



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:17 AM UTC

PDB ID : 2POH / pdb_00002poh
Title : Structure of Phage P22 Tail Needle gp26
Authors : Olia, A.S.; Cingolani, G.
Deposited on : 2007-04-26
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

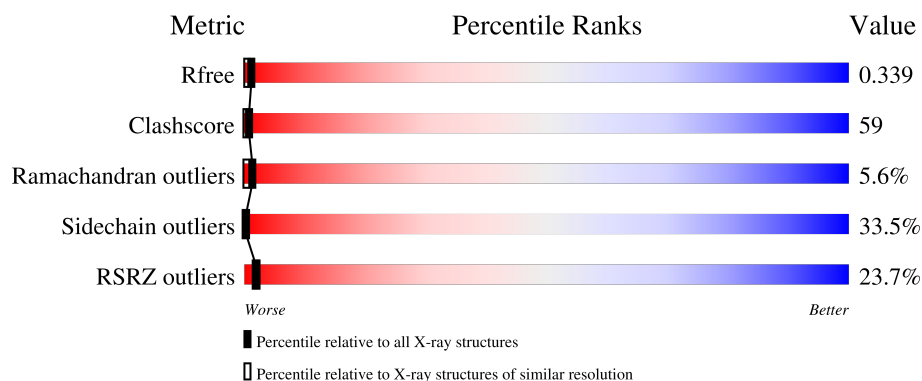
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	233	
1	B	233	
1	C	233	
1	D	233	
1	E	233	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	233	26% 27% 47% 23%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11261 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 Head completion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	Se	0	0	0
			1738	1065	311	360	2			
1	B	233	Total	C	N	O	Se	0	0	0
			1738	1065	311	360	2			
1	C	233	Total	C	N	O	Se	0	0	0
			1738	1065	311	360	2			
1	D	233	Total	C	N	O	Se	0	0	0
			1715	1045	310	358	2			
1	E	233	Total	C	N	O	Se	0	0	0
			1712	1048	308	354	2			
1	F	233	Total	C	N	O	Se	0	0	0
			1734	1062	311	359	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q8LTG5
A	222	MSE	LEU	engineered mutation	UNP Q8LTG5
B	1	MSE	MET	modified residue	UNP Q8LTG5
B	222	MSE	LEU	engineered mutation	UNP Q8LTG5
C	1	MSE	MET	modified residue	UNP Q8LTG5
C	222	MSE	LEU	engineered mutation	UNP Q8LTG5
D	1	MSE	MET	modified residue	UNP Q8LTG5
D	222	MSE	LEU	engineered mutation	UNP Q8LTG5
E	1	MSE	MET	modified residue	UNP Q8LTG5
E	222	MSE	LEU	engineered mutation	UNP Q8LTG5
F	1	MSE	MET	modified residue	UNP Q8LTG5
F	222	MSE	LEU	engineered mutation	UNP Q8LTG5

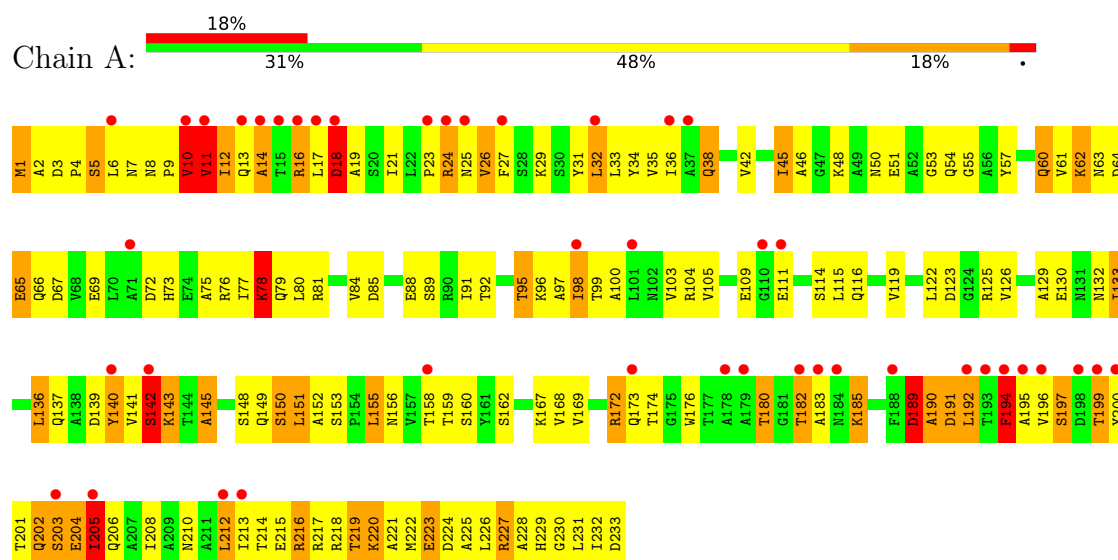
- Molecule 2 is water.

