



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:34 AM UTC

PDB ID : 4LIN / pdb_00004lin
Title : Exploring the atomic structure and conformational flexibility of a 320 angstrom long engineered viral fiber using X-ray crystallography
Authors : Bhardwaj, A.; Cingolani, G.
Deposited on : 2013-07-02
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

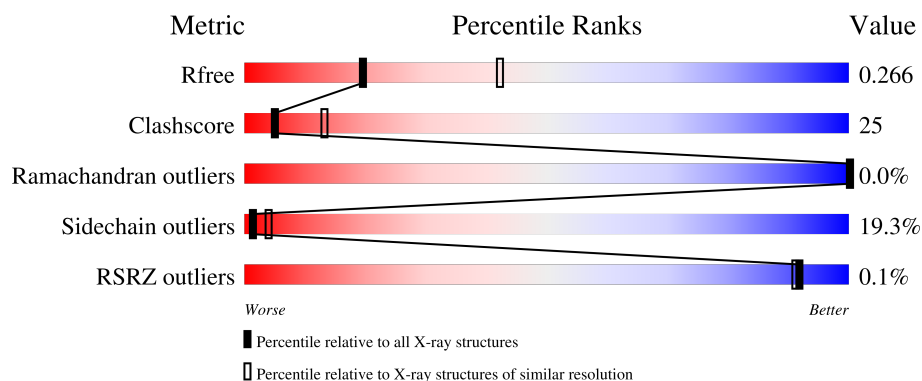
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

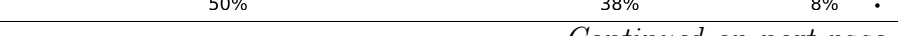
The reported resolution of this entry is 2.70 Å.

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



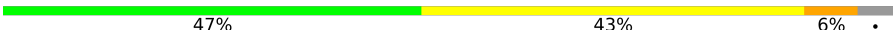
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	300	
1	B	300	
1	C	300	
1	D	300	
1	E	300	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	300	 47% 43% 6% .
1	G	300	 50% 39% 7% .
1	H	300	 45% 42% 9% .
1	I	300	 48% 40% 8% .
1	J	300	 49% 39% 8% .
1	K	300	 50% 38% 9% .
1	L	300	 49% 38% 9% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	1303	-	-	X	-
3	CL	H	1301	-	-	X	-
3	CL	I	1301	-	-	X	-
3	CL	L	1301	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26552 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 Tail needle protein gp26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	B	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	C	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	D	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	E	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	F	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	G	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	H	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	I	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	J	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	K	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			
1	L	289	Total	C	N	O	S	0	0	0
			2148	1310	386	451	1			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	E	1	Total	Ca	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total 1	Ca 1	0	0
2	J	1	Total 1	Ca 1	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Cl 2	0	0
3	D	1	Total 1	Cl 1	0	0
3	E	1	Total 1	Cl 1	0	0
3	H	1	Total 1	Cl 1	0	0
3	I	1	Total 1	Cl 1	0	0
3	K	1	Total 1	Cl 1	0	0
3	L	1	Total 1	Cl 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	70	Total 70	O 70	0	0
4	B	81	Total 81	O 81	0	0
4	C	54	Total 54	O 54	0	0
4	D	68	Total 68	O 68	0	0
4	E	61	Total 61	O 61	0	0
4	F	70	Total 70	O 70	0	0
4	G	58	Total 58	O 58	0	0
4	H	54	Total 54	O 54	0	0

Continued on next page...

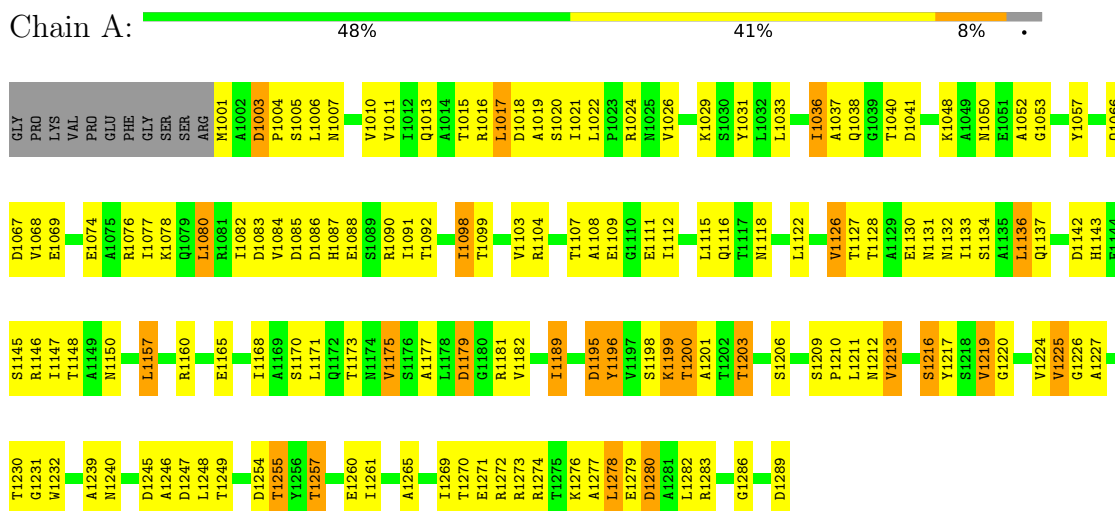
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	61	Total 61	O 61	0	0
4	J	67	Total 67	O 67	0	0
4	K	53	Total 53	O 53	0	0
4	L	67	Total 67	O 67	0	0

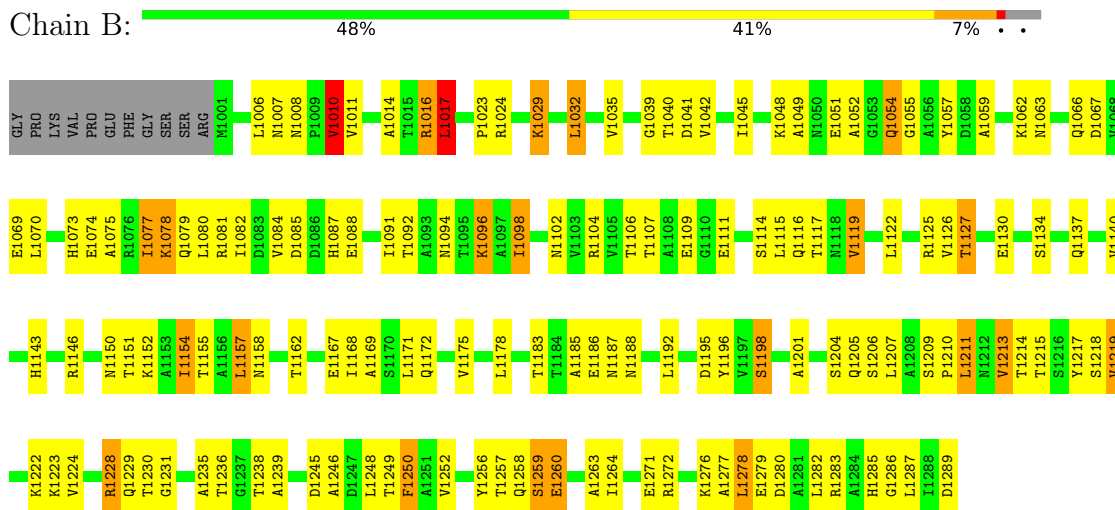
3 Residue-property plots [i](#)

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

• Molecule 1: Tail needle protein gp26

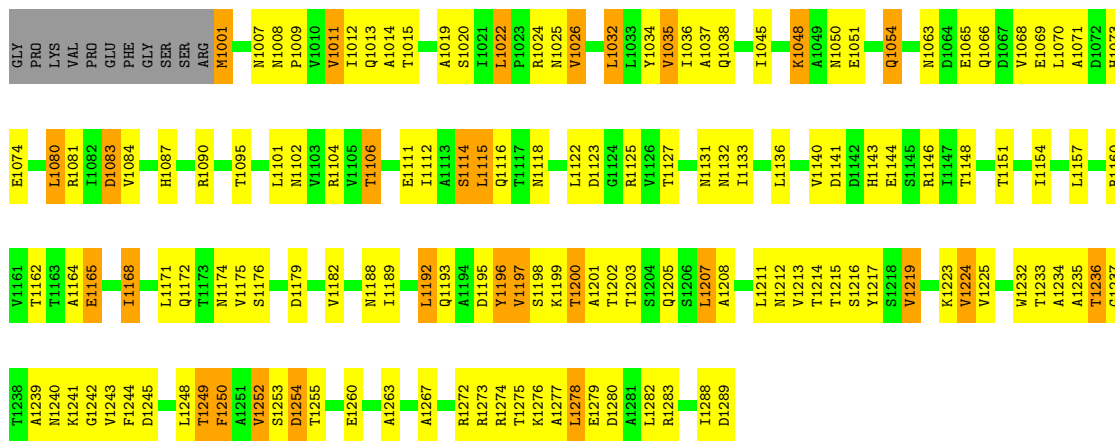


• Molecule 1: Tail needle protein gp26

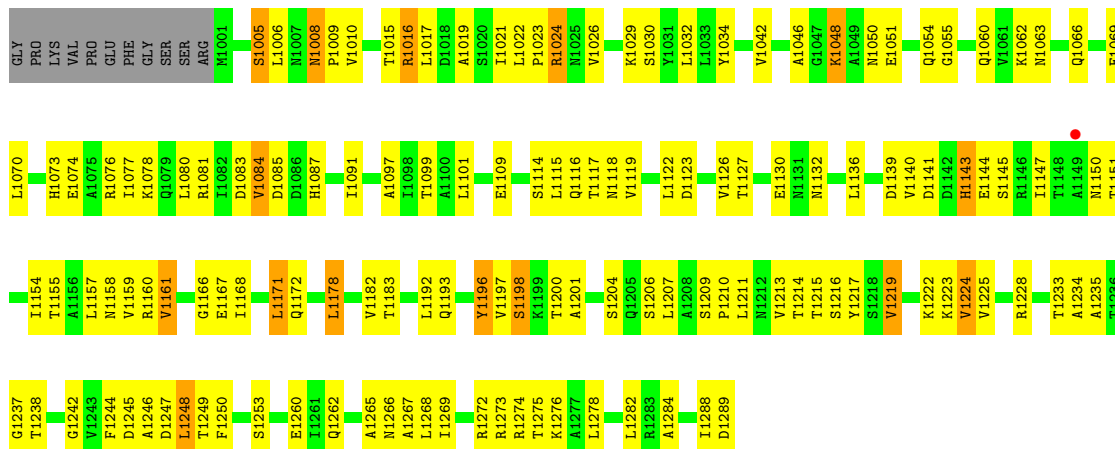


• Molecule 1: Tail needle protein gp26

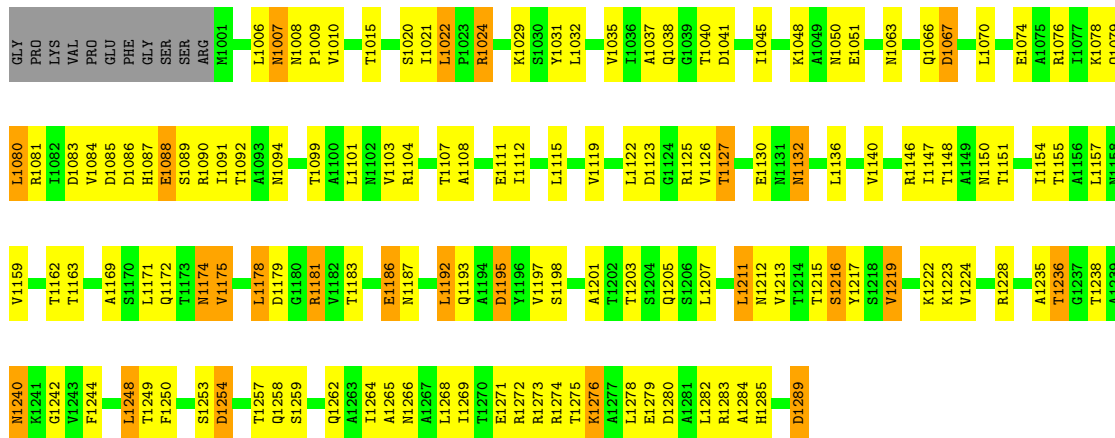




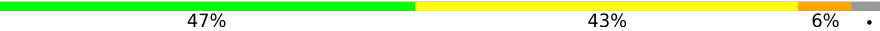
• Molecule 1: Tail needle protein gp26

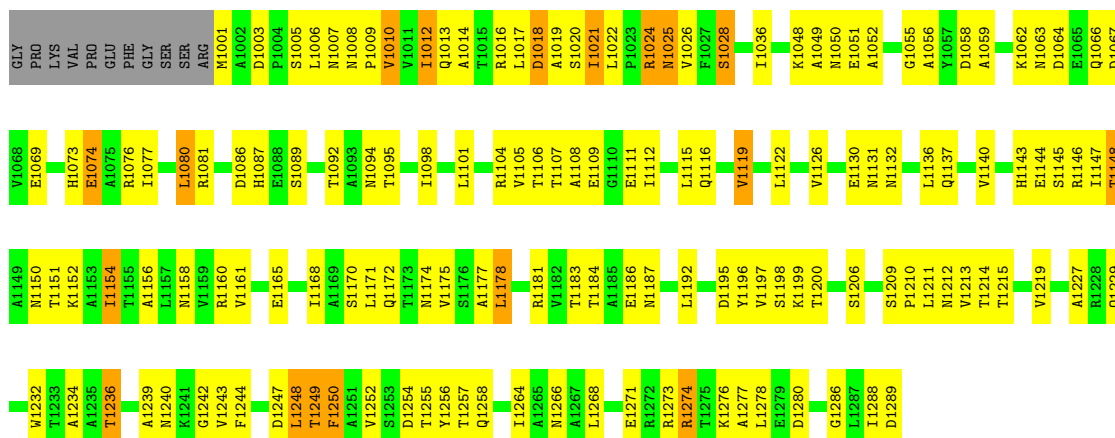


• Molecule 1: Tail needle protein gp26



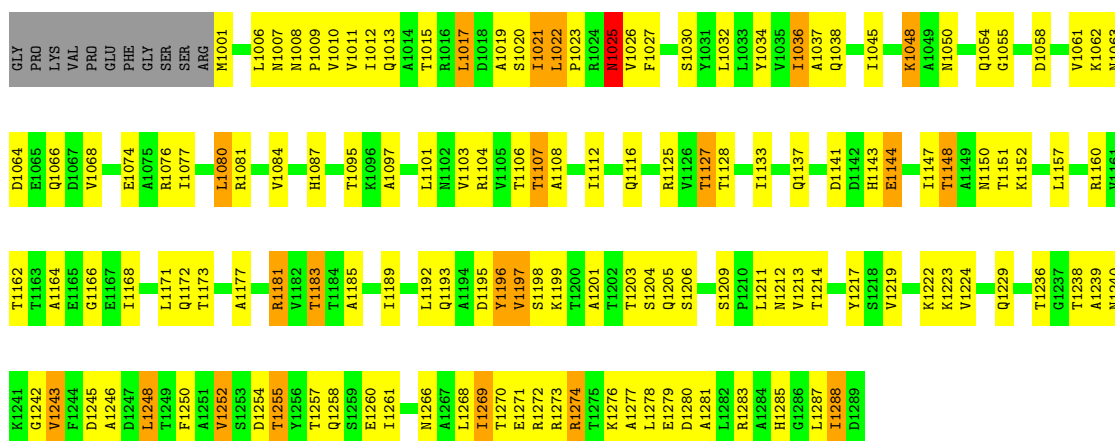
• Molecule 1: Tail needle protein gp26

Chain F:  47% 43% 6% .

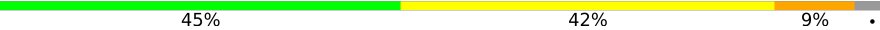


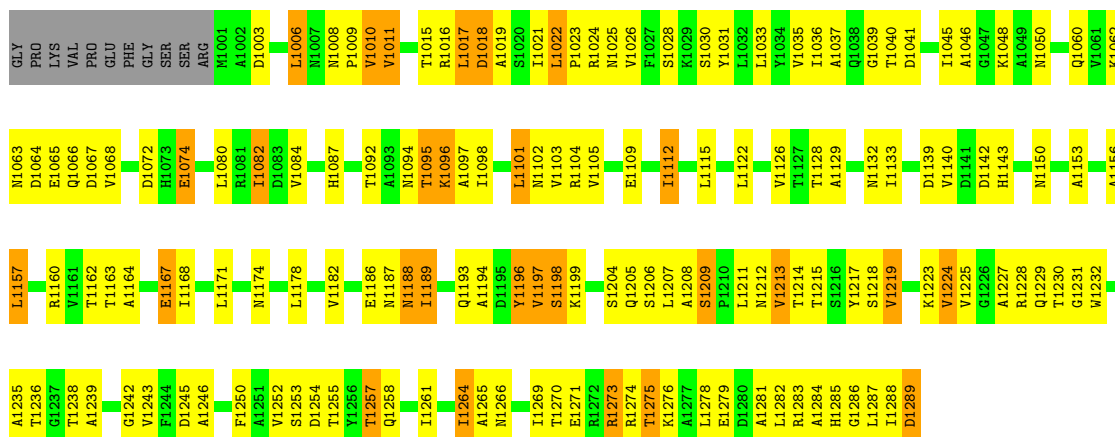
• Molecule 1: Tail needle protein gp26

Chain G:  50% 39% 7% .



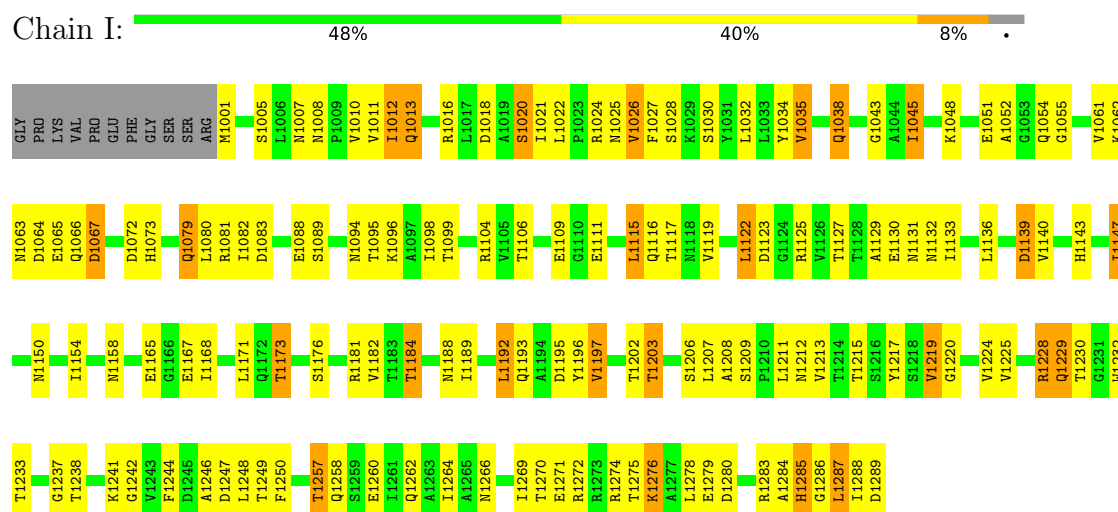
• Molecule 1: Tail needle protein gp26

Chain H:  45% 42% 9% .



