	M	249	ALA	2.2
1	M	313	GLN	2.2
1	E	42	ASP	2.2
1	K	8	LYS	2.2
1	K	315	VAL	2.2
1	W	40	VAL	2.2
1	I	245	LEU	2.2
1	T	132	GLY	2.2
1	U	132	GLY	2.2
1	K	103	THR	2.2
1	U	92	LYS	2.2
1	V	209	ARG	2.2
1	F	73	SER	2.2
1	R	39	SER	2.2
1	C	236	THR	2.2
1	W	298	THR	2.2
1	G	90	PHE	2.2
1	V	79	GLY	2.2
1	U	244	GLU	2.2
1	N	310	LYS	2.1
1	C	318	ASN	2.1
1	B	149	GLY	2.1
1	W	104	GLY	2.1
1	P	244	GLU	2.1
1	K	80	SER	2.1
1	J	42	ASP	2.1
1	P	88	ASN	2.1
1	R	315	VAL	2.1
1	F	244	GLU	2.1
1	C	312	ILE	2.1
1	J	76	ALA	2.1
1	O	312	ILE	2.1
1	D	79	GLY	2.1
1	N	40	VAL	2.1
1	G	242	ILE	2.1
1	K	312	ILE	2.1
1	V	316	ILE	2.1
1	P	42	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	N	77	GLU	2.1
1	T	319	ASP	2.1
1	P	104	GLY	2.1
1	D	92	LYS	2.1
1	C	237	SER	2.1
1	M	193	ASN	2.1
1	T	38	GLU	2.1
1	C	75	LYS	2.1
1	P	209	ARG	2.1
1	G	319	ASP	2.0
1	H	78	ASP	2.0
1	R	307	ALA	2.0
1	Q	243	VAL	2.0
1	F	306	GLN	2.0
1	A	75	LYS	2.0
1	M	76	ALA	2.0
1	A	248	GLU	2.0
1	K	243	VAL	2.0
1	B	308	SER	2.0
1	C	64	GLN	2.0
1	P	237	SER	2.0
1	B	43	GLY	2.0
1	H	207	ILE	2.0
1	I	42	ASP	2.0
1	F	41	GLU	2.0
1	G	290	GLU	2.0
1	A	131	LYS	2.0
1	K	314	THR	2.0
1	R	150	LYS	2.0
1	U	103	THR	2.0
1	W	103	THR	2.0
1	E	80	SER	2.0
1	U	80	SER	2.0
1	R	90	PHE	2.0
1	T	239	ASP	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.