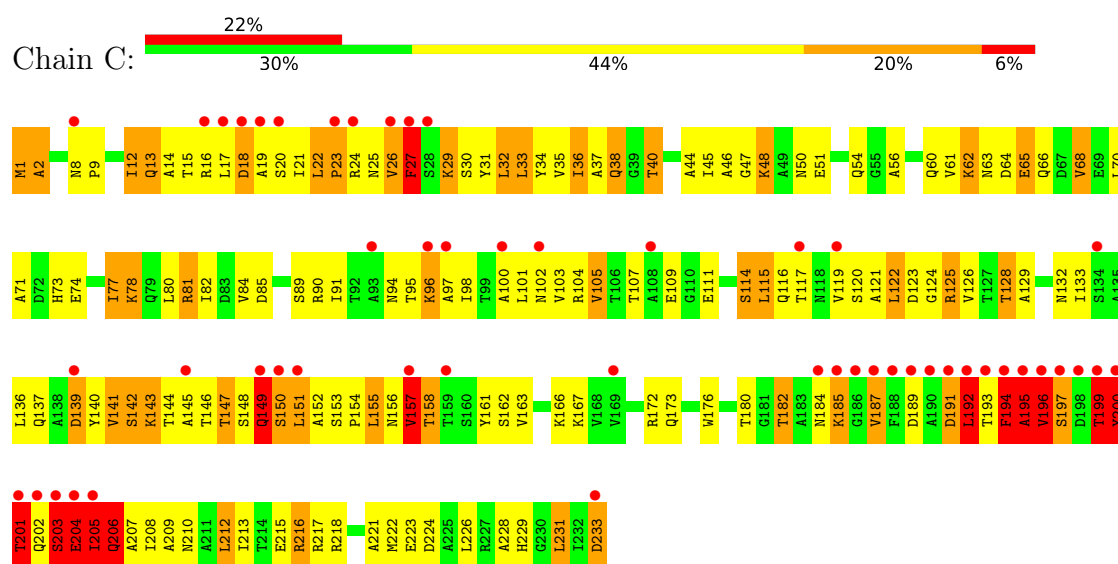
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	155	Total 155	O 155	0	0
2	B	167	Total 167	O 167	0	0
2	C	151	Total 151	O 151	0	0
2	D	124	Total 124	O 124	0	0
2	E	138	Total 138	O 138	0	0
2	F	151	Total 151	O 151	0	0

3 Residue-property plots [i](#)

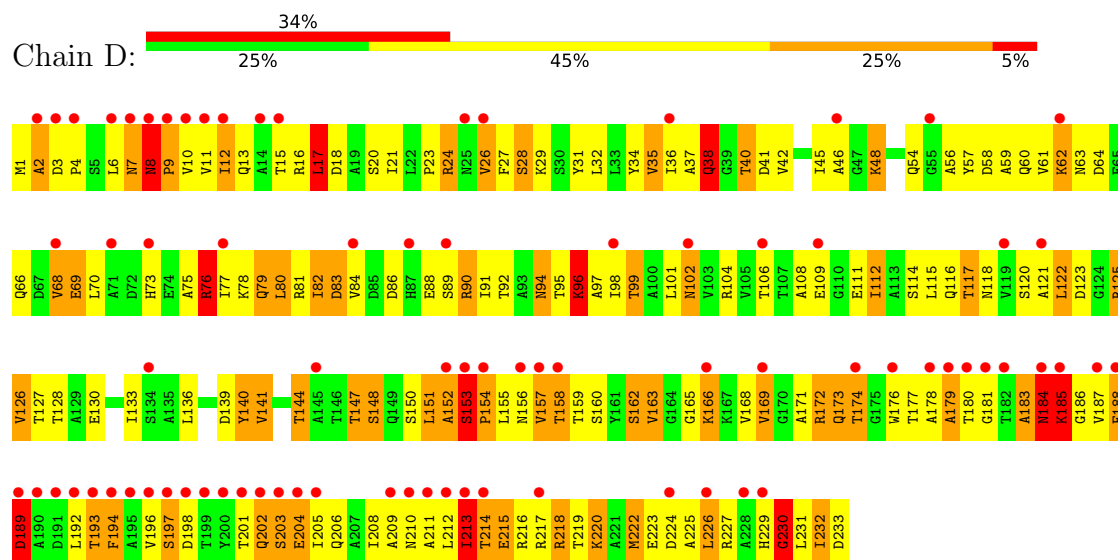
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Head completion protein