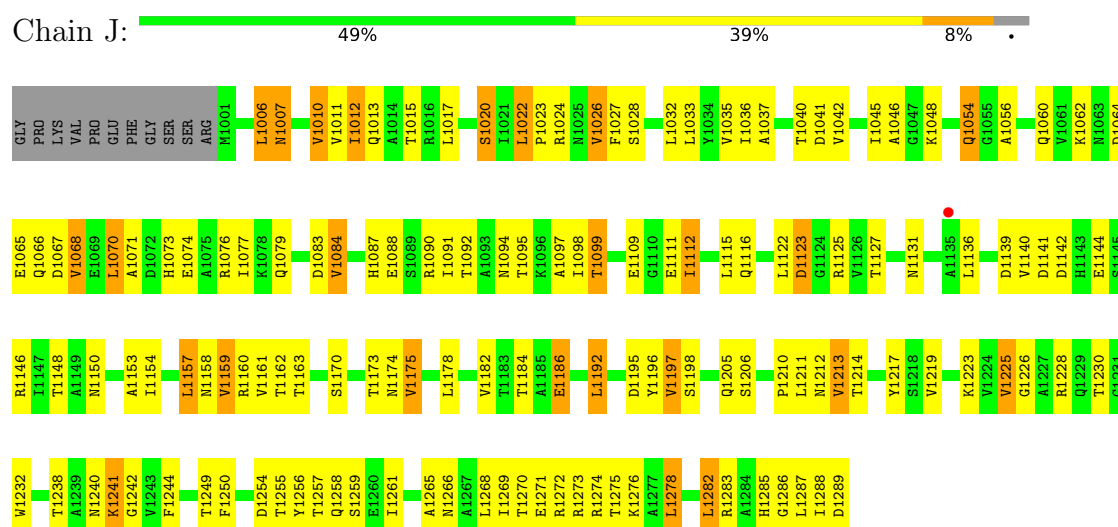
• Molecule 1: Tail needle protein gp26

Chain I:



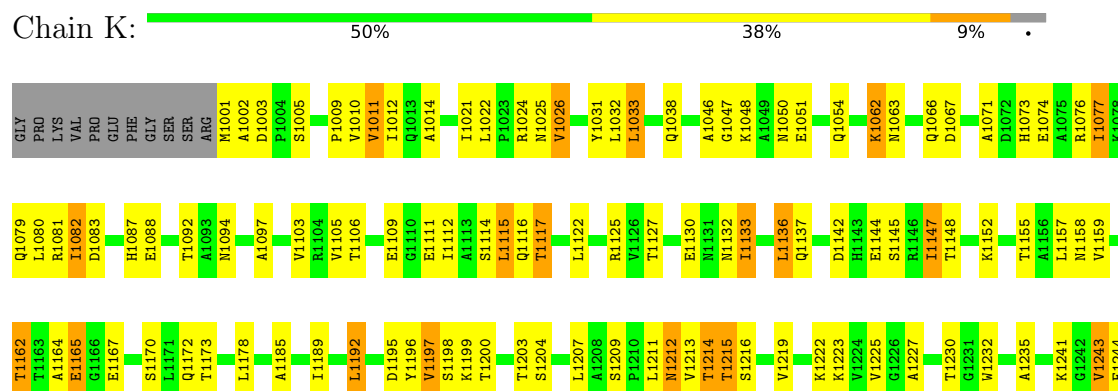
• Molecule 1: Tail needle protein gp26

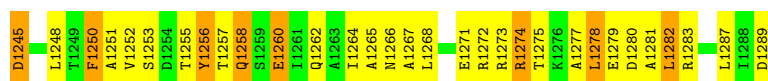
Chain J:



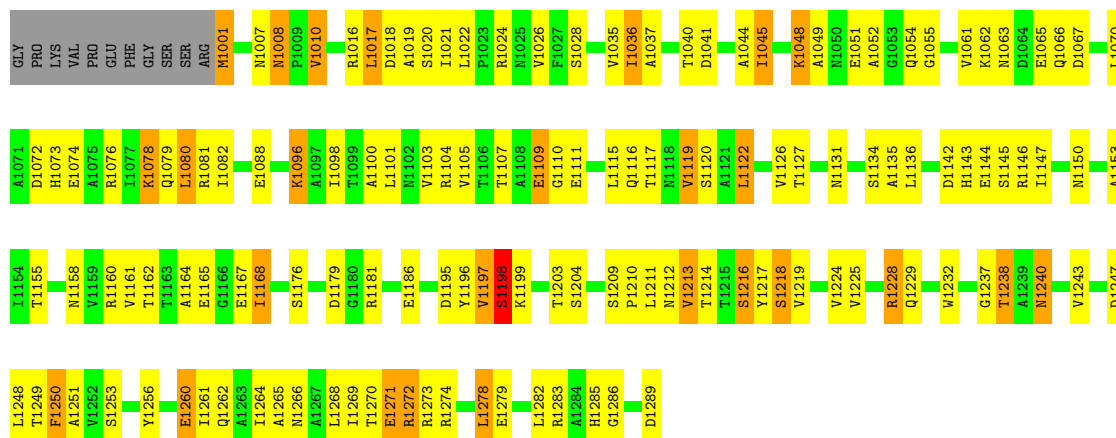
• Molecule 1: Tail needle protein gp26

Chain K:





• Molecule 1: Tail needle protein gp26



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	38.69Å 147.93Å 151.01Å 87.94° 90.05° 89.95°	Depositor
Resolution (Å)	14.99 – 2.70 14.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.5 (14.99-2.70) 73.2 (14.99-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.229 , 0.268 0.228 , 0.266	Depositor DCC
R_{free} test set	2018 reflections (2.40%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.997	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-l,k 0.000 for h,l,-k 0.430 for h,-k,-l 0.000 for -h,k,-l 0.000 for -h,-k,l 0.000 for -h,-l,-k 0.000 for -h,l,k	Xtriage
Reported twinning fraction	0.480 for h,-k,-l	Depositor
Outliers	0 of 73933 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	26552	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.51% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.40	0/2166	0.83	3/2950 (0.1%)
1	B	0.39	0/2166	0.86	5/2950 (0.2%)
1	C	0.45	2/2166 (0.1%)	0.86	4/2950 (0.1%)
1	D	0.41	0/2166	0.82	2/2950 (0.1%)
1	E	0.40	0/2166	0.83	2/2950 (0.1%)
1	F	0.39	0/2166	0.87	3/2950 (0.1%)
1	G	0.41	0/2166	0.86	1/2950 (0.0%)
1	H	0.43	0/2166	0.86	0/2950
1	I	0.42	0/2166	0.86	3/2950 (0.1%)
1	J	0.40	0/2166	0.87	2/2950 (0.1%)
1	K	0.41	0/2166	0.89	4/2950 (0.1%)
1	L	0.43	0/2166	0.89	6/2950 (0.2%)
All	All	0.41	2/25992 (0.0%)	0.86	35/35400 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1143	HIS	CE1-NE2	-6.02	1.26	1.32
1	C	1143	HIS	CG-ND1	5.69	1.44	1.38

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	1261	ILE	N-CA-C	-10.52	102.42	112.83
1	K	1250	PHE	N-CA-C	7.82	119.44	111.07
1	L	1272	ARG	N-CA-C	-6.77	104.90	113.02
1	L	1008	ASN	CA-C-N	6.72	126.90	120.31
1	L	1008	ASN	C-N-CA	6.72	126.90	120.31
1	K	1260	GLU	N-CA-C	6.57	119.42	111.40
1	F	1249	THR	N-CA-C	-6.33	105.42	113.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	1026	VAL	N-CA-C	6.19	116.36	110.42
1	L	1198	SER	N-CA-C	6.09	118.64	110.35
1	L	1218	SER	N-CA-C	6.08	116.58	108.38
1	I	1257	THR	CB-CA-C	-5.96	109.69	116.54
1	J	1214	THR	N-CA-C	5.70	117.57	111.36
1	C	1278	LEU	N-CA-C	-5.69	105.83	112.89
1	E	1195	ASP	N-CA-C	5.62	120.26	113.17
1	K	1243	VAL	N-CA-C	5.57	116.76	108.46
1	C	1224	VAL	N-CA-C	5.53	118.31	112.83
1	I	1285	HIS	N-CA-C	-5.53	102.70	110.50
1	A	1216	SER	N-CA-C	5.46	117.14	108.79
1	E	1250	PHE	N-CA-C	5.32	117.41	107.99
1	B	1152	LYS	N-CA-C	-5.25	106.87	113.28
1	B	1008	ASN	CA-C-N	5.25	126.40	119.84
1	B	1008	ASN	C-N-CA	5.25	126.40	119.84
1	I	1202	THR	N-CA-C	5.25	118.14	111.69
1	D	1008	ASN	CA-C-N	5.23	125.21	120.03
1	D	1008	ASN	C-N-CA	5.23	125.21	120.03
1	A	1003	ASP	CA-C-N	5.22	124.83	119.56
1	A	1003	ASP	C-N-CA	5.22	124.83	119.56
1	G	1025	ASN	N-CA-C	5.18	117.34	111.02
1	C	1249	THR	N-CA-C	-5.14	100.13	108.41
1	F	1008	ASN	CA-C-N	5.14	125.12	120.03
1	F	1008	ASN	C-N-CA	5.14	125.12	120.03
1	K	1216	SER	N-CA-C	5.11	116.61	108.79
1	B	1010	VAL	CB-CA-C	-5.11	104.58	111.63
1	B	1017	LEU	N-CA-C	5.04	118.16	111.30
1	C	1200	THR	N-CA-C	5.02	119.50	113.17

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	2148	0	2135	132	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2148	0	2135	135	0
1	C	2148	0	2135	130	0
1	D	2148	0	2135	137	0
1	E	2148	0	2135	125	1
1	F	2148	0	2135	129	1
1	G	2148	0	2135	127	0
1	H	2148	0	2135	158	0
1	I	2148	0	2134	148	1
1	J	2148	0	2134	168	2
1	K	2148	0	2135	164	1
1	L	2148	0	2134	150	0
2	A	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
2	J	1	0	0	0	0
3	A	2	0	0	3	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	H	1	0	0	2	0
3	I	1	0	0	4	0
3	K	1	0	0	1	0
3	L	1	0	0	2	0
4	A	70	0	0	26	0
4	B	81	0	0	26	2
4	C	54	0	0	17	0
4	D	68	0	0	28	2
4	E	61	0	0	24	0
4	F	70	0	0	21	2
4	G	58	0	0	27	0
4	H	54	0	0	23	0
4	I	61	0	0	31	0
4	J	67	0	0	18	0
4	K	53	0	0	19	0
4	L	67	0	0	25	1
All	All	26552	0	25617	1280	7