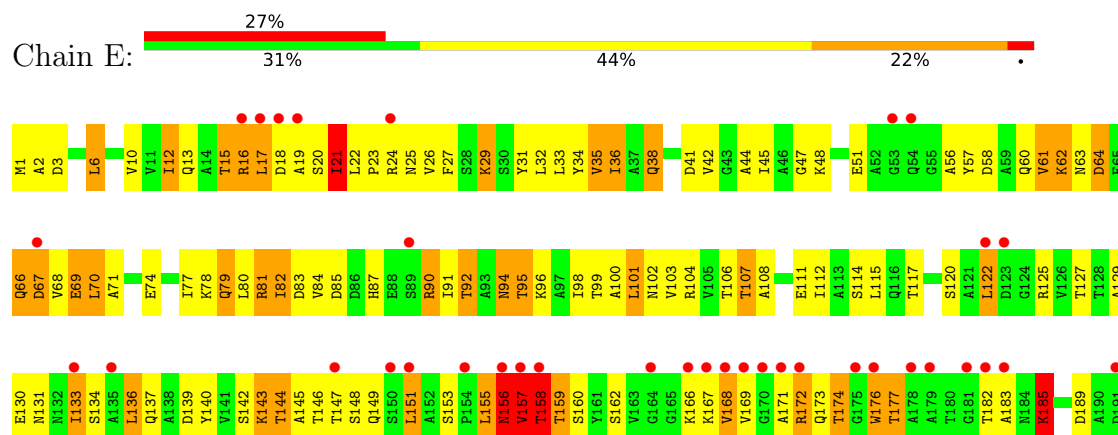




• Molecule 1: Head completion protein

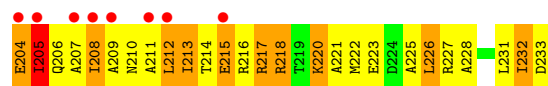
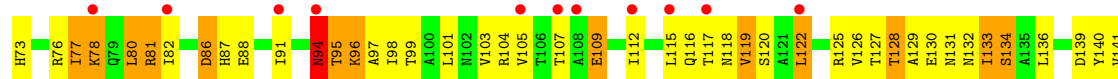
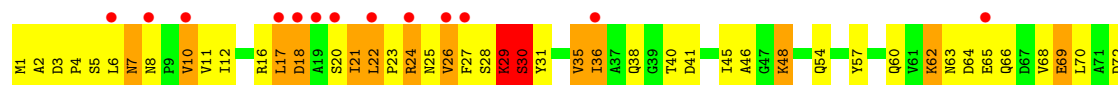


• Molecule 1: Head completion protein





• Molecule 1: Head completion protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	40.40Å 114.03Å 171.92Å 90.00° 90.74° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.10 200.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.3 ((Not available)-2.10) 99.1 (200.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.00Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.167 , 0.232 0.282 , 0.339	Depositor DCC
R_{free} test set	4967 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11261	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.34% 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	0.48	0/1754	1.54	20/2384 (0.8%)
1	B	0.46	0/1754	1.52	14/2384 (0.6%)
1	C	0.60	1/1754 (0.1%)	1.65	35/2384 (1.5%)
1	D	0.44	0/1730	1.43	18/2347 (0.8%)
1	E	0.47	0/1728	1.48	14/2347 (0.6%)
1	F	0.46	0/1750	1.47	20/2377 (0.8%)
All	All	0.49	1/10470 (0.0%)	1.52	121/14223 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	3
1	D	0	7
1	E	0	3
1	F	0	2
All	All	0	15

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	149	GLN	CD-NE2	13.36	1.61	1.33