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (1280) 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:J:1265:ALA:HB1	1:K:1250:PHE:CE2	1.41	1.49
1:H:1087:HIS:HD2	4:H:1454:HOH:O	1.08	1.35
1:K:1250:PHE:CE1	1:K:1264:ILE:HA	1.62	1.35
1:J:1217:TYR:CD2	1:J:1225:VAL:HB	1.72	1.23
1:K:1250:PHE:CD1	1:K:1264:ILE:HG12	1.73	1.22
1:J:1265:ALA:HB1	1:K:1250:PHE:CD2	1.84	1.12
1:K:1054:GLN:NE2	4:K:1440:HOH:O	1.82	1.11
1:J:1265:ALA:CB	1:K:1250:PHE:CE2	2.34	1.08
1:J:1217:TYR:HD2	1:J:1225:VAL:CB	1.69	1.05
1:L:1196:TYR:CE1	1:L:1198:SER:HB2	1.91	1.05
1:J:1197:VAL:O	1:L:1197:VAL:CG2	2.05	1.05
1:L:1196:TYR:O	1:L:1197:VAL:HG23	1.58	1.04
1:K:1250:PHE:HE1	1:K:1264:ILE:HA	0.87	1.02
1:K:1245:ASP:HB3	1:K:1248:LEU:HD11	1.41	1.00
1:I:1116:GLN:NE2	4:I:1414:HOH:O	1.95	0.97
1:B:1109:GLU:OE1	4:B:1358:HOH:O	1.83	0.96
1:J:1217:TYR:HD2	1:J:1225:VAL:HB	0.81	0.96
1:A:1279:GLU:OE1	4:A:1458:HOH:O	1.82	0.96
1:B:1024:ARG:O	4:B:1354:HOH:O	1.84	0.95
1:A:1118:ASN:ND2	4:A:1437:HOH:O	2.00	0.94
1:G:1238:THR:O	4:G:1406:HOH:O	1.84	0.94
1:E:1284:ALA:O	4:E:1451:HOH:O	1.85	0.94
1:J:1268:LEU:HD23	1:K:1250:PHE:CZ	2.02	0.94
1:E:1280:ASP:OD1	4:E:1453:HOH:O	1.86	0.93
1:J:1268:LEU:HD23	1:K:1250:PHE:HZ	1.31	0.93
1:E:1236:THR:OG1	4:E:1402:HOH:O	1.81	0.93
1:L:1134:SER:OG	4:L:1407:HOH:O	1.84	0.92
1:K:1250:PHE:CE1	1:K:1264:ILE:CA	2.53	0.92
1:B:1172:GLN:O	4:B:1334:HOH:O	1.87	0.92
1:L:1134:SER:O	4:L:1437:HOH:O	1.87	0.92
1:L:1120:SER:OG	4:L:1414:HOH:O	1.88	0.91
1:D:1166:GLY:O	4:D:1432:HOH:O	1.88	0.91
1:A:1212:ASN:ND2	4:A:1439:HOH:O	1.85	0.90
1:D:1228:ARG:NH1	4:D:1430:HOH:O	2.04	0.90
1:J:1150:ASN:ND2	3:L:1301:CL:CL	2.40	0.90
1:D:1237:GLY:O	4:D:1451:HOH:O	1.89	0.90
1:L:1150:ASN:ND2	3:L:1301:CL:CL	2.41	0.90
1:F:1227:ALA:O	4:F:1316:HOH:O	1.88	0.90
1:K:1071:ALA:O	4:K:1453:HOH:O	1.90	0.89
1:A:1150:ASN:ND2	3:A:1302:CL:CL	2.42	0.89
1:K:1289:ASP:OD2	4:K:1428:HOH:O	1.90	0.89
1:G:1177:ALA:O	4:G:1451:HOH:O	1.91	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1258:GLN:NE2	4:K:1429:HOH:O	2.03	0.88
1:A:1203:THR:OG1	4:A:1427:HOH:O	1.91	0.88
1:C:1007:ASN:OD1	1:C:1054:GLN:NE2	2.06	0.88
1:G:1222:LYS:NZ	4:G:1410:HOH:O	2.06	0.88
1:C:1001:MET:O	4:C:1313:HOH:O	1.91	0.88
1:J:1142:ASP:OD2	4:J:1410:HOH:O	1.93	0.87
1:J:1153:ALA:O	4:J:1416:HOH:O	1.92	0.87
1:G:1193:GLN:O	4:G:1449:HOH:O	1.93	0.87
1:K:1010:VAL:O	4:K:1441:HOH:O	1.93	0.86
1:K:1250:PHE:CE1	1:K:1264:ILE:HG12	2.10	0.86
1:D:1099:THR:OG1	4:D:1450:HOH:O	1.91	0.86
3:H:1301:CL:CL	1:I:1094:ASN:ND2	2.46	0.86
1:K:1087:HIS:NE2	1:L:1088:GLU:OE2	2.08	0.86
1:F:1001:MET:O	4:F:1335:HOH:O	1.93	0.86
1:C:1009:PRO:O	4:C:1306:HOH:O	1.93	0.85
1:C:1102:ASN:ND2	4:C:1349:HOH:O	2.04	0.85
1:J:1268:LEU:CD2	1:K:1250:PHE:HZ	1.89	0.85
1:J:1048:LYS:NZ	1:K:1050:ASN:OD1	2.10	0.85
1:A:1001:MET:O	4:A:1449:HOH:O	1.94	0.85
1:C:1234:ALA:O	4:C:1301:HOH:O	1.95	0.84
1:I:1203:THR:O	4:I:1457:HOH:O	1.95	0.84
1:B:1069:GLU:OE2	4:B:1308:HOH:O	1.94	0.84
1:K:1223:LYS:O	1:L:1228:ARG:NH2	2.10	0.84
1:L:1186:GLU:OE2	4:L:1444:HOH:O	1.95	0.84
1:D:1206:SER:HA	1:F:1212:ASN:HB3	1.60	0.84
1:J:1197:VAL:O	1:L:1197:VAL:HG22	1.76	0.84
1:D:1030:SER:HB2	1:E:1021:ILE:HG12	1.57	0.84
1:E:1171:LEU:HD11	1:F:1172:GLN:HG2	1.60	0.84
1:J:1265:ALA:CB	1:K:1250:PHE:CD2	2.59	0.83
1:K:1250:PHE:CD1	1:K:1264:ILE:CG1	2.61	0.83
1:D:1116:GLN:O	4:D:1437:HOH:O	1.96	0.83
1:F:1165:GLU:OE1	4:F:1323:HOH:O	1.94	0.83
1:J:1219:VAL:HG13	1:K:1215:THR:H	1.42	0.83
1:L:1196:TYR:CE1	1:L:1198:SER:CB	2.61	0.82
1:K:1172:GLN:NE2	4:K:1415:HOH:O	1.90	0.82
1:I:1079:GLN:OE1	4:I:1425:HOH:O	1.96	0.82
1:J:1232:TRP:O	4:J:1401:HOH:O	1.96	0.82
1:K:1062:LYS:HD2	1:L:1063:ASN:HD22	1.45	0.81
1:A:1274:ARG:NH2	4:A:1402:HOH:O	2.11	0.81
4:E:1402:HOH:O	1:F:1244:PHE:O	1.97	0.81
1:G:1238:THR:N	4:G:1406:HOH:O	2.13	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1212:ASN:HB3	1:I:1206:SER:HA	1.61	0.81
1:A:1050:ASN:OD1	1:C:1048:LYS:NZ	2.13	0.81
1:E:1276:LYS:NZ	4:E:1438:HOH:O	2.11	0.81
1:H:1096:LYS:NZ	4:H:1433:HOH:O	1.92	0.81
1:J:1071:ALA:O	4:J:1441:HOH:O	1.97	0.81
1:E:1099:THR:OG1	4:E:1419:HOH:O	1.96	0.81
1:H:1160:ARG:NH1	1:I:1158:ASN:OD1	2.14	0.81
1:H:1242:GLY:O	1:H:1274:ARG:NH1	2.14	0.80
1:L:1247:ASP:OD2	4:L:1467:HOH:O	1.99	0.80
1:A:1017:LEU:O	4:A:1440:HOH:O	2.00	0.80
1:G:1258:GLN:NE2	1:H:1253:SER:O	2.14	0.79
1:A:1048:LYS:HE3	1:B:1010:VAL:HG13	1.63	0.79
1:I:1208:ALA:O	4:I:1402:HOH:O	2.00	0.79
1:A:1019:ALA:O	4:A:1469:HOH:O	2.01	0.79
1:F:1106:THR:N	4:F:1367:HOH:O	2.09	0.79
1:E:1066:GLN:NE2	1:F:1067:ASP:OD1	2.16	0.79
1:H:1039:GLY:O	4:H:1405:HOH:O	2.00	0.79
1:H:1217:TYR:HB2	1:H:1225:VAL:HB	1.64	0.79
1:D:1008:ASN:O	1:F:1048:LYS:NZ	2.16	0.78
1:G:1245:ASP:O	1:I:1272:ARG:NH1	2.16	0.78
1:K:1272:ARG:HG2	1:L:1271:GLU:HG3	1.64	0.78
1:D:1246:ALA:HB2	1:F:1236:THR:HB	1.66	0.78
1:B:1073:HIS:ND1	4:B:1336:HOH:O	2.16	0.78
1:G:1162:THR:O	4:G:1457:HOH:O	2.02	0.78
1:A:1231:GLY:O	4:A:1409:HOH:O	2.02	0.78
1:I:1072:ASP:OD2	4:I:1418:HOH:O	2.01	0.77
1:H:1227:ALA:O	1:I:1285:HIS:NE2	2.17	0.77
1:I:1206:SER:O	4:I:1410:HOH:O	2.01	0.77
1:I:1130:GLU:OE2	4:I:1445:HOH:O	2.01	0.77
1:K:1279:GLU:OE2	1:K:1283:ARG:NH2	2.17	0.77
1:I:1220:GLY:N	4:I:1447:HOH:O	2.16	0.77
1:A:1066:GLN:NE2	1:B:1067:ASP:OD1	2.18	0.77
1:D:1010:VAL:O	4:D:1454:HOH:O	2.01	0.77
1:D:1026:VAL:O	4:D:1464:HOH:O	2.01	0.76
1:H:1024:ARG:NH1	4:H:1441:HOH:O	2.18	0.76
1:B:1154:ILE:HA	1:B:1157:LEU:HB2	1.66	0.76
1:F:1288:ILE:O	4:F:1311:HOH:O	2.03	0.75
1:K:1011:VAL:O	4:K:1403:HOH:O	2.05	0.75
1:L:1237:GLY:HA3	1:L:1273:ARG:HH12	1.51	0.75
1:I:1188:ASN:OD1	4:I:1427:HOH:O	2.05	0.75
1:L:1196:TYR:O	1:L:1197:VAL:CG2	2.35	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1008:ASN:ND2	4:L:1456:HOH:O	2.19	0.75
1:E:1283:ARG:NH1	1:E:1289:ASP:OD1	2.20	0.74
1:G:1019:ALA:HA	1:G:1022:LEU:H	1.52	0.74
1:G:1205:GLN:O	4:G:1402:HOH:O	2.03	0.74
1:E:1272:ARG:NH2	1:F:1247:ASP:OD2	2.20	0.74
1:C:1131:ASN:ND2	4:C:1334:HOH:O	2.18	0.74
1:B:1263:ALA:O	4:B:1311:HOH:O	2.05	0.74
1:G:1229:GLN:HE22	1:H:1284:ALA:HB3	1.51	0.74
1:I:1064:ASP:HA	1:I:1067:ASP:HB2	1.70	0.74
1:D:1260:GLU:OE2	4:D:1459:HOH:O	2.05	0.74
1:H:1239:ALA:O	4:H:1430:HOH:O	2.05	0.74
1:L:1219:VAL:HG12	1:L:1224:VAL:HG11	1.70	0.73
1:F:1051:GLU:OE1	4:F:1354:HOH:O	2.05	0.73
1:J:1206:SER:HA	1:L:1212:ASN:HB3	1.71	0.73
1:B:1185:ALA:O	4:B:1339:HOH:O	2.06	0.73
1:G:1229:GLN:NE2	4:H:1419:HOH:O	2.21	0.73
1:K:1158:ASN:OD1	4:K:1448:HOH:O	2.07	0.73
1:D:1284:ALA:HB3	1:F:1229:GLN:HE22	1.53	0.73
1:E:1242:GLY:O	1:E:1274:ARG:NH1	2.18	0.73
3:A:1303:CL:CL	1:B:1094:ASN:ND2	2.56	0.73
1:D:1130:GLU:O	4:D:1468:HOH:O	2.06	0.73
1:E:1272:ARG:O	4:E:1420:HOH:O	2.06	0.73
1:G:1199:LYS:NZ	1:I:1196:TYR:O	2.21	0.73
1:C:1116:GLN:O	4:C:1320:HOH:O	2.05	0.72
1:L:1196:TYR:O	4:L:1461:HOH:O	2.06	0.72
1:H:1198:SER:H	1:H:1205:GLN:HE22	1.37	0.72
1:E:1212:ASN:HB3	1:F:1206:SER:HA	1.71	0.72
1:J:1272:ARG:HD2	1:K:1271:GLU:HB2	1.71	0.72
1:J:1288:ILE:O	4:J:1412:HOH:O	2.07	0.72
1:K:1197:VAL:O	4:K:1430:HOH:O	2.06	0.72
1:B:1051:GLU:HA	1:B:1054:GLN:HB3	1.70	0.72
1:D:1147:ILE:HG22	1:F:1146:ARG:HH11	1.54	0.72
1:J:1097:ALA:N	4:J:1439:HOH:O	2.22	0.72
1:L:1240:ASN:O	4:L:1459:HOH:O	2.08	0.72
1:K:1250:PHE:HE1	1:K:1264:ILE:CA	1.83	0.72
1:G:1103:VAL:O	1:G:1107:THR:OG1	2.07	0.72
1:A:1257:THR:HB	1:A:1260:GLU:HB3	1.72	0.72
1:C:1011:VAL:HG23	1:C:1050:ASN:HD22	1.55	0.72
1:J:1109:GLU:OE2	4:J:1459:HOH:O	2.07	0.71
1:G:1141:ASP:O	4:G:1408:HOH:O	2.08	0.71
1:J:1073:HIS:NE2	1:K:1074:GLU:OE1	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1240:ASN:O	1:J:1274:ARG:NH1	2.24	0.71
1:K:1094:ASN:ND2	3:K:1301:CL:CL	2.57	0.71
1:B:1116:GLN:NE2	4:B:1309:HOH:O	2.24	0.71
1:D:1210:PRO:HG3	1:F:1215:THR:HB	1.73	0.71
1:D:1237:GLY:O	1:D:1276:LYS:NZ	2.20	0.71
1:L:1210:PRO:O	4:L:1465:HOH:O	2.06	0.71
1:J:1048:LYS:HZ1	1:K:1009:PRO:HA	1.55	0.71
1:B:1096:LYS:O	4:B:1312:HOH:O	2.07	0.71
1:E:1223:LYS:NZ	4:E:1436:HOH:O	2.02	0.71
1:A:1213:VAL:HG21	1:B:1211:LEU:HB2	1.71	0.71
1:A:1280:ASP:OD1	4:A:1428:HOH:O	2.08	0.71
1:E:1264:ILE:O	4:E:1401:HOH:O	2.09	0.71
1:L:1196:TYR:C	1:L:1197:VAL:CG2	2.63	0.71
1:D:1016:ARG:HA	1:D:1016:ARG:HH11	1.56	0.70
1:J:1146:ARG:NH2	1:K:1144:GLU:OE1	2.23	0.70
1:H:1250:PHE:CE2	1:H:1264:ILE:HG22	2.26	0.70
1:K:1258:GLN:O	1:K:1262:GLN:NE2	2.23	0.70
1:B:1278:LEU:HB3	1:C:1278:LEU:HD21	1.73	0.70
1:C:1071:ALA:O	4:C:1315:HOH:O	2.09	0.70
1:B:1048:LYS:NZ	1:C:1008:ASN:O	2.24	0.70
1:E:1228:ARG:O	4:E:1408:HOH:O	2.08	0.70
1:D:1063:ASN:HD22	1:F:1062:LYS:HG3	1.57	0.70
1:G:1081:ARG:NH1	1:I:1083:ASP:OD2	2.24	0.70
1:D:1083:ASP:O	4:D:1449:HOH:O	2.10	0.70
1:E:1265:ALA:O	4:E:1432:HOH:O	2.07	0.70
1:C:1208:ALA:O	4:C:1318:HOH:O	2.10	0.70
1:D:1073:HIS:ND1	4:D:1447:HOH:O	2.24	0.70
1:E:1136:LEU:HD21	1:F:1137:GLN:HG2	1.72	0.70
1:I:1150:ASN:ND2	3:I:1301:CL:CL	2.62	0.70
1:J:1226:GLY:O	4:J:1407:HOH:O	2.09	0.70
1:C:1240:ASN:O	1:C:1274:ARG:NH1	2.25	0.70
1:D:1253:SER:O	1:F:1256:TYR:OH	2.10	0.69
1:G:1106:THR:HG22	1:I:1104:ARG:HH22	1.57	0.69
1:F:1174:ASN:O	1:F:1178:LEU:N	2.25	0.69
1:D:1272:ARG:HG2	1:E:1271:GLU:HG3	1.73	0.69
1:L:1096:LYS:O	4:L:1405:HOH:O	2.09	0.69
1:D:1132:ASN:ND2	4:D:1423:HOH:O	2.24	0.69
1:D:1219:VAL:O	4:D:1402:HOH:O	2.09	0.69
1:H:1046:ALA:O	1:H:1050:ASN:ND2	2.26	0.69
1:A:1269:ILE:HD11	1:B:1248:LEU:HD13	1.75	0.69
1:J:1265:ALA:HB1	1:K:1250:PHE:HE2	1.44	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1091:ILE:HG23	3:A:1303:CL:CL	2.29	0.69
1:F:1064:ASP:OD2	4:F:1353:HOH:O	2.10	0.69
1:H:1102:ASN:N	4:H:1432:HOH:O	2.08	0.69
1:H:1264:ILE:HD12	1:H:1265:ALA:N	2.07	0.69
1:D:1234:ALA:O	4:D:1429:HOH:O	2.10	0.69
1:G:1213:VAL:HG22	1:H:1207:LEU:HD12	1.73	0.69
1:H:1087:HIS:CD2	4:H:1454:HOH:O	1.98	0.69
1:I:1242:GLY:O	1:I:1274:ARG:NH1	2.24	0.69
1:E:1037:ALA:O	1:E:1041:ASP:N	2.25	0.69
1:J:1094:ASN:O	4:J:1439:HOH:O	2.11	0.69
1:E:1125:ARG:HH21	1:F:1126:VAL:HG12	1.58	0.68
1:K:1117:THR:N	4:K:1439:HOH:O	2.20	0.68
1:J:1213:VAL:HG21	1:K:1211:LEU:HB2	1.75	0.68
1:C:1224:VAL:HG12	1:C:1224:VAL:O	1.92	0.68
1:C:1232:TRP:HB2	1:C:1289:ASP:HB3	1.74	0.68
1:E:1020:SER:O	4:E:1429:HOH:O	2.10	0.68
1:J:1219:VAL:HG13	1:K:1215:THR:N	2.08	0.68
1:B:1016:ARG:NH2	1:B:1039:GLY:O	2.27	0.68
1:D:1193:GLN:HG3	1:F:1192:LEU:HD11	1.74	0.68
1:E:1193:GLN:NE2	4:E:1414:HOH:O	2.26	0.68
1:G:1066:GLN:NE2	1:H:1067:ASP:OD1	2.24	0.68
1:H:1224:VAL:HG13	1:H:1225:VAL:HG23	1.76	0.68
1:L:1007:ASN:OD1	1:L:1054:GLN:NE2	2.26	0.68
1:B:1143:HIS:NE2	1:C:1144:GLU:OE1	2.25	0.68
1:D:1262:GLN:OE1	4:D:1439:HOH:O	2.09	0.68
1:G:1087:HIS:HD2	4:H:1454:HOH:O	1.76	0.68
1:B:1280:ASP:OD2	4:B:1342:HOH:O	2.11	0.67
4:D:1449:HOH:O	1:E:1088:GLU:OE2	2.11	0.67
1:G:1195:ASP:OD2	1:H:1196:TYR:OH	2.11	0.67
1:L:1135:ALA:O	4:L:1458:HOH:O	2.12	0.67
1:L:1196:TYR:HE1	1:L:1198:SER:HB2	1.55	0.67
1:A:1083:ASP:OD2	1:B:1081:ARG:NH2	2.27	0.67
1:K:1273:ARG:NH1	4:K:1401:HOH:O	1.89	0.67
1:B:1109:GLU:OE2	4:B:1343:HOH:O	2.11	0.67
1:B:1007:ASN:OD1	1:B:1054:GLN:NE2	2.27	0.67
1:I:1082:ILE:O	4:I:1417:HOH:O	2.12	0.67
1:I:1147:ILE:HA	1:I:1150:ASN:HB2	1.77	0.67
1:L:1017:LEU:HD13	1:L:1036:ILE:HG12	1.77	0.67
1:G:1025:ASN:HD22	1:G:1026:VAL:HG23	1.59	0.67
1:J:1265:ALA:HA	1:J:1268:LEU:HB3	1.75	0.67
1:D:1074:GLU:HG3	1:F:1073:HIS:NE2	2.10	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1235:ALA:HB3	1:D:1276:LYS:HG3	1.77	0.67
1:E:1213:VAL:HG11	1:F:1211:LEU:HB2	1.77	0.67
1:G:1007:ASN:OD1	1:G:1054:GLN:NE2	2.28	0.67
4:J:1459:HOH:O	1:L:1104:ARG:O	2.12	0.67
1:F:1089:SER:OG	4:F:1361:HOH:O	2.12	0.67
1:J:1197:VAL:HG23	1:L:1197:VAL:HG23	1.76	0.67
4:A:1402:HOH:O	1:C:1279:GLU:OE2	2.13	0.66
1:G:1010:VAL:H	1:G:1050:ASN:HD21	1.43	0.66
1:I:1026:VAL:O	4:I:1459:HOH:O	2.13	0.66
1:J:1006:LEU:HD21	1:L:1052:ALA:HA	1.77	0.66
1:B:1252:VAL:O	4:B:1333:HOH:O	2.14	0.66
1:J:1064:ASP:OD1	1:L:1062:LYS:NZ	2.27	0.66
1:K:1232:TRP:HB2	1:K:1289:ASP:HB3	1.77	0.66
1:I:1280:ASP:OD2	4:I:1434:HOH:O	2.13	0.66
1:J:1275:THR:OG1	4:L:1415:HOH:O	2.13	0.66
1:A:1283:ARG:NH1	4:A:1411:HOH:O	2.28	0.66
4:E:1452:HOH:O	1:F:1006:LEU:HD21	1.95	0.66
1:E:1031:TYR:OH	4:E:1425:HOH:O	2.04	0.66
1:I:1229:GLN:OE1	1:I:1232:TRP:NE1	2.21	0.66
1:L:1072:ASP:O	1:L:1076:ARG:HG2	1.96	0.66
4:A:1402:HOH:O	1:C:1233:THR:O	2.13	0.66
1:F:1130:GLU:OE1	4:F:1326:HOH:O	2.13	0.66
1:B:1029:LYS:HA	1:B:1032:LEU:HB2	1.78	0.66
1:B:1183:THR:O	1:B:1187:ASN:ND2	2.23	0.66
1:D:1247:ASP:OD2	1:F:1273:ARG:NE	2.28	0.66
1:C:1102:ASN:O	1:C:1106:THR:OG1	2.14	0.65
1:J:1238:THR:O	1:J:1276:LYS:NZ	2.29	0.65
1:J:1020:SER:HB2	1:J:1024:ARG:HH21	1.60	0.65
1:K:1214:THR:O	1:K:1214:THR:HG22	1.96	0.65
1:L:1155:THR:OG1	4:L:1432:HOH:O	2.14	0.65
1:G:1172:GLN:OE1	4:G:1407:HOH:O	2.15	0.65
1:H:1098:ILE:O	4:H:1432:HOH:O	2.13	0.65
1:I:1024:ARG:O	4:I:1446:HOH:O	2.13	0.65
1:J:1146:ARG:NH1	4:J:1411:HOH:O	2.28	0.65
1:G:1239:ALA:HB1	1:G:1277:ALA:HB2	1.78	0.65
1:H:1092:THR:HA	1:H:1095:THR:HG22	1.78	0.65
1:H:1275:THR:OG1	1:I:1271:GLU:OE2	2.08	0.65
1:A:1091:ILE:HB	1:C:1090:ARG:HH12	1.61	0.65
1:D:1055:GLY:HA3	1:E:1006:LEU:HD21	1.79	0.65
1:E:1107:THR:O	4:E:1441:HOH:O	2.15	0.65
1:G:1199:LYS:N	1:I:1195:ASP:O	2.28	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1235:ALA:HB2	1:F:1274:ARG:HH21	1.62	0.65
1:I:1279:GLU:OE2	1:I:1283:ARG:NH2	2.30	0.65
1:J:1060:GLN:NE2	1:L:1055:GLY:O	2.28	0.65
1:B:1137:GLN:NE2	4:B:1305:HOH:O	2.29	0.65
1:L:1074:GLU:OE2	1:L:1078:LYS:NZ	2.29	0.65
1:C:1022:LEU:HD11	1:C:1032:LEU:HD21	1.78	0.64
1:C:1165:GLU:OE2	4:C:1317:HOH:O	2.14	0.64
1:D:1048:LYS:NZ	1:E:1008:ASN:O	2.28	0.64
1:H:1196:TYR:O	4:H:1409:HOH:O	2.15	0.64
1:D:1087:HIS:CE1	1:E:1087:HIS:HB3	2.33	0.64
1:E:1198:SER:O	1:E:1205:GLN:NE2	2.30	0.64
1:H:1045:ILE:HG21	1:I:1045:ILE:HG22	1.78	0.64
1:J:1090:ARG:NH2	1:K:1092:THR:OG1	2.30	0.64
1:A:1136:LEU:HD23	1:C:1136:LEU:HD23	1.80	0.64
1:H:1171:LEU:HD21	1:I:1171:LEU:HB2	1.80	0.64
1:E:1083:ASP:OD2	1:F:1081:ARG:NH2	2.31	0.64
1:G:1196:TYR:O	4:G:1417:HOH:O	2.14	0.64
1:I:1189:ILE:HA	1:I:1192:LEU:HB2	1.80	0.64
1:L:1260:GLU:O	4:L:1423:HOH:O	2.15	0.64
1:E:1236:THR:OG1	1:F:1244:PHE:O	2.15	0.63
1:J:1074:GLU:OE1	1:L:1073:HIS:NE2	2.30	0.63
1:A:1201:ALA:N	4:A:1403:HOH:O	2.28	0.63
1:A:1246:ALA:HB2	1:C:1236:THR:HG23	1.81	0.63
1:J:1162:THR:OG1	1:L:1160:ARG:NH2	2.31	0.63
1:A:1209:SER:OG	1:B:1205:GLN:OE1	2.16	0.63
1:D:1062:LYS:HG2	1:E:1063:ASN:HB3	1.79	0.63
1:D:1073:HIS:NE2	1:E:1074:GLU:OE1	2.31	0.63
1:K:1073:HIS:NE2	1:L:1074:GLU:OE1	2.32	0.63
1:J:1272:ARG:HB3	1:K:1244:PHE:HE2	1.63	0.63
4:J:1417:HOH:O	1:L:1073:HIS:ND1	2.30	0.63
1:A:1136:LEU:HD11	1:B:1137:GLN:HG2	1.81	0.63
1:A:1272:ARG:HG2	1:B:1271:GLU:HG3	1.80	0.63
1:B:1223:LYS:NZ	4:B:1332:HOH:O	2.28	0.63
1:H:1194:ALA:O	4:H:1422:HOH:O	2.16	0.63