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ARG	NE-CZ-NH2	13.62	131.46	119.20
1	A	172	ARG	CD-NE-CZ	13.41	143.18	124.40
1	A	172	ARG	NE-CZ-NH1	-11.92	109.58	121.50
1	E	229	HIS	O-C-N	-10.85	108.28	122.39
1	C	149	GLN	CB-CG-CD	-10.62	94.54	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	201	THR	CB-CA-C	-10.61	89.31	110.42
1	C	191	ASP	CA-CB-CG	9.61	122.21	112.60
1	E	156	ASN	N-CA-C	9.11	120.65	108.07
1	A	197	SER	CA-C-N	9.10	132.82	120.54
1	A	197	SER	C-N-CA	9.10	132.82	120.54
1	C	200	TYR	CA-CB-CG	8.58	129.35	113.90
1	D	194	PHE	CA-CB-CG	8.54	122.34	113.80
1	C	202	GLN	CA-C-O	8.49	129.54	120.46
1	E	94	ASN	CA-C-N	8.25	131.17	120.44
1	E	94	ASN	C-N-CA	8.25	131.17	120.44
1	D	140	TYR	CA-C-N	-8.08	112.75	122.93
1	D	140	TYR	C-N-CA	-8.08	112.75	122.93
1	A	194	PHE	CA-CB-CG	-8.02	105.78	113.80
1	E	67	ASP	CA-CB-CG	8.01	120.61	112.60
1	E	208	ILE	CA-C-N	7.91	131.39	120.63
1	E	208	ILE	C-N-CA	7.91	131.39	120.63
1	C	201	THR	CA-C-N	7.80	134.19	123.11
1	C	201	THR	C-N-CA	7.80	134.19	123.11
1	C	199	THR	CA-C-O	-7.70	109.50	120.51
1	C	149	GLN	N-CA-CB	-7.57	98.49	110.98
1	E	228	ALA	CA-C-N	7.49	132.58	120.60
1	E	228	ALA	C-N-CA	7.49	132.58	120.60
1	D	230	GLY	CA-C-N	7.44	130.58	120.38
1	D	230	GLY	C-N-CA	7.44	130.58	120.38
1	B	190	ALA	CA-C-N	7.43	132.69	122.07
1	B	190	ALA	C-N-CA	7.43	132.69	122.07
1	B	156	ASN	OD1-CG-ND2	-7.14	115.46	122.60
1	C	206	GLN	CA-C-N	6.88	131.14	120.82
1	C	206	GLN	C-N-CA	6.88	131.14	120.82
1	E	21	ILE	N-CA-C	-6.65	107.39	113.71
1	E	185	LYS	CA-C-N	6.54	129.50	122.69
1	E	185	LYS	C-N-CA	6.54	129.50	122.69
1	C	149	GLN	CA-C-N	6.50	133.96	121.54
1	C	149	GLN	C-N-CA	6.50	133.96	121.54
1	D	90	ARG	CD-NE-CZ	6.45	133.43	124.40
1	B	65	GLU	O-C-N	6.41	128.70	122.03
1	C	195	ALA	CA-C-N	-6.34	114.77	123.46
1	C	195	ALA	C-N-CA	-6.34	114.77	123.46
1	F	133	ILE	CA-C-N	6.32	131.23	121.19
1	F	133	ILE	C-N-CA	6.32	131.23	121.19
1	C	27	PHE	CA-CB-CG	6.25	120.05	113.80
1	E	3	ASP	CA-CB-CG	6.24	118.84	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18	ASP	N-CA-C	6.20	115.62	108.49
1	F	119	VAL	CA-C-N	6.20	128.83	120.65
1	F	119	VAL	C-N-CA	6.20	128.83	120.65
1	C	205	ILE	CA-C-N	6.18	130.09	120.82
1	C	205	ILE	C-N-CA	6.18	130.09	120.82
1	C	194	PHE	CA-CB-CG	6.17	119.97	113.80
1	F	64	ASP	CA-C-N	6.13	128.49	120.28
1	F	64	ASP	C-N-CA	6.13	128.49	120.28
1	B	153	SER	O-C-N	6.08	126.67	121.20
1	A	189	ASP	CA-CB-CG	6.02	118.62	112.60
1	C	201	THR	CA-C-O	-5.98	111.96	120.51
1	C	139	ASP	CA-C-N	-5.96	112.99	122.29
1	C	139	ASP	C-N-CA	-5.96	112.99	122.29
1	D	213	ILE	CA-C-N	5.92	130.85	121.44
1	D	213	ILE	C-N-CA	5.92	130.85	121.44
1	A	228	ALA	CA-C-N	5.90	128.43	120.65
1	A	228	ALA	C-N-CA	5.90	128.43	120.65
1	E	64	ASP	CA-C-O	5.90	126.67	120.42
1	C	149	GLN	CA-CB-CG	5.89	125.88	114.10
1	B	212	LEU	CA-C-N	5.82	128.10	120.60
1	B	212	LEU	C-N-CA	5.82	128.10	120.60
1	D	94	ASN	CA-C-N	5.79	130.48	120.58
1	D	94	ASN	C-N-CA	5.79	130.48	120.58
1	F	166	LYS	CB-CG-CD	5.79	124.61	111.30
1	F	5	SER	CA-C-N	5.77	129.48	120.82
1	F	5	SER	C-N-CA	5.77	129.48	120.82
1	A	78	LYS	O-C-N	5.75	128.22	122.12
1	D	38	GLN	CA-C-N	5.74	126.31	119.94
1	D	38	GLN	C-N-CA	5.74	126.31	119.94
1	C	54	GLN	CA-C-N	5.72	126.43	120.03
1	C	54	GLN	C-N-CA	5.72	126.43	120.03
1	A	199	THR	CA-C-O	5.67	126.56	120.32
1	F	5	SER	O-C-N	5.66	128.11	122.12
1	D	197	SER	CB-CA-C	-5.49	109.25	115.79
1	B	34	TYR	CA-C-N	5.42	127.89	120.46
1	B	34	TYR	C-N-CA	5.42	127.89	120.46
1	F	69	GLU	CA-C-N	5.41	127.79	120.65
1	F	69	GLU	C-N-CA	5.41	127.79	120.65
1	C	196	VAL	CB-CA-C	-5.40	103.03	110.91
1	C	149	GLN	CA-C-O	-5.34	113.17	119.48
1	C	158	THR	N-CA-C	5.34	122.17	110.80
1	D	214	THR	N-CA-C	-5.34	105.82	114.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	133	ILE	O-C-N	5.31	127.11	121.91
1	A	205	ILE	CA-CB-CG1	5.29	119.39	110.40
1	F	198	ASP	N-CA-C	-5.26	107.42	113.88
1	A	18	ASP	CA-C-N	5.24	131.54	121.54
1	A	18	ASP	C-N-CA	5.24	131.54	121.54
1	F	147	THR	CA-C-N	5.22	131.51	121.54
1	F	147	THR	C-N-CA	5.22	131.51	121.54
1	B	102	ASN	CA-C-N	-5.19	113.04	120.42
1	B	102	ASN	C-N-CA	-5.19	113.04	120.42
1	B	129	ALA	O-C-N	5.19	127.42	122.07
1	C	148	SER	CA-C-N	5.17	130.33	122.37
1	C	148	SER	C-N-CA	5.17	130.33	122.37
1	F	119	VAL	O-C-N	5.17	126.88	121.87
1	F	97	ALA	CA-C-N	5.13	127.70	120.42
1	F	97	ALA	C-N-CA	5.13	127.70	120.42
1	C	149	GLN	CB-CA-C	-5.11	101.85	110.64
1	A	199	THR	CA-C-N	5.11	131.29	121.54
1	A	199	THR	C-N-CA	5.11	131.29	121.54
1	C	81	ARG	CA-C-N	5.07	127.40	120.46
1	C	81	ARG	C-N-CA	5.07	127.40	120.46
1	C	91	ILE	O-C-N	5.07	127.05	121.83
1	A	140	TYR	CA-C-O	-5.06	115.43	121.56
1	B	11	VAL	CA-C-N	-5.05	113.90	120.91
1	B	11	VAL	C-N-CA	-5.05	113.90	120.91
1	A	64	ASP	CA-C-N	5.04	127.35	120.54
1	A	64	ASP	C-N-CA	5.04	127.35	120.54
1	F	94	ASN	CA-CB-CG	5.03	117.63	112.60
1	D	96	LYS	CA-C-N	5.03	126.97	120.44
1	D	96	LYS	C-N-CA	5.03	126.97	120.44
1	A	18	ASP	CA-CB-CG	5.02	117.62	112.60
1	D	214	THR	CA-C-N	5.01	130.10	122.23
1	D	214	THR	C-N-CA	5.01	130.10	122.23