1:F:1183:THR:O	1:F:1187:ASN:ND2	2.32	0.63
1:I:1275:THR:HA	1:I:1278:LEU:HB2	1.81	0.63
1:J:1258:GLN:HE21	1:K:1253:SER:HA	1.63	0.63
1:C:1112:ILE:O	1:C:1116:GLN:N	2.31	0.62
1:E:1279:GLU:OE2	1:E:1283:ARG:NH2	2.32	0.62
1:J:1217:TYR:HE2	1:L:1224:VAL:HG21	1.63	0.62
1:K:1111:GLU:OE2	1:L:1116:GLN:NE2	2.31	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1024:ARG:NH1	4:B:1347:HOH:O	2.31	0.62
1:E:1083:ASP:OD1	1:E:1084:VAL:N	2.33	0.62
1:F:1048:LYS:HA	1:F:1051:GLU:HG2	1.81	0.62
1:G:1150:ASN:HB3	3:I:1301:CL:CL	2.36	0.62
1:G:1213:VAL:HA	1:H:1207:LEU:HB2	1.80	0.62
1:A:1067:ASP:OD1	1:C:1066:GLN:NE2	2.31	0.62
1:K:1142:ASP:OD2	4:K:1446:HOH:O	2.16	0.62
1:B:1045:ILE:HG21	1:C:1045:ILE:HG22	1.81	0.62
1:G:1081:ARG:NH2	4:G:1421:HOH:O	2.23	0.62
1:J:1217:TYR:CE2	1:L:1217:TYR:CE2	2.87	0.62
1:K:1227:ALA:O	1:L:1285:HIS:NE2	2.32	0.62
1:G:1038:GLN:NE2	4:G:1453:HOH:O	2.33	0.62
1:L:1018:ASP:H	1:L:1021:ILE:HD13	1.65	0.62
1:I:1237:GLY:O	1:I:1276:LYS:NZ	2.32	0.62
1:A:1048:LYS:O	1:A:1052:ALA:N	2.23	0.62
1:H:1102:ASN:HA	1:H:1105:VAL:HG12	1.82	0.62
1:H:1261:ILE:O	1:H:1264:ILE:HG13	1.99	0.62
1:J:1109:GLU:HA	1:J:1112:ILE:HD11	1.81	0.62
1:D:1192:LEU:HD13	1:E:1193:GLN:HG2	1.82	0.61
1:H:1223:LYS:O	1:I:1286:GLY:HA3	2.00	0.61
1:J:1205:GLN:N	4:L:1465:HOH:O	2.31	0.61
1:A:1245:ASP:HB3	1:A:1248:LEU:HB2	1.81	0.61
1:D:1211:LEU:HD21	1:E:1211:LEU:HD11	1.81	0.61
1:J:1223:LYS:NZ	1:J:1225:VAL:O	2.33	0.61
1:B:1041:ASP:OD1	1:B:1042:VAL:N	2.33	0.61
1:B:1134:SER:HA	1:B:1137:GLN:HB2	1.80	0.61
1:B:1073:HIS:NE2	1:C:1074:GLU:OE1	2.31	0.61
1:C:1198:SER:OG	1:C:1200:THR:OG1	2.17	0.61
1:G:1266:ASN:HA	1:G:1269:ILE:HG22	1.82	0.61
1:H:1213:VAL:HG21	1:I:1211:LEU:HB3	1.82	0.61
1:J:1076:ARG:NH1	1:K:1074:GLU:OE2	2.33	0.61
1:E:1216:SER:HB3	1:E:1223:LYS:HE3	1.82	0.61
1:G:1104:ARG:NH1	4:G:1431:HOH:O	2.30	0.61
1:A:1279:GLU:OE2	1:A:1283:ARG:NH2	2.31	0.61
1:B:1229:GLN:O	1:B:1289:ASP:N	2.34	0.61
1:D:1233:THR:OG1	4:D:1409:HOH:O	2.15	0.61
1:H:1080:LEU:HD21	1:I:1080:LEU:HD13	1.81	0.61
1:J:1196:TYR:HA	4:K:1430:HOH:O	1.99	0.61
1:L:1216:SER:OG	1:L:1217:TYR:N	2.34	0.61
1:B:1228:ARG:NE	1:B:1286:GLY:O	2.29	0.61
1:G:1206:SER:HA	1:I:1212:ASN:HB3	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:ARG:O	4:B:1343:HOH:O	2.16	0.61
1:G:1127:THR:OG1	1:I:1125:ARG:NH2	2.33	0.61
1:L:1212:ASN:OD1	1:L:1213:VAL:N	2.33	0.61
1:I:1150:ASN:HB3	3:I:1301:CL:CL	2.38	0.60
1:L:1262:GLN:O	1:L:1266:ASN:N	2.29	0.60
1:D:1250:PHE:HE2	1:F:1268:LEU:HD23	1.65	0.60
1:K:1062:LYS:O	1:K:1066:GLN:N	2.27	0.60
1:L:1251:ALA:O	4:L:1402:HOH:O	2.16	0.60
1:H:1193:GLN:NE2	4:H:1446:HOH:O	2.34	0.60
1:H:1230:THR:OG1	1:H:1231:GLY:N	2.34	0.60
1:A:1147:ILE:HG21	1:C:1146:ARG:HE	1.67	0.60
1:C:1083:ASP:OD1	1:C:1084:VAL:N	2.34	0.60
1:I:1005:SER:OG	4:I:1450:HOH:O	2.17	0.60
1:B:1192:LEU:HD21	1:C:1193:GLN:HG3	1.83	0.60
1:H:1168:ILE:HD11	1:I:1168:ILE:HG12	1.83	0.60
1:D:1147:ILE:HG22	1:F:1146:ARG:NH1	2.16	0.60
1:G:1054:GLN:HG3	4:G:1412:HOH:O	2.02	0.60
1:H:1186:GLU:HA	1:H:1189:ILE:HB	1.82	0.60
1:J:1077:ILE:HG21	1:L:1076:ARG:HE	1.67	0.60
1:B:1048:LYS:O	1:B:1052:ALA:N	2.34	0.60
1:K:1225:VAL:HG21	1:L:1225:VAL:HG21	1.84	0.60
1:A:1007:ASN:ND2	4:A:1450:HOH:O	2.34	0.60
1:J:1228:ARG:NH1	4:J:1420:HOH:O	2.31	0.60
1:L:1262:GLN:HA	1:L:1265:ALA:HB3	1.84	0.60
1:C:1132:ASN:ND2	4:C:1319:HOH:O	2.35	0.59
1:I:1007:ASN:OD1	1:I:1008:ASN:N	2.34	0.59
1:G:1272:ARG:NH1	1:H:1245:ASP:OD1	2.34	0.59
1:J:1242:GLY:O	1:J:1274:ARG:NH2	2.33	0.59
1:D:1021:ILE:O	1:F:1028:SER:OG	2.17	0.59
1:E:1268:LEU:N	4:E:1401:HOH:O	2.34	0.59
1:G:1144:GLU:O	1:G:1148:THR:OG1	2.19	0.59
1:F:1048:LYS:O	1:F:1052:ALA:N	2.33	0.59
1:H:1019:ALA:HB2	1:H:1036:ILE:HD13	1.85	0.59
1:I:1279:GLU:OE1	4:I:1434:HOH:O	2.16	0.59
1:L:1037:ALA:O	1:L:1040:THR:OG1	2.20	0.59
1:D:1269:ILE:HD13	1:E:1248:LEU:HA	1.85	0.59
1:J:1195:ASP:O	4:K:1430:HOH:O	2.17	0.59
1:D:1213:VAL:HG11	1:E:1211:LEU:HD12	1.85	0.59
1:K:1282:LEU:HG	1:K:1287:LEU:HD13	1.85	0.59
1:J:1017:LEU:HD23	1:J:1036:ILE:HG22	1.84	0.59
1:J:1116:GLN:HG2	1:L:1115:LEU:HD21	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1210:PRO:HG3	1:C:1215:THR:HG22	1.85	0.59
1:B:1198:SER:OG	1:B:1201:ALA:N	2.36	0.59
1:B:1239:ALA:HB1	1:B:1277:ALA:HB2	1.85	0.59
1:J:1076:ARG:HD3	1:K:1077:ILE:HG21	1.84	0.59
1:L:1209:SER:N	4:L:1464:HOH:O	2.36	0.59
1:D:1207:LEU:HB2	1:F:1213:VAL:HA	1.84	0.58
1:K:1115:LEU:HD11	1:L:1115:LEU:HB3	1.85	0.58
1:C:1217:TYR:HB2	1:C:1225:VAL:HB	1.85	0.58
1:E:1248:LEU:HD12	1:E:1248:LEU:H	1.67	0.58
1:A:1217:TYR:HB2	1:A:1225:VAL:HB	1.84	0.58
1:D:1161:VAL:HG11	1:F:1160:ARG:HE	1.66	0.58
1:I:1266:ASN:HA	1:I:1269:ILE:HG12	1.85	0.58
1:J:1160:ARG:O	1:J:1163:THR:OG1	2.19	0.58
4:A:1424:HOH:O	1:C:1160:ARG:NH1	2.37	0.58
1:J:1125:ARG:NH2	1:K:1127:THR:OG1	2.36	0.58
1:J:1139:ASP:OD1	1:J:1140:VAL:N	2.37	0.58
1:J:1197:VAL:HG23	1:L:1197:VAL:CG2	2.34	0.58
1:K:1063:ASN:OD1	1:L:1063:ASN:ND2	2.37	0.58
1:E:1104:ARG:NH2	1:F:1106:THR:OG1	2.35	0.58
1:F:1248:LEU:H	1:F:1248:LEU:HD23	1.68	0.58
1:J:1178:LEU:HD13	1:K:1178:LEU:HD23	1.86	0.58
1:D:1015:THR:O	1:D:1016:ARG:NH1	2.37	0.58
1:E:1079:GLN:NE2	4:E:1445:HOH:O	1.93	0.58
1:F:1016:ARG:HH12	1:F:1018:ASP:HA	1.69	0.58
1:J:1198:SER:O	1:J:1205:GLN:NE2	2.29	0.58
1:A:1271:GLU:HG3	1:C:1272:ARG:HG2	1.86	0.58
1:K:1162:THR:HA	1:K:1165:GLU:HG2	1.86	0.58
1:A:1224:VAL:HG13	1:B:1287:LEU:HA	1.85	0.58
1:H:1003:ASP:HB3	1:H:1006:LEU:HB2	1.86	0.58
1:A:1076:ARG:NH1	1:B:1074:GLU:OE1	2.37	0.57
1:A:1122:LEU:HD23	1:C:1122:LEU:HD23	1.84	0.57
1:A:1247:ASP:OD1	1:C:1273:ARG:NH2	2.35	0.57
1:B:1192:LEU:HD13	1:C:1192:LEU:HD12	1.85	0.57
1:F:1144:GLU:O	1:F:1148:THR:OG1	2.16	0.57
1:J:1272:ARG:NH1	1:K:1267:ALA:O	2.37	0.57
1:A:1240:ASN:ND2	4:A:1425:HOH:O	2.28	0.57
1:C:1224:VAL:O	1:C:1225:VAL:HG23	2.05	0.57
1:H:1228:ARG:HG3	1:H:1286:GLY:O	2.05	0.57
1:J:1275:THR:OG1	1:K:1271:GLU:OE2	2.17	0.57
1:A:1080:LEU:HB3	1:C:1080:LEU:HD21	1.86	0.57
1:E:1024:ARG:HA	1:E:1024:ARG:NE	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1211:LEU:HD23	1:I:1217:TYR:HD1	1.68	0.57
1:G:1268:LEU:O	1:G:1272:ARG:HG3	2.04	0.57
1:K:1047:GLY:HA2	1:K:1050:ASN:HD22	1.68	0.57
1:F:1018:ASP:HB2	1:F:1020:SER:O	2.04	0.57
1:H:1197:VAL:HG11	1:I:1197:VAL:HG13	1.86	0.57
1:L:1016:ARG:NH2	4:L:1436:HOH:O	2.20	0.57
1:F:1017:LEU:HD11	1:F:1022:LEU:HD13	1.87	0.57
1:F:1019:ALA:HB3	1:F:1036:ILE:HD11	1.85	0.57
1:G:1008:ASN:O	1:I:1048:LYS:NZ	2.32	0.57
1:H:1011:VAL:O	4:H:1412:HOH:O	2.17	0.57
1:J:1007:ASN:ND2	1:J:1054:GLN:OE1	2.36	0.57
1:L:1164:ALA:HA	1:L:1167:GLU:HG2	1.86	0.57
1:A:1272:ARG:NH2	1:B:1245:ASP:O	2.37	0.57
1:F:1131:ASN:ND2	4:F:1315:HOH:O	2.09	0.57
1:I:1111:GLU:OE2	4:I:1431:HOH:O	2.17	0.57
1:J:1115:LEU:HD11	1:K:1116:GLN:HG2	1.85	0.57
1:A:1130:GLU:HA	1:A:1133:ILE:HD12	1.86	0.57
1:G:1045:ILE:HA	1:H:1010:VAL:HG11	1.87	0.57
1:G:1212:ASN:HB3	1:H:1206:SER:HA	1.87	0.57
1:I:1165:GLU:OE2	4:I:1437:HOH:O	2.17	0.57
1:A:1104:ARG:HH12	1:B:1106:THR:HG22	1.68	0.57
1:B:1235:ALA:O	1:B:1276:LYS:NZ	2.38	0.57
1:E:1268:LEU:HD22	1:F:1264:ILE:HG23	1.87	0.57
1:J:1026:VAL:CG1	1:K:1026:VAL:HG11	2.35	0.57
1:K:1012:ILE:HG22	1:K:1014:ALA:H	1.70	0.57
1:A:1200:THR:OG1	1:C:1195:ASP:OD2	2.17	0.56
1:B:1146:ARG:NH1	1:C:1144:GLU:OE2	2.35	0.56
1:I:1054:GLN:OE1	4:I:1430:HOH:O	2.17	0.56
1:J:1217:TYR:O	1:J:1223:LYS:HA	2.04	0.56
1:A:1230:THR:HA	1:A:1289:ASP:HB2	1.87	0.56
1:F:1063:ASN:HA	1:F:1066:GLN:HB2	1.87	0.56
1:K:1235:ALA:HB2	1:L:1274:ARG:HH21	1.69	0.56
1:B:1259:SER:HB3	1:C:1252:VAL:HG12	1.87	0.56
1:D:1046:ALA:O	1:D:1050:ASN:ND2	2.30	0.56
1:D:1192:LEU:HD21	1:E:1192:LEU:HD12	1.86	0.56
1:F:1086:ASP:OD1	4:F:1319:HOH:O	2.18	0.56
1:G:1048:LYS:NZ	1:H:1008:ASN:O	2.26	0.56
1:L:1238:THR:H	1:L:1273:ARG:CZ	2.19	0.56
1:F:1081:ARG:NH1	4:F:1337:HOH:O	2.39	0.56
1:F:1242:GLY:O	1:F:1274:ARG:NH1	2.38	0.56
1:J:1192:LEU:O	1:J:1196:TYR:HB3	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1126:VAL:HG11	1:C:1125:ARG:HE	1.70	0.56
1:G:1211:LEU:HD23	1:I:1217:TYR:CD1	2.41	0.56
1:H:1094:ASN:ND2	3:H:1301:CL:CL	2.63	0.56
1:H:1187:ASN:ND2	4:H:1437:HOH:O	2.38	0.56
1:A:1010:VAL:HG22	1:C:1048:LYS:HE2	1.88	0.56
1:A:1227:ALA:O	1:B:1285:HIS:NE2	2.37	0.56
1:H:1104:ARG:NH2	1:I:1106:THR:OG1	2.37	0.56
1:H:1187:ASN:OD1	1:H:1188:ASN:N	2.38	0.56
1:D:1196:TYR:OH	1:F:1195:ASP:OD2	2.14	0.56
1:G:1160:ARG:NH2	1:H:1162:THR:OG1	2.30	0.56
1:H:1232:TRP:HH2	1:I:1278:LEU:HD12	1.70	0.56
1:J:1091:ILE:HA	1:J:1094:ASN:HB2	1.88	0.56
1:G:1171:LEU:HB3	1:I:1171:LEU:HD13	1.87	0.56
1:H:1264:ILE:HD12	1:H:1264:ILE:C	2.30	0.56
1:B:1279:GLU:OE2	1:B:1283:ARG:NH2	2.39	0.56
4:B:1336:HOH:O	1:C:1073:HIS:ND1	2.33	0.56
1:H:1289:ASP:OD1	1:H:1289:ASP:N	2.29	0.56
1:A:1212:ASN:OD1	1:A:1213:VAL:N	2.38	0.55
1:D:1157:LEU:HD21	1:E:1157:LEU:HB3	1.86	0.55
1:H:1115:LEU:HD21	1:I:1116:GLN:HA	1.87	0.55
1:H:1276:LYS:HD3	1:I:1244:PHE:HD2	1.71	0.55
1:J:1048:LYS:HZ1	1:K:1010:VAL:H	1.54	0.55
1:J:1136:LEU:HD11	1:K:1137:GLN:HG3	1.89	0.55
1:A:1142:ASP:O	1:A:1145:SER:OG	2.20	0.55
1:J:1186:GLU:OE1	1:L:1181:ARG:NH2	2.39	0.55
1:G:1270:THR:OG1	1:I:1272:ARG:NH2	2.39	0.55
1:A:1126:VAL:HG12	1:C:1125:ARG:HH21	1.72	0.55
1:D:1217:TYR:HE2	1:F:1219:VAL:HG23	1.71	0.55
1:G:1006:LEU:HD21	1:I:1055:GLY:HA3	1.88	0.55
1:J:1066:GLN:NE2	1:K:1067:ASP:OD1	2.35	0.55
1:C:1224:VAL:O	1:C:1224:VAL:CG1	2.55	0.55
1:D:1244:PHE:O	1:F:1236:THR:OG1	2.23	0.55
1:J:1217:TYR:CE2	1:L:1217:TYR:CZ	2.78	0.55
1:K:1080:LEU:HD21	1:L:1080:LEU:HB3	1.89	0.55
1:K:1207:LEU:HD22	1:L:1199:LYS:HA	1.89	0.55
1:B:1066:GLN:NE2	1:C:1066:GLN:OE1	2.34	0.55
1:E:1146:ARG:HH21	1:F:1147:ILE:HG13	1.71	0.55
1:G:1195:ASP:OD1	1:H:1199:LYS:N	2.40	0.55
1:B:1258:GLN:NE2	1:B:1260:GLU:OE1	2.40	0.55
1:D:1242:GLY:O	1:D:1274:ARG:NH2	2.36	0.55
1:I:1013:GLN:HB3	4:I:1452:HOH:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1165:GLU:OE2	4:L:1413:HOH:O	2.18	0.55
1:A:1245:ASP:HB2	1:C:1272:ARG:HH12	1.71	0.55
1:D:1150:ASN:O	1:D:1154:ILE:HG12	2.07	0.55
1:G:1001:MET:O	1:I:1062:LYS:NZ	2.39	0.55
1:J:1225:VAL:HG12	1:J:1226:GLY:H	1.72	0.55
1:A:1212:ASN:HB3	1:B:1206:SER:HA	1.89	0.55
1:A:1220:GLY:N	4:B:1349:HOH:O	2.35	0.55
1:A:1066:GLN:HA	1:A:1069:GLU:HG2	1.88	0.55
1:D:1034:TYR:OH	4:D:1408:HOH:O	2.18	0.55
1:D:1062:LYS:O	1:D:1066:GLN:N	2.39	0.55
1:G:1077:ILE:HA	1:G:1080:LEU:HB2	1.88	0.55
1:H:1273:ARG:HG3	1:I:1246:ALA:HB1	1.89	0.55
1:J:1283:ARG:HH21	1:J:1288:ILE:HD12	1.72	0.55
1:F:1022:LEU:O	1:F:1024:ARG:N	2.40	0.54
1:H:1269:ILE:O	1:H:1273:ARG:HD3	2.07	0.54
1:J:1175:VAL:N	4:J:1464:HOH:O	2.38	0.54
1:B:1062:LYS:HB3	1:C:1063:ASN:HD22	1.72	0.54
1:G:1246:ALA:HA	1:I:1272:ARG:HH11	1.71	0.54
1:J:1062:LYS:NZ	1:K:1067:ASP:OD2	2.36	0.54
1:D:1022:LEU:HD23	1:D:1032:LEU:HD12	1.88	0.54
1:A:1087:HIS:O	1:A:1091:ILE:HG13	2.07	0.54
1:F:1058:ASP:OD1	1:F:1059:ALA:N	2.41	0.54
1:I:1219:VAL:HG13	1:I:1224:VAL:HG21	1.90	0.54
4:A:1402:HOH:O	1:C:1235:ALA:N	2.40	0.54
1:C:1277:ALA:HA	1:C:1280:ASP:HB2	1.88	0.54
1:J:1219:VAL:CG1	1:K:1215:THR:HA	2.38	0.54
1:D:1060:GLN:NE2	1:F:1058:ASP:OD1	2.41	0.54
1:D:1224:VAL:HG13	1:D:1225:VAL:HG23	1.90	0.54
1:E:1197:VAL:N	4:E:1404:HOH:O	2.40	0.54
1:J:1197:VAL:C	1:L:1197:VAL:CG2	2.78	0.54
1:C:1111:GLU:O	1:C:1115:LEU:N	2.34	0.54
1:I:1027:PHE:HA	4:I:1459:HOH:O	2.06	0.54
1:L:1228:ARG:NE	1:L:1286:GLY:O	2.29	0.54
1:D:1278:LEU:HB2	1:E:1278:LEU:HD21	1.90	0.54
1:K:1250:PHE:CE1	1:K:1264:ILE:CG1	2.88	0.54
1:A:1066:GLN:OE1	1:B:1066:GLN:NE2	2.41	0.54
1:B:1195:ASP:OD1	1:B:1196:TYR:N	2.40	0.54
1:H:1150:ASN:HB3	3:I:1301:CL:CL	2.44	0.54
1:J:1232:TRP:HB3	1:J:1283:ARG:HH22	1.72	0.54
1:K:1250:PHE:CG	1:K:1264:ILE:HG12	2.39	0.54
1:E:1178:LEU:HA	1:E:1181:ARG:HD3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1235:ALA:HB1	1:I:1244:PHE:O	2.09	0.53
1:J:1210:PRO:HG2	1:K:1204:SER:HB2	1.90	0.53
1:L:1196:TYR:CZ	1:L:1198:SER:HB3	2.43	0.53
1:B:1230:THR:HG22	1:B:1289:ASP:HB3	1.89	0.53
1:H:1109:GLU:HA	1:H:1112:ILE:HD11	1.89	0.53
1:H:1225:VAL:HA	1:I:1285:HIS:HB3	1.90	0.53
1:J:1275:THR:HA	1:J:1278:LEU:HD22	1.90	0.53
1:B:1195:ASP:OD2	1:C:1196:TYR:OH	2.17	0.53
1:C:1035:VAL:HA	1:C:1038:GLN:HG2	1.89	0.53
1:J:1197:VAL:HG22	1:K:1197:VAL:O	2.08	0.53
1:L:1240:ASN:HB3	1:L:1273:ARG:HG3	1.90	0.53
1:C:1279:GLU:OE2	1:C:1283:ARG:NH2	2.36	0.53
1:C:1282:LEU:HB3	1:C:1288:ILE:HG12	1.89	0.53
1:D:1048:LYS:HD2	1:E:1010:VAL:HG13	1.90	0.53
1:B:1114:SER:OG	4:B:1363:HOH:O	2.19	0.53
1:J:1048:LYS:NZ	1:K:1010:VAL:H	2.06	0.53
1:K:1256:TYR:C	1:K:1258:GLN:H	2.16	0.53
1:L:1196:TYR:CZ	1:L:1198:SER:CB	2.91	0.53
1:B:1256:TYR:OH	1:C:1253:SER:O	2.15	0.53
1:C:1012:ILE:HG13	1:C:1014:ALA:N	2.23	0.53
1:F:1007:ASN:O	1:F:1009:PRO:HD3	2.09	0.53
1:J:1010:VAL:HG12	1:J:1011:VAL:O	2.09	0.53
1:C:1216:SER:HB2	1:C:1223:LYS:HG3	1.90	0.53
1:E:1238:THR:N	4:E:1424:HOH:O	2.42	0.53
1:J:1197:VAL:O	1:L:1197:VAL:HG23	2.01	0.53
1:K:1212:ASN:HD22	1:K:1213:VAL:N	2.07	0.53
1:G:1112:ILE:HG23	1:I:1115:LEU:HD22	1.91	0.53
1:K:1209:SER:OG	1:L:1203:THR:O	2.19	0.53
1:L:1161:VAL:O	1:L:1165:GLU:N	2.42	0.53
1:D:1023:PRO:HB2	1:D:1026:VAL:HG12	1.90	0.53
1:D:1265:ALA:HA	1:D:1268:LEU:HB3	1.91	0.53
1:B:1014:ALA:HB3	1:L:1107:THR:HG23	1.91	0.52
1:B:1102:ASN:O	1:B:1106:THR:HG23	2.09	0.52
1:D:1022:LEU:HG	1:D:1023:PRO:HD2	1.91	0.52
1:G:1164:ALA:O	1:G:1168:ILE:HG12	2.09	0.52
1:H:1213:VAL:HG23	1:I:1207:LEU:HD12	1.89	0.52
1:L:1270:THR:O	1:L:1273:ARG:HB2	2.08	0.52
1:A:1003:ASP:HB3	1:A:1006:LEU:HD13	1.91	0.52
1:A:1157:LEU:HD21	1:B:1158:ASN:OD1	2.10	0.52
1:D:1245:ASP:O	4:D:1458:HOH:O	2.19	0.52
1:A:1265:ALA:HB1	1:B:1250:PHE:HD2	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1214:THR:HG23	1:D:1215:THR:HG23	1.92	0.52
1:E:1259:SER:HA	1:E:1262:GLN:HB2	1.90	0.52
1:A:1109:GLU:HG3	1:A:1112:ILE:HB	1.91	0.52
1:C:1034:TYR:O	1:C:1038:GLN:N	2.38	0.52
1:D:1005:SER:OG	4:D:1452:HOH:O	2.19	0.52
1:D:1087:HIS:ND1	4:D:1448:HOH:O	2.23	0.52
1:E:1006:LEU:HD12	1:E:1006:LEU:H	1.74	0.52
1:G:1011:VAL:HA	1:G:1013:GLN:HG2	1.91	0.52
1:G:1287:LEU:HD22	1:H:1287:LEU:HD11	1.92	0.52
1:G:1223:LYS:O	1:H:1286:GLY:HA3	2.09	0.52
1:H:1017:LEU:HD23	1:H:1036:ILE:HD12	1.90	0.52
1:A:1004:PRO:HA	1:A:1057:TYR:CE1	2.44	0.52
1:G:1022:LEU:HD21	1:G:1032:LEU:HD22	1.92	0.52
1:G:1240:ASN:O	1:G:1274:ARG:NH1	2.42	0.52
1:K:1271:GLU:HG3	1:L:1271:GLU:OE2	2.10	0.52
1:B:1024:ARG:N	4:B:1329:HOH:O	2.13	0.52
1:D:1115:LEU:HD21	1:E:1115:LEU:HD23	1.91	0.52
1:D:1209:SER:HB3	1:E:1201:ALA:O	2.09	0.52
1:G:1211:LEU:HD12	1:G:1212:ASN:H	1.75	0.52
1:H:1230:THR:HA	1:H:1289:ASP:OD2	2.10	0.52
1:J:1175:VAL:HA	1:J:1178:LEU:HB2	1.91	0.52
1:D:1182:VAL:HG12	1:F:1181:ARG:HH21	1.74	0.52
1:E:1240:ASN:HB2	1:E:1273:ARG:HB3	1.92	0.52
1:H:1031:TYR:HB2	1:I:1021:ILE:HG22	1.92	0.52
1:D:1024:ARG:NH1	1:D:1032:LEU:HD21	2.23	0.51