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	196	VAL	Peptide
1	C	199	THR	Peptide
1	C	203	SER	Peptide
1	D	1	MSE	Peptide
1	D	152	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	153	SER	Peptide
1	D	188	PHE	Peptide
1	D	189	ASP	Peptide
1	D	2	ALA	Peptide
1	D	7	ASN	Peptide
1	E	156	ASN	Peptide
1	E	158	THR	Peptide
1	E	229	HIS	Mainchain
1	F	168	VAL	Peptide
1	F	169	VAL	Peptide

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	1738	0	1731	236	0
1	B	1738	0	1731	212	0
1	C	1738	0	1731	246	0
1	D	1715	0	1677	319	0
1	E	1712	0	1688	271	0
1	F	1734	0	1721	284	0
2	A	155	0	0	34	0
2	B	167	0	0	32	0
2	C	151	0	0	27	0
2	D	124	0	0	34	0
2	E	138	0	0	20	0
2	F	151	0	0	39	0
All	All	11261	0	10279	1210	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 59.

All (1210) 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:D:222:MSE:SE	1:E:222:MSE:HE3	1.31	1.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:MSE:SE	1:E:222:MSE:CE	2.22	1.36
1:E:157:VAL:HG23	1:F:164:GLY:CA	1.54	1.35
1:D:153:SER:OG	1:E:158:THR:HB	1.36	1.25
1:E:157:VAL:CG2	1:E:158:THR:H	1.44	1.23
1:F:168:VAL:O	1:F:169:VAL:HG23	1.40	1.19
1:E:156:ASN:ND2	1:E:157:VAL:HG12	1.59	1.14
1:E:157:VAL:HG22	1:E:158:THR:N	1.43	1.13
1:D:172:ARG:HH11	1:D:172:ARG:HG2	1.14	1.12
1:E:157:VAL:HG23	1:F:164:GLY:HA2	1.13	1.11
1:B:189:ASP:HB3	1:B:192:LEU:HD12	1.11	1.10
1:D:163:VAL:HG22	1:F:171:ALA:HB2	1.19	1.10
1:D:152:ALA:HB2	2:D:293:HOH:O	1.49	1.09
1:E:231:LEU:HD13	1:F:168:VAL:HG22	1.30	1.07
1:D:150:SER:HB2	1:E:156:ASN:HD22	1.20	1.06
1:B:189:ASP:CB	1:B:192:LEU:HD12	1.87	1.05
1:D:8:ASN:H	1:D:9:PRO:CD	1.69	1.04
1:C:157:VAL:CG1	1:C:158:THR:H	1.70	1.03
1:E:157:VAL:CG2	1:F:164:GLY:HA2	1.88	1.03
1:D:189:ASP:OD1	1:E:216:ARG:HD2	1.56	1.02
1:D:106:THR:HG22	1:E:104:ARG:HH12	1.25	1.02
1:B:29:LYS:HE3	1:B:33:LEU:HD21	1.43	1.01
1:E:157:VAL:CG2	1:E:158:THR:N	2.12	1.01
1:D:8:ASN:H	1:D:9:PRO:HD3	1.25	1.00
1:F:17:LEU:HD13	1:F:36:ILE:HD12	1.37	1.00
1:E:157:VAL:CG2	1:F:164:GLY:CA	2.42	0.97
1:A:1:MSE:SE	1:A:2:ALA:N	2.48	0.97
1:F:176:TRP:HB2	1:F:233:ASP:HB3	1.48	0.96
1:B:189:ASP:HB3	1:B:192:LEU:CD1	1.96	0.95
1:C:191:ASP:C	1:C:192:LEU:HD23	1.93	0.94
1:D:188:PHE:CZ	1:E:216:ARG:HD3	2.03	0.94
1:F:169:VAL:HG12	1:F:170:GLY:H	1.33	0.93
1:B:62:LYS:HG3	1:C:1:MSE:HE2	1.51	0.93
1:C:157:VAL:HG13	1:C:158:THR:H	1.29	0.93
1:D:212:LEU:H	1:E:216:ARG:HH21	1.16	0.92
1:D:176:TRP:H	1:F:185:LYS:HD3	1.32	0.92
1:A:203:SER:HA	1:A:206:GLN:HE21	1.34	0.92
1:E:231:LEU:HD13	1:F:168:VAL:CG2	1.98	0.91
1:A:173:GLN:HE22	1:B:228:ALA:HB3	1.33	0.91
1:D:163:VAL:CG2	1:F:171:ALA:HB2	2.01	0.89
1:F:168:VAL:O	1:F:168:VAL:HG22	1.71	0.89
1:C:157:VAL:CG1	1:C:158:THR:N	2.30	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:GLN:HE21	1:F:203:SER:H	1.21	0.88
1:E:142:SER:H	1:E:149:GLN:HE22	1.22	0.88
1:D:4:PRO:HB2	2:D:248:HOH:O	1.72	0.87
1:F:183:ALA:HB1	1:F:221:ALA:HB2	1.56	0.87
1:E:156:ASN:CG	1:E:157:VAL:N	2.33	0.86
1:A:226:LEU:HD22	1:A:231:LEU:HD12	1.57	0.85
1:E:168:VAL:HG12	1:E:168:VAL:O	1.74	0.85
1:B:192:LEU:HD23	1:B:193:THR:O	1.76	0.85
1:D:174:THR:HA	1:D:233:ASP:HB2	1.57	0.85
1:E:157:VAL:HG23	1:F:164:GLY:N	1.92	0.85
1:F:183:ALA:HB2	1:F:220:LYS:HE3	1.58	0.85
1:A:183:ALA:HB2	1:A:220:LYS:HG3	1.59	0.85
1:D:4:PRO:CG	1:D:64:ASP:OD2	2.25	0.85
1:D:91:ILE:HG12	1:E:91:ILE:HG12	1.57	0.84
1:D:3:ASP:N	1:D:4:PRO:HD3	1.92	0.84
1:C:157:VAL:HG12	1:C:158:THR:N	1.93	0.83
1:D:172:ARG:NH1	1:E:166:LYS:CE	2.42	0.83
1:E:183:ALA:HB2	1:E:220:LYS:HB3	1.61	0.83
1:E:156:ASN:CG	1:E:157:VAL:H	1.85	0.83
1:E:160:SER:CB	1:E:167:LYS:HE2	2.08	0.83
1:C:226:LEU:HD23	1:C:231:LEU:HD23	1.61	0.83
1:D:3:ASP:H	1:D:4:PRO:HD3	1.41	0.83
1:D:172:ARG:HH11	1:E:166:LYS:HG2	1.44	0.82
1:D:172:ARG:NH1	1:E:166:LYS:HE2	1.94	0.82
1:D:226:LEU:HD12	1:F:222:MSE:HE3	1.59	0.82
1:B:31:TYR:HB2	1:C:21:ILE:HD12	1.61	0.81
1:E:157:VAL:CG2	1:F:164:GLY:O	2.28	0.81
1:D:172:ARG:HG2	1:D:172:ARG:NH1	1.91	0.81
1:D:3:ASP:N	1:D:4:PRO:CD	2.43	0.81
1:E:205:ILE:HA	1:E:208:ILE:HD11	1.62	0.81
1:D:176:TRP:HA	1:F:185:LYS:HG2	1.63	0.81
1:D:151:LEU:HB3	1:F:143:LYS:HA	1.61	0.81
1:D:222:MSE:SE	1:E:226:LEU:HG	2.30	0.81
1:B:192:LEU:HD22	1:B:192:LEU:O	1.81	0.81
1:E:160:SER:HB3	1:E:167:LYS:HE2	1.63	0.81
1:D:163:VAL:HG11	1:F:170:GLY:C	2.06	0.80
1:B:69:GLU:HG2	1:C:70:LEU:HD13	1.62	0.80
1:D:6:LEU:HG	1:D:6:LEU:O	1.82	0.80
1:A:105:VAL:O	1:A:109:GLU:HG3	1.83	0.79
1:D:172:ARG:HB3	1:E:168:VAL:CG2	2.12	0.79
1:B:106:THR:HA	1:B:109:GLU:OE2	1.83	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:SER:HB3	1:C:156:ASN:HD22	1.47	0.79
1:F:87:HIS:O	1:F:91:ILE:HG22	1.83	0.79
1:F:212:LEU:O	1:F:216:ARG:HG2	1.83	0.79
1:D:215:GLU:O	1:D:219:THR:HG23	1.83	0.78
1:A:5:SER:HB2	2:C:344:HOH:O	1.84	0.78
1:F:169:VAL:CG1	1:F:170:GLY:H	1.97	0.78
1:B:129:ALA:O	1:B:133:ILE:HG23	1.83	0.78
1:D:8:ASN:N	1:D:9:PRO:CD	2.41	0.78
1:B:1:MSE:HG2	2:B:254:HOH:O	1.84	0.78
1:B:172:ARG:HB2	1:B:230:GLY:O	1.83	0.78
1:D:66:GLN:O	1:D:70:LEU:HD12	1.84	0.78
1:D:91:ILE:HG13	1:F:91:ILE:HD13	1.63	0.78
1:B:101:LEU:HD21	1:C:102:ASN:OD1	1.84	0.78
1:A:182:THR:HG23	2:A:345:HOH:O	1.84	0.78
1:C:201:THR:O	1:C:201:THR:HG22	1.83	0.78
1:E:155:LEU:HB2	1:F:157:VAL:HG21	1.66	0.78
1:E:157:VAL:HG21	1:F:164:GLY:O	1.84	0.78
1:E:206:GLN:O	1:E:209:ALA:HB3	1.84	0.77
1:E:226:LEU:HD12	1:E:232:ILE:HD11	1.66	0.77
1:B:163:VAL:HG12	1:B:168:VAL:HG21	1.64	0.77
1:F:62:LYS:O	1:F:66:GLN:HG3	1.84	0.77
1:A:216:ARG:NH2	1:B:192:LEU:HD11	1.99	0.77
1:C:1:MSE:HB2	1:C:64:ASP:OD1	1.84	0.77
1:A:142:SER:HA	1:C:139:ASP:O	1.85	0.77
1:F:130:GLU:HA	1:F:133:ILE:HD12	1.67	0.77
1:A:57:TYR:O	1:A:61:VAL:HG23	1.85	0.77