1:F:1063:ASN:OD1	1:F:1066:GLN:NE2	2.43	0.51
1:J:1027:PHE:HB2	1:J:1032:LEU:HD12	1.93	0.51
1:K:1198:SER:HA	4:K:1430:HOH:O	2.10	0.51
1:C:1212:ASN:ND2	4:C:1344:HOH:O	2.43	0.51
1:H:1265:ALA:O	1:H:1269:ILE:HG12	2.10	0.51
1:J:1268:LEU:O	1:J:1271:GLU:HB3	2.10	0.51
1:K:1255:THR:O	1:K:1257:THR:OG1	2.23	0.51
1:K:1282:LEU:HD21	1:L:1282:LEU:HD21	1.91	0.51
1:A:1261:ILE:HG22	1:B:1252:VAL:HG21	1.91	0.51
1:B:1104:ARG:NH1	1:C:1102:ASN:OD1	2.38	0.51
1:E:1195:ASP:O	1:F:1199:LYS:NZ	2.29	0.51
1:H:1266:ASN:O	1:H:1270:THR:HG23	2.10	0.51
1:K:1083:ASP:OD2	1:L:1081:ARG:NH2	2.32	0.51
1:C:1114:SER:OG	4:C:1321:HOH:O	2.19	0.51
1:H:1273:ARG:NH1	1:I:1247:ASP:HA	2.25	0.51
1:J:1041:ASP:O	1:J:1045:ILE:N	2.38	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1083:ASP:OD1	1:J:1084:VAL:N	2.44	0.51
1:D:1019:ALA:O	1:D:1024:ARG:NH2	2.32	0.51
1:D:1248:LEU:HD13	1:D:1250:PHE:CE1	2.45	0.51
1:K:1213:VAL:HG11	1:L:1211:LEU:HB2	1.90	0.51
1:D:1118:ASN:O	1:D:1122:LEU:HG	2.10	0.51
1:E:1174:ASN:C	1:E:1174:ASN:HD22	2.18	0.51
1:H:1208:ALA:O	4:H:1402:HOH:O	2.19	0.51
1:J:1020:SER:HB2	1:J:1024:ARG:NH2	2.25	0.51
1:J:1241:LYS:H	1:J:1241:LYS:HD3	1.76	0.51
1:L:1269:ILE:HA	1:L:1272:ARG:HG2	1.92	0.51
1:C:1164:ALA:O	4:C:1323:HOH:O	2.19	0.51
1:F:1012:ILE:HG23	1:F:1014:ALA:N	2.26	0.51
1:I:1063:ASN:O	1:I:1066:GLN:HG2	2.10	0.51
1:J:1197:VAL:C	1:L:1197:VAL:HG21	2.36	0.51
1:J:1249:THR:HG21	1:L:1265:ALA:HB1	1.92	0.51
1:F:1108:ALA:HA	1:F:1111:GLU:HB2	1.92	0.51
1:F:1232:TRP:HB2	1:F:1289:ASP:OD1	2.11	0.51
1:G:1080:LEU:O	1:G:1084:VAL:HG23	2.11	0.51
1:H:1264:ILE:HD11	1:I:1264:ILE:HG21	1.93	0.51
1:A:1074:GLU:OE1	1:C:1073:HIS:NE2	2.40	0.51
1:D:1213:VAL:HG12	1:E:1207:LEU:HD12	1.93	0.51
1:G:1258:GLN:HE21	1:H:1253:SER:C	2.18	0.51
1:G:1281:ALA:HA	1:I:1229:GLN:HE21	1.76	0.51
1:A:1170:SER:O	1:A:1173:THR:OG1	2.27	0.51
1:B:1204:SER:O	4:B:1355:HOH:O	2.20	0.51
1:C:1242:GLY:O	1:C:1274:ARG:NH2	2.44	0.51
1:D:1114:SER:HA	1:D:1117:THR:HG22	1.93	0.51
1:D:1172:GLN:HG2	1:F:1171:LEU:HD11	1.93	0.51
1:G:1254:ASP:OD1	1:G:1255:THR:N	2.44	0.51
1:H:1189:ILE:O	1:H:1193:GLN:HG3	2.11	0.51
1:G:1173:THR:OG1	4:G:1419:HOH:O	2.19	0.50
4:G:1402:HOH:O	1:I:1211:LEU:HD12	2.10	0.50
1:H:1160:ARG:HD2	4:H:1429:HOH:O	2.09	0.50
1:H:1212:ASN:OD1	1:H:1213:VAL:N	2.45	0.50
1:F:1105:VAL:N	4:F:1367:HOH:O	2.44	0.50
1:G:1271:GLU:HA	1:G:1274:ARG:HB2	1.92	0.50
1:I:1212:ASN:OD1	1:I:1213:VAL:N	2.44	0.50
1:E:1235:ALA:HB2	1:F:1274:ARG:NH2	2.25	0.50
1:F:1186:GLU:OE1	4:F:1307:HOH:O	2.19	0.50
1:J:1046:ALA:HB2	1:L:1045:ILE:HD13	1.92	0.50
1:A:1024:ARG:O	4:A:1420:HOH:O	2.19	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1204:SER:OG	4:G:1422:HOH:O	2.19	0.50
1:J:1027:PHE:HD2	1:J:1032:LEU:HD12	1.75	0.50
1:L:1109:GLU:HG3	1:L:1110:GLY:N	2.27	0.50
1:A:1195:ASP:OD2	1:B:1196:TYR:OH	2.23	0.50
1:B:1077:ILE:HA	1:B:1080:LEU:HB2	1.94	0.50
1:D:1023:PRO:HD3	4:F:1370:HOH:O	2.11	0.50
1:D:1160:ARG:NH2	1:E:1162:THR:OG1	2.39	0.50
1:D:1204:SER:HB2	1:F:1210:PRO:HG2	1.93	0.50
1:E:1224:VAL:O	1:F:1286:GLY:N	2.45	0.50
1:G:1022:LEU:O	4:G:1456:HOH:O	2.19	0.50
1:H:1273:ARG:O	1:H:1276:LYS:N	2.44	0.50
1:L:1076:ARG:O	1:L:1080:LEU:HB2	2.12	0.50
1:L:1115:LEU:O	1:L:1119:VAL:HG23	2.12	0.50
1:A:1022:LEU:O	4:A:1469:HOH:O	2.19	0.50
1:B:1006:LEU:HB2	1:B:1057:TYR:HB2	1.94	0.50
1:D:1141:ASP:HA	1:D:1144:GLU:HB3	1.93	0.50
1:G:1266:ASN:HB3	4:G:1430:HOH:O	2.11	0.50
1:E:1253:SER:OG	1:E:1254:ASP:OD1	2.30	0.50
1:F:1156:ALA:O	4:F:1302:HOH:O	2.19	0.50
1:H:1018:ASP:OD1	1:H:1018:ASP:N	2.45	0.50
1:H:1115:LEU:HD21	1:I:1116:GLN:HG2	1.92	0.50
1:K:1148:THR:HG22	1:K:1152:LYS:HD3	1.94	0.50
1:B:1087:HIS:O	1:B:1091:ILE:N	2.42	0.49
1:F:1239:ALA:HB1	1:F:1277:ALA:HB2	1.93	0.49
1:G:1272:ARG:HA	1:H:1271:GLU:OE2	2.11	0.49
1:J:1205:GLN:HB3	1:K:1199:LYS:HE2	1.94	0.49
1:J:1256:TYR:OH	1:K:1253:SER:O	2.25	0.49
1:J:1275:THR:HG23	1:K:1278:LEU:HD22	1.94	0.49
1:H:1028:SER:HB3	1:I:1021:ILE:HG23	1.93	0.49
1:A:1168:ILE:HD13	4:C:1323:HOH:O	2.11	0.49
1:K:1164:ALA:HA	1:K:1167:GLU:HG2	1.95	0.49
1:K:1214:THR:C	1:K:1215:THR:OG1	2.56	0.49
1:L:1211:LEU:HA	4:L:1465:HOH:O	2.12	0.49
1:D:1116:GLN:HG3	1:F:1115:LEU:HD11	1.94	0.49
1:E:1089:SER:OG	1:E:1090:ARG:N	2.45	0.49
1:E:1132:ASN:O	1:E:1136:LEU:HG	2.12	0.49
1:K:1031:TYR:HD1	1:L:1021:ILE:HG22	1.77	0.49
1:L:1041:ASP:O	1:L:1045:ILE:N	2.40	0.49
1:B:1250:PHE:HB3	1:B:1264:ILE:HG12	1.93	0.49
1:C:1024:ARG:NH2	4:C:1316:HOH:O	2.33	0.49
1:F:1249:THR:HB	1:F:1264:ILE:HG12	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1258:GLN:NE2	4:F:1334:HOH:O	2.06	0.49
1:G:1137:GLN:HG2	1:I:1136:LEU:HD11	1.94	0.49
1:G:1203:THR:OG1	4:G:1401:HOH:O	2.20	0.49
1:K:1048:LYS:HG2	1:L:1010:VAL:HG12	1.94	0.49
1:G:1143:HIS:O	1:G:1147:ILE:HG13	2.13	0.49
1:B:1209:SER:OG	1:C:1205:GLN:OE1	2.26	0.49
1:F:1010:VAL:HG23	1:F:1050:ASN:HD21	1.77	0.49
1:H:1198:SER:N	1:H:1205:GLN:HE22	2.08	0.49
1:J:1154:ILE:O	1:J:1158:ASN:ND2	2.45	0.49
1:L:1211:LEU:HD12	1:L:1212:ASN:H	1.77	0.49
1:A:1274:ARG:HH21	1:C:1235:ALA:HB2	1.77	0.49
1:D:1078:LYS:NZ	4:D:1422:HOH:O	2.46	0.49
1:D:1216:SER:OG	1:D:1217:TYR:N	2.45	0.49
1:G:1272:ARG:HD2	1:H:1245:ASP:OD1	2.13	0.49
1:E:1275:THR:OG1	1:F:1271:GLU:OE2	2.27	0.49
1:F:1104:ARG:O	1:F:1107:THR:OG1	2.31	0.49
1:G:1081:ARG:HH11	1:I:1080:LEU:HD23	1.77	0.49
1:I:1012:ILE:HG12	1:I:1013:GLN:H	1.78	0.49
1:K:1079:GLN:HA	1:K:1082:ILE:HD11	1.95	0.49
1:C:1219:VAL:HG13	1:C:1224:VAL:HG21	1.94	0.49
1:D:1076:ARG:O	1:D:1080:LEU:HB2	2.12	0.49
1:K:1076:ARG:NH1	1:L:1074:GLU:OE2	2.43	0.49
1:G:1076:ARG:O	1:G:1080:LEU:HB2	2.12	0.48
1:I:1048:LYS:O	1:I:1052:ALA:N	2.46	0.48
1:J:1010:VAL:HG11	1:L:1048:LYS:HZ3	1.77	0.48
1:K:1199:LYS:NZ	4:K:1411:HOH:O	2.41	0.48
1:B:1125:ARG:HH22	1:C:1127:THR:HG23	1.77	0.48
1:D:1109:GLU:OE1	4:D:1428:HOH:O	2.20	0.48
1:F:1025:ASN:OD1	1:F:1025:ASN:N	2.46	0.48
1:J:1041:ASP:OD1	1:J:1042:VAL:N	2.46	0.48
1:L:1119:VAL:HA	1:L:1122:LEU:HB2	1.94	0.48
1:A:1232:TRP:CH2	1:B:1278:LEU:HD12	2.48	0.48
1:D:1132:ASN:O	1:D:1136:LEU:HG	2.14	0.48
1:F:1140:VAL:HA	1:F:1143:HIS:HB2	1.95	0.48
1:I:1184:THR:O	1:I:1188:ASN:N	2.46	0.48
1:J:1154:ILE:HD13	1:L:1153:ALA:HB3	1.95	0.48
1:C:1252:VAL:N	1:C:1260:GLU:OE2	2.47	0.48
1:D:1115:LEU:O	1:D:1119:VAL:HG23	2.14	0.48
1:G:1023:PRO:HG3	4:I:1459:HOH:O	2.13	0.48
1:G:1197:VAL:HG13	4:G:1404:HOH:O	2.12	0.48
1:J:1122:LEU:HD12	1:J:1125:ARG:HD3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1189:ILE:HD11	1:C:1188:ASN:HB3	1.94	0.48
1:B:1218:SER:HA	1:B:1224:VAL:HG22	1.95	0.48
1:D:1060:GLN:NE2	1:F:1055:GLY:O	2.47	0.48
1:D:1066:GLN:OE1	1:F:1066:GLN:NE2	2.29	0.48
1:E:1041:ASP:O	1:E:1045:ILE:HG12	2.14	0.48
1:I:1196:TYR:O	4:I:1412:HOH:O	2.20	0.48
1:J:1112:ILE:HD12	1:L:1111:GLU:OE1	2.14	0.48
1:J:1170:SER:O	1:J:1173:THR:OG1	2.31	0.48
1:K:1136:LEU:HD21	1:L:1136:LEU:HB3	1.95	0.48
1:E:1195:ASP:O	1:F:1198:SER:HA	2.14	0.48
1:E:1244:PHE:N	4:E:1410:HOH:O	2.06	0.48
1:L:1016:ARG:HH12	1:L:1040:THR:HA	1.78	0.48
1:A:1278:LEU:HG	1:C:1282:LEU:HD22	1.96	0.48
1:B:1213:VAL:HA	1:C:1207:LEU:HB2	1.96	0.48
1:D:1217:TYR:HD1	1:E:1217:TYR:CE1	2.32	0.48
1:G:1279:GLU:OE2	1:G:1283:ARG:NH2	2.47	0.48
1:J:1150:ASN:OD1	4:J:1425:HOH:O	2.20	0.48
1:J:1269:ILE:O	1:J:1273:ARG:HG3	2.14	0.48
1:A:1177:ALA:O	1:A:1181:ARG:HG3	2.14	0.48
1:B:1066:GLN:O	1:B:1070:LEU:HG	2.12	0.48
1:B:1167:GLU:O	1:B:1171:LEU:HB2	2.13	0.48
1:I:1079:GLN:HA	1:I:1082:ILE:HG22	1.96	0.48
1:C:1012:ILE:HG13	1:C:1013:GLN:C	2.39	0.48
1:E:1259:SER:N	4:E:1448:HOH:O	2.46	0.48
1:H:1133:ILE:HD11	1:I:1133:ILE:HG21	1.96	0.48
1:J:1150:ASN:HD21	1:K:1147:ILE:HG12	1.77	0.48
1:K:1076:ARG:HH12	1:L:1074:GLU:CD	2.22	0.48
1:L:1018:ASP:O	1:L:1020:SER:N	2.36	0.48
1:A:1109:GLU:HA	1:A:1112:ILE:HB	1.96	0.48
1:H:1022:LEU:HG	1:H:1023:PRO:HD2	1.96	0.48
1:H:1109:GLU:HA	1:H:1112:ILE:CD1	2.42	0.48
1:H:1115:LEU:HD13	1:I:1115:LEU:HB3	1.95	0.48
1:H:1284:ALA:HB1	4:H:1423:HOH:O	2.14	0.48
1:K:1277:ALA:HA	1:K:1280:ASP:HB2	1.96	0.48
1:A:1239:ALA:HB1	1:A:1277:ALA:HB2	1.96	0.47
1:C:1036:ILE:O	4:C:1305:HOH:O	2.20	0.47
1:E:1101:LEU:HD23	1:F:1101:LEU:HD23	1.95	0.47
1:C:1022:LEU:O	1:C:1024:ARG:N	2.45	0.47
1:G:1166:GLY:N	4:G:1457:HOH:O	2.15	0.47
1:G:1217:TYR:HB3	1:H:1217:TYR:CZ	2.49	0.47
1:A:1225:VAL:HG12	1:A:1226:GLY:H	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1143:HIS:CE1	1:H:1140:VAL:HG13	2.50	0.47
1:J:1197:VAL:HB	1:L:1197:VAL:HG21	1.97	0.47
1:L:1248:LEU:HD11	1:L:1250:PHE:O	2.14	0.47
1:B:1209:SER:HB3	1:C:1201:ALA:O	2.14	0.47
1:C:1188:ASN:O	1:C:1192:LEU:HB2	2.15	0.47
1:D:1081:ARG:NH1	1:D:1085:ASP:OD1	2.46	0.47
1:D:1213:VAL:HA	1:E:1207:LEU:HB2	1.95	0.47
1:G:1224:VAL:O	1:H:1286:GLY:N	2.46	0.47
1:E:1254:ASP:OD1	1:E:1254:ASP:N	2.47	0.47
1:H:1258:GLN:HA	1:H:1261:ILE:HD13	1.96	0.47
1:A:1143:HIS:O	1:A:1147:ILE:HG12	2.14	0.47
1:B:1063:ASN:OD1	1:B:1066:GLN:NE2	2.48	0.47
1:E:1279:GLU:HB2	1:F:1278:LEU:HD21	1.96	0.47
1:F:1106:THR:HA	1:F:1109:GLU:OE1	2.15	0.47
1:G:1050:ASN:HA	1:I:1048:LYS:HE2	1.97	0.47
1:H:1094:ASN:OD1	1:I:1095:THR:OG1	2.30	0.47
1:I:1129:ALA:O	1:I:1133:ILE:HG23	2.14	0.47
1:K:1268:LEU:HD11	1:L:1268:LEU:HB2	1.96	0.47
1:B:1119:VAL:HG23	1:B:1122:LEU:HD12	1.97	0.47
1:B:1210:PRO:HD2	1:C:1202:THR:O	2.15	0.47
1:D:1214:THR:HA	1:D:1215:THR:HA	1.72	0.47
1:E:1021:ILE:HA	4:E:1429:HOH:O	2.14	0.47
1:G:1074:GLU:OE1	1:I:1073:HIS:NE2	2.46	0.47
1:J:1232:TRP:HB3	1:J:1283:ARG:NH2	2.28	0.47
1:K:1214:THR:CG2	1:K:1215:THR:OG1	2.63	0.47
1:D:1282:LEU:HD21	1:E:1282:LEU:HD21	1.95	0.47
1:E:1108:ALA:O	1:E:1112:ILE:N	2.47	0.47
1:E:1169:ALA:HA	1:E:1172:GLN:HE21	1.80	0.47
1:G:1063:ASN:HD22	1:I:1062:LYS:HE3	1.80	0.47
1:L:1196:TYR:C	1:L:1197:VAL:HG22	2.40	0.47
1:E:1244:PHE:HZ	1:E:1271:GLU:HG2	1.80	0.47
1:D:1136:LEU:HA	1:D:1139:ASP:HB2	1.97	0.47
1:H:1033:LEU:HA	1:H:1036:ILE:HG22	1.96	0.47
1:H:1101:LEU:N	4:H:1432:HOH:O	2.47	0.47
1:K:1262:GLN:O	1:K:1266:ASN:N	2.43	0.47
1:A:1006:LEU:HB3	1:A:1053:GLY:O	2.15	0.46
1:A:1175:VAL:O	1:A:1179:ASP:HB3	2.14	0.46
1:A:1195:ASP:O	1:B:1198:SER:HA	2.15	0.46
1:A:1232:TRP:HB2	1:A:1289:ASP:HB3	1.97	0.46
1:F:1012:ILE:HA	1:F:1013:GLN:HB2	1.97	0.46
1:F:1197:VAL:O	1:F:1199:LYS:NZ	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1198:SER:HB3	1:G:1201:ALA:HB2	1.97	0.46
1:H:1197:VAL:CG1	1:I:1197:VAL:HG13	2.45	0.46
1:A:1198:SER:HA	1:C:1195:ASP:O	2.14	0.46
1:B:1122:LEU:HD11	1:C:1123:ASP:OD1	2.15	0.46
1:G:1019:ALA:HA	1:G:1022:LEU:N	2.27	0.46
1:H:1218:SER:HA	1:H:1224:VAL:H	1.80	0.46
1:L:1041:ASP:O	1:L:1045:ILE:HG13	2.15	0.46
1:D:1091:ILE:HD11	1:E:1091:ILE:CD1	2.46	0.46
1:F:1018:ASP:OD1	1:F:1018:ASP:N	2.48	0.46
1:H:1253:SER:OG	1:H:1257:THR:OG1	2.32	0.46
1:I:1176:SER:OG	4:I:1421:HOH:O	2.20	0.46
1:K:1185:ALA:O	1:K:1189:ILE:HG13	2.15	0.46
1:G:1287:LEU:HB3	1:H:1285:HIS:CE1	2.51	0.46
1:H:1037:ALA:O	1:H:1040:THR:OG1	2.28	0.46
1:H:1217:TYR:CE1	1:I:1211:LEU:HD23	2.51	0.46
1:J:1197:VAL:HG21	1:K:1197:VAL:HG22	1.98	0.46
1:K:1167:GLU:HG3	1:L:1168:ILE:HG21	1.98	0.46
1:G:1269:ILE:HD12	1:G:1272:ARG:HH21	1.80	0.46
1:H:1164:ALA:O	1:H:1168:ILE:HG12	2.16	0.46
1:I:1150:ASN:O	1:I:1154:ILE:HG13	2.15	0.46
1:J:1123:ASP:O	1:J:1127:THR:OG1	2.33	0.46
1:L:1131:ASN:ND2	4:L:1448:HOH:O	2.24	0.46
1:C:1168:ILE:N	4:C:1323:HOH:O	2.48	0.46
1:E:1253:SER:OG	1:E:1254:ASP:N	2.49	0.46
1:K:1250:PHE:HB2	1:K:1251:ALA:HA	1.96	0.46
1:E:1275:THR:HG23	1:F:1278:LEU:HD11	1.98	0.46
1:F:1184:THR:HA	1:F:1187:ASN:HD21	1.81	0.46
1:J:1112:ILE:H	1:J:1112:ILE:HG12	1.61	0.46
1:E:1081:ARG:O	1:E:1085:ASP:N	2.40	0.46
1:G:1252:VAL:CG2	1:I:1262:GLN:HG2	2.45	0.46
1:D:1069:GLU:OE1	1:E:1070:LEU:HB3	2.16	0.46
1:G:1020:SER:HA	1:G:1021:ILE:C	2.41	0.46
1:L:1100:ALA:HA	1:L:1103:VAL:HG12	1.97	0.46
1:B:1169:ALA:HA	1:B:1172:GLN:HB2	1.97	0.46
1:F:1248:LEU:C	1:F:1250:PHE:H	2.23	0.46
1:G:1236:THR:HB	1:H:1246:ALA:HB2	1.98	0.46
1:G:1269:ILE:HG13	1:G:1273:ARG:HE	1.80	0.46
1:H:1041:ASP:O	1:H:1045:ILE:HG12	2.15	0.46
1:H:1218:SER:O	1:I:1212:ASN:HA	2.16	0.46
1:H:1279:GLU:OE1	1:I:1274:ARG:NE	2.33	0.46
1:A:1086:ASP:O	1:A:1090:ARG:HD3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1048:LYS:HB3	1:F:1049:ALA:HB1	1.99	0.45
1:E:1262:GLN:O	1:E:1266:ASN:N	2.49	0.45
1:G:1197:VAL:HG12	4:H:1413:HOH:O	2.15	0.45
1:J:1087:HIS:NE2	1:K:1088:GLU:OE2	2.33	0.45
1:K:1256:TYR:CG	1:L:1256:TYR:HB2	2.51	0.45
1:L:1273:ARG:HA	1:L:1273:ARG:HD3	1.56	0.45
1:B:1049:ALA:HA	1:B:1052:ALA:HB3	1.98	0.45
1:H:1218:SER:N	1:I:1217:TYR:OH	2.50	0.45
1:I:1167:GLU:OE2	4:I:1424:HOH:O	2.21	0.45
1:D:1222:LYS:HB2	1:D:1222:LYS:HE3	1.75	0.45
1:F:1115:LEU:O	1:F:1119:VAL:HB	2.17	0.45
1:H:1153:ALA:O	1:H:1157:LEU:HB2	2.16	0.45
1:J:1026:VAL:HG11	1:K:1026:VAL:HG11	1.98	0.45
1:J:1217:TYR:CE2	1:L:1224:VAL:HG21	2.49	0.45
1:D:1147:ILE:HD11	1:E:1147:ILE:HG12	1.97	0.45
1:G:1270:THR:HA	1:G:1273:ARG:HD2	1.99	0.45
1:H:1139:ASP:O	1:H:1142:ASP:HB3	2.15	0.45
1:J:1266:ASN:N	4:J:1456:HOH:O	2.50	0.45
1:D:1073:HIS:O	1:D:1077:ILE:HG13	2.17	0.45
1:E:1076:ARG:O	1:E:1080:LEU:HB2	2.17	0.45
1:G:1243:VAL:N	4:G:1409:HOH:O	2.28	0.45
1:I:1188:ASN:ND2	4:I:1460:HOH:O	2.38	0.45
1:J:1020:SER:OG	1:J:1022:LEU:N	2.50	0.45
1:L:1274:ARG:HA	4:L:1459:HOH:O	2.17	0.45
1:A:1270:THR:OG1	1:C:1272:ARG:NH2	2.49	0.45
1:B:1178:LEU:HD11	1:C:1179:ASP:OD1	2.15	0.45
1:D:1238:THR:N	4:D:1431:HOH:O	2.10	0.45
1:E:1108:ALA:O	1:E:1112:ILE:HG13	2.17	0.45
1:H:1082:ILE:HD12	1:H:1082:ILE:HA	1.75	0.45
1:K:1062:LYS:HE2	1:L:1001:MET:HE1	1.99	0.45
1:A:1247:ASP:N	4:A:1455:HOH:O	2.46	0.45
1:D:1062:LYS:HB3	1:E:1063:ASN:HD22	1.82	0.45
1:F:1112:ILE:HG22	1:F:1116:GLN:OE1	2.17	0.45
1:G:1148:THR:O	1:G:1152:LYS:HB2	2.17	0.45
1:J:1048:LYS:HZ1	1:K:1010:VAL:N	2.13	0.45
1:A:1195:ASP:HB3	1:B:1196:TYR:HE2	1.81	0.45
1:A:1213:VAL:HG22	1:B:1209:SER:O	2.16	0.45
1:B:1055:GLY:O	1:B:1059:ALA:N	2.50	0.45
1:C:1011:VAL:HG23	1:C:1050:ASN:ND2	2.28	0.45
1:D:1140:VAL:HG21	1:F:1136:LEU:HD22	1.98	0.45
1:G:1034:TYR:O	1:G:1037:ALA:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1229:GLN:HE21	1:I:1284:ALA:HB3	1.81	0.45
1:J:1062:LYS:HA	1:J:1065:GLU:HG2	1.99	0.45
1:A:1013:GLN:HB2	1:C:1037:ALA:HB1	1.99	0.45
1:B:1168:ILE:O	1:B:1172:GLN:N	2.50	0.45
1:D:1217:TYR:HB2	1:D:1225:VAL:HB	1.97	0.45
1:G:1285:HIS:CE1	1:I:1287:LEU:HD12	2.52	0.45
1:J:1026:VAL:HG13	1:K:1026:VAL:HG11	1.97	0.45
1:J:1157:LEU:HD21	1:K:1157:LEU:HB2	1.99	0.45
1:J:1285:HIS:NE2	1:L:1228:ARG:HA	2.31	0.45
1:L:1218:SER:HA	1:L:1224:VAL:HG22	1.98	0.45
1:A:1182:VAL:N	4:A:1445:HOH:O	2.49	0.45
1:D:1123:ASP:O	1:D:1127:THR:OG1	2.22	0.45
1:E:1186:GLU:HG3	1:E:1187:ASN:N	2.32	0.45
1:F:1147:ILE:HA	1:F:1150:ASN:HB2	1.99	0.45
1:K:1214:THR:HG23	1:K:1215:THR:OG1	2.17	0.45
1:K:1244:PHE:HZ	1:K:1271:GLU:HA	1.82	0.45
1:B:1040:THR:O	4:B:1365:HOH:O	2.21	0.44