1:E:80:LEU:O	1:E:84:VAL:HG23	1.85	0.77
1:F:103:VAL:O	1:F:107:THR:HG23	1.85	0.77
1:F:151:LEU:HD21	1:F:155:LEU:HD12	1.66	0.77
1:E:209:ALA:O	1:E:213:ILE:HG13	1.84	0.76
1:C:103:VAL:O	1:C:107:THR:HG23	1.84	0.76
1:D:189:ASP:CG	1:E:216:ARG:HD2	2.09	0.76
1:A:192:LEU:H	1:A:192:LEU:HD22	1.49	0.76
1:D:168:VAL:HG11	1:F:171:ALA:HA	1.67	0.76
1:D:172:ARG:NE	1:D:233:ASP:HA	2.00	0.76
1:E:21:ILE:HD12	1:F:31:TYR:HB2	1.66	0.76
1:E:208:ILE:O	1:E:212:LEU:HB2	1.85	0.76
1:D:108:ALA:O	1:D:112:ILE:HD12	1.86	0.76
1:F:29:LYS:HE3	1:F:29:LYS:H	1.51	0.76
1:A:1:MSE:SE	1:A:2:ALA:H	2.19	0.76
1:B:176:TRP:HB2	1:B:233:ASP:HB3	1.68	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:VAL:O	1:A:130:GLU:HG3	1.85	0.75
1:C:73:HIS:O	1:C:77:ILE:HG12	1.87	0.75
1:D:62:LYS:O	1:D:66:GLN:HG3	1.86	0.75
1:D:172:ARG:HG2	1:E:166:LYS:HG2	1.66	0.75
1:E:157:VAL:CG2	1:F:164:GLY:C	2.60	0.75
1:C:115:LEU:O	1:C:119:VAL:HG23	1.86	0.75
1:C:47:GLY:O	1:C:51:GLU:HG3	1.87	0.75
1:D:172:ARG:HB2	1:D:230:GLY:O	1.86	0.75
1:E:62:LYS:O	1:E:66:GLN:HG2	1.87	0.74
1:A:229:HIS:O	1:C:167:LYS:HE2	1.88	0.74
1:F:169:VAL:HG12	1:F:170:GLY:N	1.98	0.74
1:B:17:LEU:HD23	1:B:21:ILE:HD11	1.69	0.74
1:D:81:ARG:HD2	2:D:316:HOH:O	1.87	0.74
1:E:41:ASP:O	1:E:45:ILE:HG13	1.88	0.74
1:A:227:ARG:HD2	2:A:352:HOH:O	1.87	0.74
1:C:129:ALA:O	1:C:133:ILE:HG13	1.88	0.74
1:D:144:THR:HB	1:E:139:ASP:OD2	1.87	0.74
1:A:133:ILE:O	1:A:137:GLN:HG3	1.88	0.73
1:E:12:ILE:HD11	2:E:318:HOH:O	1.87	0.73
1:D:151:LEU:HB2	2:F:324:HOH:O	1.87	0.73
1:E:157:VAL:HG23	1:F:164:GLY:C	2.13	0.73
1:F:168:VAL:O	1:F:169:VAL:CG2	2.30	0.73
1:A:145:ALA:O	1:C:153:SER:HB3	1.88	0.73
1:A:50:ASN:OD1	1:C:48:LYS:HD2	1.88	0.73
1:E:91:ILE:HA	2:E:325:HOH:O	1.87	0.73
1:D:172:ARG:HE	1:D:233:ASP:HA	1.52	0.73
1:D:212:LEU:N	1:E:216:ARG:HH21	1.86	0.73
1:B:29:LYS:O	1:B:33:LEU:HG	1.89	0.73
1:A:148:SER:HB2	1:C:154:PRO:HB2	1.70	0.73
1:F:94:ASN:O	1:F:98:ILE:HG13	1.89	0.73
1:E:156:ASN:ND2	1:E:157:VAL:CG1	2.47	0.72
1:A:156:ASN:ND2	1:B:150:SER:HB3	2.04	0.72
1:E:108:ALA:O	1:E:112:ILE:HG13	1.89	0.72
1:B:1:MSE:HB3	1:B:64:ASP:OD1	1.89	0.72
1:A:122:LEU:O	1:A:126:VAL:HG23	1.89	0.72
1:D:162:SER:HB3	1:F:156:ASN:HB2	1.71	0.72
1:B:189:ASP:OD1	1:B:192:LEU:HB3	1.88	0.72
1:F:188:PHE:HZ	1:F:215:GLU:HA	1.54	0.72
1:B:125:ARG:HH21	1:C:126:VAL:HG12	1.52	0.72
1:D:23:PRO:HB2	1:D:26:VAL:HG11	1.72	0.72
1:A:206:GLN:HG2	1:B:196:VAL:HG11	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:ASP:OD2	1:E:216:ARG:HB3	1.90	0.72
1:B:192:LEU:HD22	1:B:192:LEU:C	2.15	0.72
1:C:94:ASN:O	1:C:98:ILE:HG23	1.90	0.72
1:C:18:ASP:O	1:C:22:LEU:HD22	1.90	0.72
1:C:95:THR:O	1:C:98:ILE:HG13	1.89	0.72
1:B:101:LEU:O	1:B:105:VAL:HG23	1.89	0.71
1:B:104:ARG:NH1	1:C:105:VAL:HB	2.05	0.71
1:C:19:ALA:HA	1:C:22:LEU:HB2	1.72	0.71
1:C:124:GLY:O	1:C:128:THR:HG23	1.90	0.71