1:B:1231:GLY:O	1:C:1241:LYS:HB3	2.17	0.44
1:D:1168:ILE:HG12	1:F:1168:ILE:HD11	1.99	0.44
1:D:1198:SER:O	4:D:1440:HOH:O	2.21	0.44
1:F:1020:SER:HA	1:F:1021:ILE:HA	1.74	0.44
1:G:1144:GLU:N	4:G:1408:HOH:O	2.50	0.44
1:J:1144:GLU:OE1	1:L:1143:HIS:NE2	2.48	0.44
1:E:1008:ASN:HA	1:E:1009:PRO:HD3	1.82	0.44
1:F:1158:ASN:HA	1:F:1161:VAL:HG22	1.98	0.44
1:G:1181:ARG:HH21	1:H:1182:VAL:HB	1.83	0.44
1:H:1030:SER:HB2	1:I:1021:ILE:HG21	1.99	0.44
1:J:1022:LEU:HD12	1:J:1023:PRO:HD2	1.99	0.44
1:J:1278:LEU:HD23	1:K:1278:LEU:HD23	1.99	0.44
1:K:1047:GLY:O	1:K:1051:GLU:HG2	2.18	0.44
1:A:1029:LYS:O	1:A:1033:LEU:HG	2.17	0.44
1:A:1088:GLU:OE1	1:C:1087:HIS:NE2	2.50	0.44
1:A:1104:ARG:O	1:A:1107:THR:OG1	2.30	0.44
1:G:1055:GLY:O	1:H:1060:GLN:NE2	2.47	0.44
1:H:1023:PRO:HB2	1:H:1026:VAL:HG12	2.00	0.44
1:I:1189:ILE:O	1:I:1193:GLN:N	2.42	0.44
1:J:1174:ASN:O	1:J:1178:LEU:N	2.41	0.44
1:C:1212:ASN:OD1	1:C:1213:VAL:N	2.51	0.44
1:E:1150:ASN:O	1:E:1154:ILE:HG13	2.18	0.44
1:H:1026:VAL:HG23	1:I:1026:VAL:HG21	1.99	0.44
1:I:1229:GLN:HB2	1:I:1288:ILE:HA	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1258:GLN:NE2	1:J:1230:THR:O	2.48	0.44
1:J:1232:TRP:HA	1:K:1241:LYS:HD2	1.98	0.44
1:A:1196:TYR:CZ	1:A:1198:SER:HB2	2.52	0.44
1:B:1134:SER:N	4:B:1317:HOH:O	1.98	0.44
1:D:1062:LYS:HE2	1:E:1067:ASP:CG	2.42	0.44
1:J:1136:LEU:HD21	1:K:1137:GLN:HA	1.99	0.44
1:L:1088:GLU:HG3	4:L:1452:HOH:O	2.18	0.44
1:F:1074:GLU:OE2	4:F:1340:HOH:O	2.21	0.44
1:H:1062:LYS:NZ	1:H:1065:GLU:OE2	2.38	0.44
1:H:1129:ALA:O	1:H:1132:ASN:N	2.51	0.44
1:H:1174:ASN:O	1:H:1178:LEU:HB2	2.17	0.44
1:J:1012:ILE:HG21	4:J:1465:HOH:O	2.16	0.44
1:J:1037:ALA:O	1:J:1040:THR:OG1	2.32	0.44
1:K:1274:ARG:O	1:K:1278:LEU:N	2.46	0.44
1:A:1115:LEU:HD13	1:B:1115:LEU:HD23	2.00	0.44
1:A:1273:ARG:HG2	1:B:1246:ALA:HB1	1.99	0.44
1:I:1022:LEU:HD21	1:I:1035:VAL:HG11	2.00	0.44
1:J:1067:ASP:HA	1:J:1070:LEU:HB2	2.00	0.44
1:K:1279:GLU:HB2	1:L:1278:LEU:HD11	2.00	0.44
1:A:1132:ASN:O	1:A:1136:LEU:HB2	2.18	0.44
1:B:1098:ILE:HD12	1:B:1098:ILE:HA	1.85	0.44
1:C:1066:GLN:O	1:C:1070:LEU:HG	2.17	0.44
1:C:1080:LEU:HD12	1:C:1080:LEU:HA	1.83	0.44
1:G:1081:ARG:NH2	4:G:1414:HOH:O	2.35	0.44
1:I:1173:THR:OG1	4:I:1426:HOH:O	2.14	0.44
1:K:1170:SER:O	1:K:1173:THR:OG1	2.34	0.44
1:A:1219:VAL:HG12	1:B:1217:TYR:HE2	1.82	0.44
1:E:1050:ASN:OD1	1:E:1051:GLU:N	2.51	0.44
1:E:1123:ASP:O	1:E:1127:THR:HB	2.17	0.44
1:I:1139:ASP:O	1:I:1143:HIS:N	2.45	0.44
1:I:1165:GLU:CD	4:I:1437:HOH:O	2.61	0.44
1:I:1224:VAL:HG12	1:I:1225:VAL:HG23	2.00	0.44
1:J:1011:VAL:HA	1:J:1012:ILE:HA	1.73	0.44
1:J:1219:VAL:HG22	1:K:1213:VAL:HG23	1.99	0.44
1:C:1132:ASN:O	1:C:1136:LEU:HD13	2.18	0.43
1:C:1239:ALA:HB1	1:C:1277:ALA:HB2	2.00	0.43
1:F:1111:GLU:O	4:F:1324:HOH:O	2.20	0.43
1:F:1175:VAL:HA	1:F:1178:LEU:HB2	1.99	0.43
1:F:1229:GLN:HB2	1:F:1288:ILE:HD13	1.99	0.43
1:G:1036:ILE:HD12	1:G:1036:ILE:HA	1.78	0.43
1:J:1283:ARG:HE	1:J:1283:ARG:HB2	1.57	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1024:ARG:HG2	4:L:1430:HOH:O	2.18	0.43
1:D:1008:ASN:HA	1:D:1009:PRO:HD3	1.77	0.43
1:H:1219:VAL:HG21	1:I:1215:THR:O	2.17	0.43
1:K:1250:PHE:CB	1:K:1251:ALA:HA	2.47	0.43
1:A:1165:GLU:OE1	4:A:1424:HOH:O	2.21	0.43
1:A:1213:VAL:HG12	1:C:1219:VAL:HG12	2.00	0.43
1:C:1011:VAL:O	1:C:1013:GLN:HB2	2.18	0.43
1:G:1242:GLY:HA2	4:G:1409:HOH:O	2.18	0.43
1:I:1248:LEU:HG	1:I:1250:PHE:O	2.19	0.43
1:J:1228:ARG:HD3	1:J:1289:ASP:HB3	2.00	0.43
1:K:1080:LEU:HD13	1:L:1081:ARG:HD3	1.99	0.43
1:C:1019:ALA:HB1	1:C:1024:ARG:HD3	1.99	0.43
1:E:1007:ASN:OD1	1:E:1007:ASN:N	2.49	0.43
1:G:1048:LYS:HG3	1:H:1010:VAL:HG22	1.99	0.43
1:I:1131:ASN:OD1	4:I:1461:HOH:O	2.21	0.43
1:L:1143:HIS:O	1:L:1147:ILE:HG12	2.18	0.43
1:B:1195:ASP:O	1:C:1199:LYS:HG3	2.18	0.43
1:H:1230:THR:O	1:I:1241:LYS:HD3	2.17	0.43
1:H:1253:SER:HG	1:H:1257:THR:HG1	1.60	0.43
1:H:1278:LEU:O	1:H:1282:LEU:HG	2.18	0.43
1:I:1061:VAL:O	1:I:1065:GLU:HG3	2.19	0.43
1:K:1012:ILE:HG22	1:K:1014:ALA:N	2.33	0.43
1:K:1275:THR:HA	1:K:1278:LEU:HB2	2.00	0.43
1:L:1101:LEU:O	1:L:1105:VAL:HG23	2.18	0.43
1:L:1104:ARG:O	1:L:1107:THR:HB	2.19	0.43
1:L:1238:THR:H	1:L:1273:ARG:NH2	2.15	0.43
1:A:1160:ARG:HH22	1:B:1162:THR:HG23	1.84	0.43
1:C:1011:VAL:N	1:C:1050:ASN:HD21	2.16	0.43
1:E:1219:VAL:HA	1:F:1213:VAL:O	2.18	0.43
1:H:1197:VAL:HA	1:H:1205:GLN:HE22	1.82	0.43
1:H:1235:ALA:HB3	1:H:1276:LYS:CE	2.49	0.43
1:I:1228:ARG:HB2	1:I:1286:GLY:O	2.18	0.43
1:B:1122:LEU:HD21	1:C:1123:ASP:HA	2.01	0.43
1:B:1127:THR:HA	1:B:1130:GLU:HB2	2.00	0.43
1:D:1016:ARG:HA	1:D:1016:ARG:HD3	1.78	0.43
1:D:1024:ARG:HH12	1:D:1032:LEU:HD21	1.82	0.43
1:D:1201:ALA:O	1:F:1209:SER:HB3	2.18	0.43
1:H:1074:GLU:N	4:H:1431:HOH:O	2.51	0.43
1:H:1198:SER:H	1:H:1205:GLN:NE2	2.11	0.43
1:J:1006:LEU:HD22	1:J:1056:ALA:HB3	2.01	0.43
1:K:1122:LEU:HD12	1:K:1122:LEU:HA	1.86	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:THR:OG1	1:A:1041:ASP:N	2.52	0.43
1:A:1261:ILE:HG22	1:B:1252:VAL:CG2	2.49	0.43
1:B:1278:LEU:O	1:B:1282:LEU:HG	2.19	0.43
1:C:1118:ASN:O	1:C:1122:LEU:HD13	2.19	0.43
1:D:1209:SER:O	1:F:1213:VAL:HG13	2.18	0.43
1:H:1062:LYS:HD2	1:H:1062:LYS:HA	1.92	0.43
1:A:1038:GLN:NE2	4:A:1416:HOH:O	2.12	0.43
1:I:1241:LYS:HB2	1:I:1241:LYS:HE3	1.81	0.43
1:I:1260:GLU:O	1:I:1264:ILE:HG12	2.18	0.43
1:J:1282:LEU:HA	1:J:1287:LEU:HD13	2.01	0.43
1:K:1003:ASP:OD2	1:K:1005:SER:OG	2.36	0.43
1:K:1047:GLY:CA	1:K:1050:ASN:HD22	2.31	0.43
1:K:1109:GLU:O	4:K:1425:HOH:O	2.21	0.43
1:A:1098:ILE:HD12	1:B:1098:ILE:HD11	1.99	0.43
1:A:1171:LEU:HD11	1:B:1172:GLN:HG2	2.01	0.43
1:A:1232:TRP:HH2	1:B:1278:LEU:HD12	1.83	0.43
1:D:1197:VAL:HG23	4:D:1412:HOH:O	2.19	0.43
1:E:1148:THR:O	1:E:1151:THR:OG1	2.35	0.43
1:G:1125:ARG:NH1	4:G:1426:HOH:O	2.52	0.43
1:I:1132:ASN:O	1:I:1136:LEU:HD13	2.19	0.43
1:J:1065:GLU:O	1:J:1068:VAL:HG12	2.19	0.43
1:J:1241:LYS:HE2	1:J:1241:LYS:HB2	1.82	0.43
1:L:1048:LYS:HG2	1:L:1049:ALA:N	2.33	0.43
1:A:1131:ASN:O	1:A:1134:SER:OG	2.31	0.42
1:B:1183:THR:HA	1:B:1186:GLU:HG2	2.01	0.42
1:I:1285:HIS:N	1:I:1285:HIS:CD2	2.87	0.42
1:J:1268:LEU:CD2	1:K:1250:PHE:CZ	2.76	0.42
1:K:1001:MET:HG2	1:K:1002:ALA:H	1.84	0.42
1:K:1033:LEU:HD12	1:K:1033:LEU:HA	1.85	0.42
1:K:1115:LEU:HD22	1:K:1115:LEU:HA	1.86	0.42
1:C:1001:MET:HE2	1:C:1001:MET:HB2	1.86	0.42
1:D:1143:HIS:HB2	1:F:1143:HIS:CE1	2.54	0.42
1:E:1269:ILE:O	1:E:1273:ARG:N	2.49	0.42
1:F:1094:ASN:O	1:F:1098:ILE:HG13	2.19	0.42
1:I:1280:ASP:OD1	4:I:1429:HOH:O	2.21	0.42
1:J:1211:LEU:HD23	1:J:1212:ASN:N	2.34	0.42
1:J:1217:TYR:CZ	1:L:1219:VAL:HB	2.53	0.42
1:A:1219:VAL:HG13	1:A:1224:VAL:HG21	2.00	0.42
1:A:1224:VAL:O	1:B:1287:LEU:HG	2.19	0.42
1:H:1008:ASN:HA	1:H:1009:PRO:HD3	1.79	0.42
1:H:1122:LEU:O	1:H:1126:VAL:HG23	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1038:GLN:HE21	1:I:1038:GLN:HB3	1.58	0.42
1:J:1144:GLU:OE2	1:L:1146:ARG:NH1	2.52	0.42
1:A:1076:ARG:HD3	1:B:1077:ILE:HD12	2.01	0.42
1:F:1012:ILE:HG23	1:F:1013:GLN:C	2.44	0.42
1:H:1167:GLU:O	1:H:1171:LEU:HB2	2.20	0.42
1:K:1256:TYR:CD1	1:L:1256:TYR:HB2	2.55	0.42
1:B:1023:PRO:HA	4:B:1329:HOH:O	2.18	0.42
1:B:1059:ALA:O	1:B:1063:ASN:ND2	2.53	0.42
1:B:1078:LYS:HG3	1:B:1079:GLN:N	2.34	0.42
1:B:1150:ASN:HD21	1:C:1151:THR:HG23	1.85	0.42
1:C:1224:VAL:O	1:C:1225:VAL:CG2	2.68	0.42
1:F:1177:ALA:O	4:F:1301:HOH:O	2.22	0.42
1:D:1097:ALA:O	1:D:1101:LEU:HG	2.19	0.42
1:J:1033:LEU:O	1:J:1036:ILE:HG12	2.19	0.42
1:K:1274:ARG:HG2	1:K:1278:LEU:HD13	2.01	0.42
1:A:1254:ASP:OD1	1:A:1255:THR:OG1	2.37	0.42
1:C:1263:ALA:O	1:C:1267:ALA:N	2.53	0.42
1:H:1213:VAL:HA	1:I:1207:LEU:HB2	2.02	0.42
1:I:1122:LEU:HD22	1:I:1122:LEU:HA	1.86	0.42
1:J:1079:GLN:HG3	1:K:1081:ARG:HH22	1.85	0.42
1:L:1048:LYS:O	1:L:1051:GLU:HG2	2.19	0.42
1:A:1274:ARG:NH2	1:C:1235:ALA:HB2	2.34	0.42
1:B:1032:LEU:HD23	1:B:1032:LEU:HA	1.86	0.42
1:C:1048:LYS:HE3	1:C:1048:LYS:HB3	1.61	0.42
1:D:1265:ALA:O	1:D:1269:ILE:HG13	2.20	0.42
1:E:1035:VAL:HA	1:E:1038:GLN:HB3	2.01	0.42
1:H:1189:ILE:HD12	1:I:1189:ILE:HD11	2.00	0.42
1:I:1008:ASN:HB3	4:I:1458:HOH:O	2.18	0.42
4:B:1339:HOH:O	1:C:1189:ILE:HG21	2.19	0.42
1:C:1254:ASP:OD1	1:C:1254:ASP:N	2.34	0.42
1:D:1123:ASP:HA	1:D:1126:VAL:HG12	2.02	0.42
1:H:1276:LYS:HD3	1:I:1244:PHE:CD2	2.52	0.42
1:K:1097:ALA:HB3	1:L:1098:ILE:HD13	2.02	0.42
1:L:1041:ASP:O	1:L:1044:ALA:N	2.47	0.42
1:A:1286:GLY:HA2	4:A:1401:HOH:O	2.19	0.42
1:B:1272:ARG:NH1	1:C:1245:ASP:O	2.51	0.42
1:D:1167:GLU:O	1:D:1171:LEU:HB2	2.20	0.42
1:D:1262:GLN:O	1:D:1266:ASN:HB2	2.20	0.42
1:G:1097:ALA:O	1:G:1101:LEU:HG	2.20	0.42
1:G:1185:ALA:O	1:G:1189:ILE:HG13	2.20	0.42
1:H:1171:LEU:HD12	1:H:1171:LEU:HA	1.86	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1241:LYS:HE3	1:K:1241:LYS:HB3	1.61	0.42
1:L:1122:LEU:O	1:L:1126:VAL:HG23	2.20	0.42
1:A:1031:TYR:CE1	1:B:1017:LEU:HD11	2.55	0.41
1:G:1213:VAL:HG13	1:H:1209:SER:O	2.20	0.41
1:G:1287:LEU:HA	1:I:1224:VAL:HG13	2.02	0.41
1:H:1224:VAL:HG22	1:I:1287:LEU:HD13	2.01	0.41
1:I:1027:PHE:O	4:I:1446:HOH:O	2.22	0.41
1:J:1159:VAL:O	1:J:1163:THR:HG23	2.19	0.41
1:K:1066:GLN:OE1	1:L:1066:GLN:NE2	2.52	0.41
1:A:1026:VAL:HG21	1:C:1026:VAL:HG12	2.02	0.41
1:A:1211:LEU:HD21	1:B:1211:LEU:CD1	2.50	0.41
1:E:1172:GLN:HA	1:E:1175:VAL:HB	2.02	0.41
1:E:1223:LYS:O	1:F:1286:GLY:HA3	2.19	0.41
1:H:1142:ASP:OD2	1:H:1143:HIS:ND1	2.43	0.41
1:H:1197:VAL:HG12	1:I:1197:VAL:O	2.19	0.41
1:A:1108:ALA:O	1:A:1112:ILE:HG12	2.21	0.41
1:G:1229:GLN:HB2	1:G:1288:ILE:HG13	2.01	0.41
1:H:1150:ASN:ND2	1:I:1147:ILE:HG23	2.35	0.41
1:H:1156:ALA:HB1	4:H:1429:HOH:O	2.21	0.41
1:K:1222:LYS:HE3	1:L:1228:ARG:HH12	1.84	0.41
1:K:1232:TRP:CH2	1:L:1278:LEU:HD12	2.55	0.41
1:K:1241:LYS:O	1:K:1241:LYS:HG2	2.20	0.41
1:C:1007:ASN:O	1:C:1009:PRO:HD3	2.20	0.41
1:D:1080:LEU:HD12	1:D:1080:LEU:HA	1.86	0.41
1:D:1273:ARG:NH2	1:E:1248:LEU:HG	2.35	0.41
1:E:1094:ASN:ND2	1:F:1095:THR:OG1	2.43	0.41
1:E:1111:GLU:O	1:E:1115:LEU:HB2	2.20	0.41
1:J:1232:TRP:HB2	1:J:1289:ASP:C	2.45	0.41
1:K:1244:PHE:O	4:K:1450:HOH:O	2.21	0.41
1:A:1206:SER:HA	1:C:1212:ASN:HB3	2.02	0.41
1:F:1148:THR:O	1:F:1152:LYS:HD3	2.21	0.41
1:F:1266:ASN:ND2	4:F:1312:HOH:O	1.92	0.41
1:G:1062:LYS:HB3	1:H:1063:ASN:ND2	2.36	0.41
1:G:1108:ALA:O	1:G:1112:ILE:HG13	2.20	0.41
1:G:1209:SER:O	1:I:1213:VAL:HG13	2.20	0.41
1:H:1097:ALA:HB1	1:I:1098:ILE:HG21	2.03	0.41
1:H:1276:LYS:HD2	1:H:1276:LYS:HA	1.78	0.41
1:K:1125:ARG:HH21	1:L:1126:VAL:HG12	1.86	0.41
1:L:1217:TYR:CD1	1:L:1218:SER:N	2.87	0.41
1:A:1112:ILE:O	1:A:1116:GLN:N	2.53	0.41
1:A:1195:ASP:HB3	1:B:1196:TYR:CE2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1272:ARG:CG	1:B:1271:GLU:HG3	2.49	0.41
1:B:1014:ALA:CB	1:L:1107:THR:HG23	2.51	0.41
1:D:1091:ILE:HD11	1:E:1091:ILE:HG12	2.03	0.41
1:G:1001:MET:HG2	1:G:1064:ASP:OD2	2.20	0.41
1:G:1248:LEU:HD23	1:G:1248:LEU:HA	1.92	0.41
1:H:1017:LEU:CD2	1:H:1036:ILE:HD12	2.51	0.41
1:J:1213:VAL:HG22	1:K:1207:LEU:HB2	2.02	0.41
1:B:1150:ASN:O	1:B:1154:ILE:HG12	2.21	0.41
1:D:1219:VAL:HG21	1:E:1215:THR:O	2.21	0.41
1:G:1027:PHE:HD1	1:H:1023:PRO:HG3	1.85	0.41
1:H:1281:ALA:O	4:H:1419:HOH:O	2.22	0.41
1:K:1274:ARG:O	1:K:1277:ALA:N	2.53	0.41
1:L:1016:ARG:HH12	1:L:1040:THR:HG22	1.85	0.41
1:A:1036:ILE:HG13	1:A:1037:ALA:N	2.36	0.41
1:A:1199:LYS:CE	1:C:1197:VAL:HG12	2.51	0.41
1:G:1217:TYR:CZ	1:I:1217:TYR:HB3	2.55	0.41
1:H:1026:VAL:HG21	1:I:1026:VAL:HG11	2.02	0.41
1:H:1031:TYR:O	1:H:1035:VAL:HG23	2.21	0.41
1:J:1127:THR:O	1:J:1131:ASN:ND2	2.54	0.41
1:J:1232:TRP:HZ2	1:K:1281:ALA:HB2	1.85	0.41
1:J:1244:PHE:HZ	1:J:1271:GLU:OE1	2.03	0.41
1:K:1132:ASN:O	1:K:1136:LEU:HB2	2.21	0.41
1:B:1188:ASN:HB2	4:B:1339:HOH:O	2.21	0.41
1:B:1213:VAL:HG11	1:C:1211:LEU:HB2	2.03	0.41
1:B:1219:VAL:HG21	1:C:1215:THR:O	2.20	0.41
1:C:1244:PHE:CD1	1:C:1274:ARG:HG3	2.55	0.41
1:D:1147:ILE:O	1:D:1151:THR:HG22	2.20	0.41
1:D:1178:LEU:HD11	1:E:1179:ASP:HA	2.03	0.41
1:D:1237:GLY:CA	4:D:1431:HOH:O	2.68	0.41
1:E:1080:LEU:HD11	1:F:1081:ARG:HA	2.03	0.41
1:E:1103:VAL:O	1:E:1107:THR:OG1	2.23	0.41
1:F:1003:ASP:HB3	1:F:1006:LEU:HD13	2.03	0.41
1:G:1007:ASN:O	1:G:1009:PRO:HD3	2.20	0.41
1:G:1017:LEU:HD13	1:I:1034:TYR:CD2	2.55	0.41
1:H:1066:GLN:NE2	1:I:1063:ASN:O	2.54	0.41
1:H:1211:LEU:O	1:H:1217:TYR:OH	2.39	0.41
1:J:1098:ILE:HG13	1:J:1099:THR:N	2.35	0.41
1:K:1130:GLU:HA	1:K:1133:ILE:HB	2.03	0.41
1:K:1132:ASN:N	1:K:1132:ASN:HD22	2.19	0.41
1:K:1144:GLU:HA	1:K:1147:ILE:HG22	2.03	0.41
1:K:1265:ALA:HB2	1:L:1264:ILE:HD13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1001:MET:HB2	1:L:1001:MET:HE3	1.78	0.41
1:L:1232:TRP:HB3	1:L:1283:ARG:NH2	2.35	0.41
1:E:1022:LEU:HA	1:E:1022:LEU:HD12	1.89	0.41
1:F:1076:ARG:O	1:F:1080:LEU:HB2	2.21	0.41
1:G:1116:GLN:O	1:G:1116:GLN:HG3	2.22	0.41
1:G:1151:THR:OG1	1:I:1150:ASN:ND2	2.46	0.41
1:H:1182:VAL:HG22	1:I:1182:VAL:HG11	2.02	0.41
1:J:1048:LYS:HZ1	1:K:1009:PRO:CA	2.29	0.41
1:J:1286:GLY:HA2	4:J:1412:HOH:O	2.21	0.41
1:K:1109:GLU:HB3	4:K:1425:HOH:O	2.21	0.41
1:A:1128:THR:OG1	4:A:1438:HOH:O	2.21	0.40
1:A:1211:LEU:HD21	1:B:1211:LEU:HD13	2.03	0.40
1:B:1115:LEU:HD11	1:C:1116:GLN:HA	2.03	0.40
1:C:1236:THR:OG1	1:C:1237:GLY:N	2.54	0.40
1:D:1223:LYS:NZ	1:E:1285:HIS:O	2.54	0.40
1:E:1122:LEU:HG	1:E:1126:VAL:HG23	2.03	0.40
1:J:1192:LEU:HD22	1:K:1192:LEU:HD21	2.03	0.40
1:K:1197:VAL:HG13	4:L:1461:HOH:O	2.21	0.40
1:L:1101:LEU:HD23	1:L:1101:LEU:HA	1.95	0.40
1:L:1279:GLU:HG2	1:L:1283:ARG:HH12	1.87	0.40
1:A:1017:LEU:HD12	1:A:1017:LEU:HA	1.85	0.40
1:A:1080:LEU:HD23	1:C:1080:LEU:HD23	2.03	0.40
1:B:1258:GLN:HG2	1:B:1259:SER:N	2.36	0.40
1:C:1101:LEU:O	1:C:1104:ARG:N	2.54	0.40
1:C:1250:PHE:H	1:C:1250:PHE:HD2	1.67	0.40
1:D:1006:LEU:HD21	1:F:1055:GLY:HA3	2.03	0.40
1:E:1029:LYS:O	1:E:1032:LEU:HB3	2.21	0.40
1:I:1012:ILE:CD1	1:I:1043:GLY:HA2	2.51	0.40
1:J:1111:GLU:O	1:J:1115:LEU:HB2	2.21	0.40
1:L:1061:VAL:O	1:L:1065:GLU:HG3	2.20	0.40
1:L:1224:VAL:HG23	1:L:1225:VAL:N	2.36	0.40
1:D:1084:VAL:HG13	1:F:1087:HIS:HE1	1.86	0.40
1:D:1260:GLU:OE1	4:D:1461:HOH:O	2.22	0.40
1:E:1074:GLU:O	1:E:1078:LYS:HG3	2.21	0.40
1:F:1240:ASN:O	1:F:1274:ARG:HD3	2.21	0.40
1:J:1212:ASN:OD1	1:J:1213:VAL:N	2.54	0.40
1:B:1171:LEU:HD11	1:C:1172:GLN:HA	2.02	0.40
1:D:1250:PHE:HZ	1:D:1267:ALA:HB3	1.87	0.40
1:E:1076:ARG:HE	1:F:1077:ILE:HG21	1.86	0.40
1:G:1183:THR:OG1	1:I:1181:ARG:NH2	2.53	0.40
1:I:1018:ASP:C	1:I:1020:SER:H	2.30	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1046:ALA:O	1:K:1050:ASN:ND2	2.55	0.40
1:A:1137:GLN:HG2	1:C:1136:LEU:HD11	2.03	0.40
1:B:1075:ALA:HA	1:B:1078:LYS:HG2	2.02	0.40
1:D:1207:LEU:HD12	1:F:1213:VAL:HG22	2.04	0.40
1:D:1235:ALA:HB2	1:E:1244:PHE:HB3	2.02	0.40
4:E:1452:HOH:O	1:F:1056:ALA:HB3	2.22	0.40
1:F:1151:THR:HA	1:F:1154:ILE:HB	2.03	0.40
1:H:1213:VAL:HG22	1:I:1209:SER:O	2.21	0.40

All (7) 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:J:1244:PHE:O	4:F:1345:HOH:O[1_455]	1.98	0.22
1:J:1244:PHE:N	4:F:1345:HOH:O[1_455]	2.04	0.16
4:B:1346:HOH:O	4:D:1419:HOH:O[1_446]	2.06	0.14
1:F:1234:ALA:O	4:L:1408:HOH:O[1_655]	2.16	0.04
4:B:1338:HOH:O	4:D:1465:HOH:O[1_446]	2.18	0.02
1:A:1146:ARG:NH2	1:I:1025:ASN:OD1[1_474]	2.19	0.01
1:E:1024:ARG:NE	1:K:1142:ASP:OD1[1_636]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	287/300 (96%)	276 (96%)	11 (4%)	0	100	100
1	B	287/300 (96%)	279 (97%)	8 (3%)	0	100	100
1	C	287/300 (96%)	276 (96%)	11 (4%)	0	100	100
1	D	287/300 (96%)	281 (98%)	6 (2%)	0	100	100
1	E	287/300 (96%)	277 (96%)	10 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	287/300 (96%)	274 (96%)	13 (4%)	0	100	100
1	G	287/300 (96%)	281 (98%)	6 (2%)	0	100	100
1	H	287/300 (96%)	278 (97%)	9 (3%)	0	100	100
1	I	287/300 (96%)	277 (96%)	10 (4%)	0	100	100
1	J	287/300 (96%)	275 (96%)	12 (4%)	0	100	100
1	K	287/300 (96%)	273 (95%)	14 (5%)	0	100	100
1	L	287/300 (96%)	270 (94%)	16 (6%)	1 (0%)	36	60
All	All	3444/3600 (96%)	3317 (96%)	126 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	1019	ALA

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	229/238 (96%)	184 (80%)	45 (20%)	1	4
1	B	229/238 (96%)	183 (80%)	46 (20%)	1	4
1	C	229/238 (96%)	176 (77%)	53 (23%)	1	2
1	D	229/238 (96%)	199 (87%)	30 (13%)	4	10
1	E	229/238 (96%)	190 (83%)	39 (17%)	2	6
1	F	229/238 (96%)	194 (85%)	35 (15%)	3	7
1	G	229/238 (96%)	187 (82%)	42 (18%)	2	5
1	H	229/238 (96%)	178 (78%)	51 (22%)	1	3
1	I	229/238 (96%)	180 (79%)	49 (21%)	1	3
1	J	229/238 (96%)	186 (81%)	43 (19%)	1	4
1	K	229/238 (96%)	182 (80%)	47 (20%)	1	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	229/238 (96%)	180 (79%)	49 (21%)	1	3
All	All	2748/2856 (96%)	2219 (81%)	529 (19%)	1	4

All (529) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1005	SER
1	A	1011	VAL
1	A	1015	THR
1	A	1016	ARG
1	A	1017	LEU
1	A	1018	ASP
1	A	1020	SER
1	A	1021	ILE
1	A	1036	ILE
1	A	1068	VAL
1	A	1077	ILE
1	A	1078	LYS
1	A	1080	LEU
1	A	1082	ILE
1	A	1084	VAL
1	A	1085	ASP
1	A	1092	THR
1	A	1098	ILE
1	A	1099	THR
1	A	1103	VAL
1	A	1111	GLU
1	A	1126	VAL
1	A	1127	THR
1	A	1136	LEU
1	A	1148	THR
1	A	1157	LEU
1	A	1175	VAL
1	A	1179	ASP
1	A	1189	ILE
1	A	1195	ASP
1	A	1196	TYR
1	A	1199	LYS
1	A	1200	THR
1	A	1203	THR
1	A	1213	VAL
1	A	1216	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1219	VAL
1	A	1225	VAL
1	A	1249	THR
1	A	1255	THR
1	A	1257	THR
1	A	1276	LYS
1	A	1278	LEU
1	A	1280	ASP
1	A	1282	LEU
1	B	1010	VAL
1	B	1011	VAL
1	B	1016	ARG
1	B	1017	LEU
1	B	1029	LYS
1	B	1032	LEU
1	B	1035	VAL
1	B	1054	GLN
1	B	1077	ILE
1	B	1078	LYS
1	B	1082	ILE
1	B	1084	VAL
1	B	1085	ASP
1	B	1088	GLU
1	B	1092	THR
1	B	1096	LYS
1	B	1098	ILE
1	B	1107	THR
1	B	1111	GLU
1	B	1117	THR
1	B	1119	VAL
1	B	1126	VAL
1	B	1127	THR
1	B	1140	VAL
1	B	1151	THR
1	B	1154	ILE
1	B	1155	THR
1	B	1157	LEU
1	B	1175	VAL
1	B	1198	SER
1	B	1207	LEU
1	B	1211	LEU
1	B	1213	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1214	THR
1	B	1215	THR
1	B	1219	VAL
1	B	1222	LYS
1	B	1228	ARG
1	B	1236	THR
1	B	1238	THR
1	B	1249	THR
1	B	1250	PHE
1	B	1257	THR
1	B	1259	SER
1	B	1260	GLU
1	B	1278	LEU
1	C	1001	MET
1	C	1011	VAL
1	C	1015	THR
1	C	1020	SER
1	C	1022	LEU
1	C	1025	ASN
1	C	1026	VAL
1	C	1032	LEU
1	C	1035	VAL
1	C	1048	LYS
1	C	1051	GLU
1	C	1054	GLN
1	C	1065	GLU
1	C	1068	VAL
1	C	1069	GLU
1	C	1080	LEU
1	C	1081	ARG
1	C	1083	ASP
1	C	1095	THR
1	C	1106	THR
1	C	1114	SER
1	C	1115	LEU
1	C	1133	ILE
1	C	1140	VAL
1	C	1141	ASP
1	C	1148	THR
1	C	1154	ILE
1	C	1157	LEU
1	C	1162	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1165	GLU
1	C	1168	ILE
1	C	1171	LEU
1	C	1174	ASN
1	C	1175	VAL
1	C	1176	SER
1	C	1182	VAL
1	C	1192	LEU
1	C	1196	TYR
1	C	1197	VAL
1	C	1203	THR
1	C	1207	LEU
1	C	1214	THR
1	C	1219	VAL
1	C	1236	THR
1	C	1243	VAL
1	C	1248	LEU
1	C	1249	THR
1	C	1250	PHE
1	C	1252	VAL
1	C	1254	ASP
1	C	1255	THR
1	C	1275	THR
1	C	1276	LYS
1	D	1005	SER
1	D	1016	ARG
1	D	1017	LEU
1	D	1024	ARG
1	D	1029	LYS
1	D	1042	VAL
1	D	1048	LYS
1	D	1051	GLU
1	D	1054	GLN
1	D	1070	LEU
1	D	1084	VAL
1	D	1143	HIS
1	D	1145	SER
1	D	1155	THR
1	D	1158	ASN
1	D	1159	VAL
1	D	1161	VAL
1	D	1171	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1178	LEU
1	D	1183	THR
1	D	1196	TYR
1	D	1198	SER
1	D	1200	THR
1	D	1219	VAL
1	D	1224	VAL
1	D	1248	LEU
1	D	1249	THR
1	D	1275	THR
1	D	1288	ILE
1	D	1289	ASP
1	E	1007	ASN
1	E	1015	THR
1	E	1022	LEU
1	E	1024	ARG
1	E	1040	THR
1	E	1067	ASP
1	E	1080	LEU
1	E	1086	ASP
1	E	1088	GLU
1	E	1092	THR
1	E	1119	VAL
1	E	1127	THR
1	E	1130	GLU
1	E	1132	ASN
1	E	1140	VAL
1	E	1155	THR
1	E	1159	VAL
1	E	1163	THR
1	E	1174	ASN
1	E	1175	VAL
1	E	1178	LEU
1	E	1181	ARG
1	E	1183	THR
1	E	1186	GLU
1	E	1192	LEU
1	E	1203	THR
1	E	1211	LEU
1	E	1216	SER
1	E	1219	VAL
1	E	1222	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	1236	THR
1	E	1240	ASN
1	E	1248	LEU
1	E	1249	THR
1	E	1254	ASP
1	E	1257	THR
1	E	1258	GLN
1	E	1276	LYS
1	E	1289	ASP
1	F	1005	SER
1	F	1010	VAL
1	F	1012	ILE
1	F	1018	ASP
1	F	1021	ILE
1	F	1024	ARG
1	F	1025	ASN
1	F	1026	VAL
1	F	1028	SER
1	F	1069	GLU
1	F	1074	GLU
1	F	1080	LEU
1	F	1092	THR
1	F	1119	VAL
1	F	1122	LEU
1	F	1132	ASN
1	F	1145	SER
1	F	1148	THR
1	F	1154	ILE
1	F	1170	SER
1	F	1178	LEU
1	F	1196	TYR
1	F	1200	THR
1	F	1214	THR
1	F	1236	THR
1	F	1243	VAL
1	F	1248	LEU
1	F	1250	PHE
1	F	1252	VAL
1	F	1254	ASP
1	F	1255	THR
1	F	1257	THR
1	F	1274	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	1276	LYS
1	F	1280	ASP
1	G	1012	ILE
1	G	1015	THR
1	G	1017	LEU
1	G	1021	ILE
1	G	1022	LEU
1	G	1025	ASN
1	G	1030	SER
1	G	1036	ILE
1	G	1048	LYS
1	G	1058	ASP
1	G	1061	VAL
1	G	1068	VAL
1	G	1080	LEU
1	G	1095	THR
1	G	1107	THR
1	G	1127	THR
1	G	1128	THR
1	G	1133	ILE
1	G	1144	GLU
1	G	1148	THR
1	G	1157	LEU
1	G	1181	ARG
1	G	1183	THR
1	G	1192	LEU
1	G	1196	TYR
1	G	1197	VAL
1	G	1214	THR
1	G	1219	VAL
1	G	1243	VAL
1	G	1248	LEU
1	G	1250	PHE
1	G	1252	VAL
1	G	1255	THR
1	G	1257	THR
1	G	1260	GLU
1	G	1261	ILE
1	G	1269	ILE
1	G	1274	ARG
1	G	1276	LYS
1	G	1278	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	1280	ASP
1	G	1288	ILE
1	H	1006	LEU
1	H	1010	VAL
1	H	1011	VAL
1	H	1015	THR
1	H	1016	ARG
1	H	1017	LEU
1	H	1018	ASP
1	H	1021	ILE
1	H	1022	LEU
1	H	1025	ASN
1	H	1048	LYS
1	H	1064	ASP
1	H	1068	VAL
1	H	1072	ASP
1	H	1074	GLU
1	H	1082	ILE
1	H	1084	VAL
1	H	1095	THR
1	H	1096	LYS
1	H	1101	LEU
1	H	1103	VAL
1	H	1112	ILE
1	H	1128	THR
1	H	1157	LEU
1	H	1163	THR
1	H	1167	GLU
1	H	1188	ASN
1	H	1189	ILE
1	H	1196	TYR
1	H	1197	VAL
1	H	1198	SER
1	H	1204	SER
1	H	1209	SER
1	H	1213	VAL
1	H	1214	THR
1	H	1215	THR
1	H	1219	VAL
1	H	1224	VAL
1	H	1236	THR
1	H	1238	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	1243	VAL
1	H	1252	VAL
1	H	1254	ASP
1	H	1255	THR
1	H	1257	THR
1	H	1264	ILE
1	H	1273	ARG
1	H	1275	THR
1	H	1283	ARG
1	H	1288	ILE
1	H	1289	ASP
1	I	1001	MET
1	I	1010	VAL
1	I	1011	VAL
1	I	1012	ILE
1	I	1013	GLN
1	I	1016	ARG
1	I	1020	SER
1	I	1026	VAL
1	I	1028	SER
1	I	1030	SER
1	I	1032	LEU
1	I	1035	VAL
1	I	1038	GLN
1	I	1045	ILE
1	I	1051	GLU
1	I	1067	ASP
1	I	1079	GLN
1	I	1081	ARG
1	I	1088	GLU
1	I	1089	SER
1	I	1096	LYS
1	I	1099	THR
1	I	1109	GLU
1	I	1115	LEU
1	I	1117	THR
1	I	1119	VAL
1	I	1122	LEU
1	I	1123	ASP
1	I	1127	THR
1	I	1139	ASP
1	I	1140	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	1147	ILE
1	I	1173	THR
1	I	1184	THR
1	I	1192	LEU
1	I	1197	VAL
1	I	1203	THR
1	I	1219	VAL
1	I	1228	ARG
1	I	1229	GLN
1	I	1230	THR
1	I	1233	THR
1	I	1238	THR
1	I	1249	THR
1	I	1257	THR
1	I	1270	THR
1	I	1276	LYS
1	I	1287	LEU
1	I	1289	ASP
1	J	1006	LEU
1	J	1007	ASN
1	J	1010	VAL
1	J	1012	ILE
1	J	1013	GLN
1	J	1015	THR
1	J	1020	SER
1	J	1022	LEU
1	J	1028	SER
1	J	1035	VAL
1	J	1054	GLN
1	J	1068	VAL
1	J	1070	LEU
1	J	1084	VAL
1	J	1088	GLU
1	J	1092	THR
1	J	1095	THR
1	J	1099	THR
1	J	1112	ILE
1	J	1123	ASP
1	J	1141	ASP
1	J	1148	THR
1	J	1157	LEU
1	J	1159	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	1161	VAL
1	J	1175	VAL
1	J	1182	VAL
1	J	1184	THR
1	J	1186	GLU
1	J	1192	LEU
1	J	1197	VAL
1	J	1213	VAL
1	J	1225	VAL
1	J	1241	LYS
1	J	1250	PHE
1	J	1254	ASP
1	J	1255	THR
1	J	1257	THR
1	J	1259	SER
1	J	1261	ILE
1	J	1270	THR
1	J	1278	LEU
1	J	1282	LEU
1	K	1011	VAL
1	K	1021	ILE
1	K	1022	LEU
1	K	1024	ARG
1	K	1025	ASN
1	K	1026	VAL
1	K	1032	LEU
1	K	1033	LEU
1	K	1038	GLN
1	K	1062	LYS
1	K	1077	ILE
1	K	1082	ILE
1	K	1103	VAL
1	K	1105	VAL
1	K	1106	THR
1	K	1112	ILE
1	K	1114	SER
1	K	1115	LEU
1	K	1117	THR
1	K	1133	ILE
1	K	1136	LEU
1	K	1145	SER
1	K	1147	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	1155	THR
1	K	1159	VAL
1	K	1162	THR
1	K	1165	GLU
1	K	1192	LEU
1	K	1195	ASP
1	K	1196	TYR
1	K	1197	VAL
1	K	1200	THR
1	K	1203	THR
1	K	1212	ASN
1	K	1214	THR
1	K	1215	THR
1	K	1219	VAL
1	K	1230	THR
1	K	1243	VAL
1	K	1245	ASP
1	K	1252	VAL
1	K	1256	TYR
1	K	1258	GLN
1	K	1260	GLU
1	K	1274	ARG
1	K	1278	LEU
1	K	1282	LEU
1	L	1001	MET
1	L	1010	VAL
1	L	1017	LEU
1	L	1022	LEU
1	L	1026	VAL
1	L	1028	SER
1	L	1035	VAL
1	L	1036	ILE
1	L	1045	ILE
1	L	1048	LYS
1	L	1067	ASP
1	L	1070	LEU
1	L	1078	LYS
1	L	1079	GLN
1	L	1080	LEU
1	L	1082	ILE
1	L	1096	LYS
1	L	1109	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	1117	THR
1	L	1119	VAL
1	L	1122	LEU
1	L	1127	THR
1	L	1142	ASP
1	L	1144	GLU
1	L	1145	SER
1	L	1158	ASN
1	L	1162	THR
1	L	1168	ILE
1	L	1176	SER
1	L	1179	ASP
1	L	1195	ASP
1	L	1197	VAL
1	L	1198	SER
1	L	1204	SER
1	L	1213	VAL
1	L	1214	THR
1	L	1216	SER
1	L	1228	ARG
1	L	1229	GLN
1	L	1238	THR
1	L	1240	ASN
1	L	1243	VAL
1	L	1249	THR
1	L	1250	PHE
1	L	1253	SER
1	L	1260	GLU
1	L	1271	GLU
1	L	1278	LEU
1	L	1289	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1073	HIS
1	A	1137	GLN
1	B	1038	GLN
1	B	1054	GLN
1	B	1079	GLN
1	C	1007	ASN
1	C	1038	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1054	GLN
1	C	1063	ASN
1	C	1116	GLN
1	D	1060	GLN
1	E	1174	ASN
1	F	1187	ASN
1	F	1229	GLN
1	G	1025	ASN
1	G	1054	GLN
1	G	1087	HIS
1	G	1193	GLN
1	G	1205	GLN
1	G	1229	GLN
1	H	1079	GLN
1	H	1087	HIS
1	H	1137	GLN
1	H	1188	ASN
1	H	1205	GLN
1	I	1054	GLN
1	J	1258	GLN
1	J	1262	GLN
1	K	1008	ASN
1	K	1066	GLN
1	K	1116	GLN
1	K	1132	ASN
1	K	1212	ASN
1	K	1285	HIS
1	L	1025	ASN
1	L	1063	ASN
1	L	1066	GLN
1	L	1172	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	289/300 (96%)	-0.96	0 100 100	29, 61, 89, 114	0
1	B	289/300 (96%)	-0.90	0 100 100	29, 59, 80, 96	0
1	C	289/300 (96%)	-0.82	0 100 100	26, 64, 92, 122	0
1	D	289/300 (96%)	-0.75	1 (0%) 90 89	26, 73, 101, 118	0
1	E	289/300 (96%)	-0.82	0 100 100	28, 64, 93, 115	0
1	F	289/300 (96%)	-0.85	0 100 100	28, 60, 98, 124	0
1	G	289/300 (96%)	-0.85	0 100 100	33, 67, 100, 141	0
1	H	289/300 (96%)	-0.77	0 100 100	32, 68, 99, 114	0
1	I	289/300 (96%)	-0.84	0 100 100	33, 65, 97, 125	0
1	J	289/300 (96%)	-0.83	1 (0%) 90 89	36, 67, 97, 116	0
1	K	289/300 (96%)	-0.85	0 100 100	37, 66, 102, 123	0
1	L	289/300 (96%)	-0.82	0 100 100	39, 65, 99, 119	0
All	All	3468/3600 (96%)	-0.84	2 (0%) 92 91	26, 65, 97, 141	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1149	ALA	3.0
1	J	1135	ALA	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	I	1301	1/1	0.97	0.12	171,171,171,171	0
3	CL	A	1303	1/1	0.98	0.04	60,60,60,60	0
3	CL	D	1301	1/1	0.98	0.03	58,58,58,58	0
3	CL	H	1301	1/1	0.98	0.07	38,38,38,38	0
3	CL	A	1302	1/1	0.98	0.05	50,50,50,50	0
2	CA	G	1301	1/1	0.99	0.02	36,36,36,36	0
3	CL	E	1302	1/1	0.99	0.03	61,61,61,61	0
2	CA	A	1301	1/1	0.99	0.03	79,79,79,79	0
2	CA	E	1301	1/1	0.99	0.04	54,54,54,54	0
3	CL	K	1301	1/1	0.99	0.04	52,52,52,52	0
3	CL	L	1301	1/1	0.99	0.05	49,49,49,49	0
2	CA	J	1301	1/1	1.00	0.06	99,99,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.