1:D:156:ASN:HB2	1:F:150:SER:HA	1.71	0.71
1:D:172:ARG:NH1	1:E:166:LYS:HG2	2.04	0.71
1:E:205:ILE:HG12	1:F:205:ILE:HG21	1.71	0.71
1:E:157:VAL:HG22	1:E:158:THR:H	0.60	0.71
1:A:26:VAL:HG21	1:C:26:VAL:HG21	1.71	0.71
1:C:145:ALA:HB3	2:C:326:HOH:O	1.89	0.71
1:A:223:GLU:O	1:A:227:ARG:HG2	1.90	0.71
1:D:70:LEU:HD22	1:E:69:GLU:HG2	1.73	0.70
1:D:77:ILE:HG23	1:E:80:LEU:HD11	1.73	0.70
1:E:171:ALA:HB2	2:E:259:HOH:O	1.91	0.70
1:E:129:ALA:O	1:E:133:ILE:HG22	1.90	0.70
1:E:156:ASN:HD21	1:E:157:VAL:HG12	1.55	0.70
1:A:176:TRP:HB2	1:A:233:ASP:HB3	1.72	0.70
1:A:215:GLU:HG3	1:B:215:GLU:OE2	1.91	0.70
1:C:100:ALA:HB3	2:C:251:HOH:O	1.91	0.70
1:E:102:ASN:ND2	1:F:104:ARG:HH12	1.90	0.70
1:C:114:SER:HA	1:C:117:THR:OG1	1.91	0.70
1:A:202:GLN:O	1:A:206:GLN:HG3	1.90	0.70
1:B:134:SER:HA	1:B:137:GLN:HE21	1.56	0.70
1:B:173:GLN:HE22	1:C:228:ALA:HB3	1.55	0.70
1:D:172:ARG:HE	1:D:233:ASP:CA	2.05	0.70
1:E:215:GLU:HA	2:E:345:HOH:O	1.92	0.70
1:D:45:ILE:HD13	2:F:378:HOH:O	1.91	0.69
1:A:155:LEU:HB2	1:C:157:VAL:HG21	1.74	0.69
1:F:202:GLN:HE21	1:F:203:SER:N	1.91	0.69
1:B:104:ARG:HD3	1:C:109:GLU:OE2	1.92	0.69
1:E:82:ILE:HG23	2:E:348:HOH:O	1.89	0.69
1:C:8:ASN:HB2	2:C:346:HOH:O	1.91	0.69
1:A:220:LYS:HE3	1:A:224:ASP:OD1	1.93	0.69
1:C:194:PHE:HA	2:C:336:HOH:O	1.92	0.69
1:D:46:ALA:HB2	1:E:45:ILE:HD13	1.73	0.69
1:D:83:ASP:O	1:D:86:ASP:HB3	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:ALA:O	1:D:125:ARG:HG3	1.93	0.69
1:A:23:PRO:HB3	1:C:27:PHE:HB3	1.75	0.69
1:D:165:GLY:H	1:F:156:ASN:HD21	1.39	0.69
1:A:197:SER:HB2	1:A:199:THR:O	1.91	0.69
1:B:120:SER:HB2	2:F:331:HOH:O	1.92	0.69
1:B:158:THR:OG1	1:C:152:ALA:HA	1.93	0.69
1:D:4:PRO:HG3	1:D:64:ASP:OD2	1.92	0.69
1:D:226:LEU:HD22	1:D:231:LEU:HD12	1.74	0.69
1:A:215:GLU:OE2	1:C:215:GLU:HG3	1.93	0.69
1:C:121:ALA:HA	2:C:249:HOH:O	1.91	0.69
1:D:91:ILE:HG23	2:E:325:HOH:O	1.93	0.68
1:F:189:ASP:HB3	1:F:192:LEU:HB2	1.74	0.68
1:B:104:ARG:HH11	1:C:105:VAL:HB	1.58	0.68
1:B:87:HIS:O	1:B:91:ILE:HG13	1.94	0.68
1:C:191:ASP:HB3	2:C:345:HOH:O	1.92	0.68
2:A:315:HOH:O	1:B:222:MSE:HE1	1.94	0.68
1:D:38:GLN:O	1:D:42:VAL:HG23	1.94	0.68
1:A:95:THR:HA	1:A:98:ILE:HG22	1.75	0.68
1:D:28:SER:HB3	2:D:279:HOH:O	1.93	0.68
1:D:172:ARG:HH11	1:D:172:ARG:CG	1.97	0.68
1:D:172:ARG:NH1	1:E:166:LYS:CG	2.57	0.68
1:E:185:LYS:HE3	1:F:176:TRP:NE1	2.09	0.68
1:F:45:ILE:HA	2:F:367:HOH:O	1.93	0.68
1:B:226:LEU:HD22	1:C:222:MSE:SE	2.44	0.67
1:A:156:ASN:HB3	1:B:150:SER:HA	1.76	0.67
1:B:134:SER:HA	1:B:137:GLN:NE2	2.08	0.67
1:B:225:ALA:HB3	2:B:317:HOH:O	1.92	0.67
1:D:181:GLY:HA2	1:F:190:ALA:HB2	1.75	0.67
1:D:185:LYS:HD2	1:E:176:TRP:HA	1.77	0.67
1:F:225:ALA:O	1:F:228:ALA:HB3	1.95	0.67
1:F:204:GLU:O	1:F:205:ILE:HB	1.94	0.67
1:A:220:LYS:HA	2:A:357:HOH:O	1.94	0.67
1:E:155:LEU:HD23	1:E:156:ASN:H	1.60	0.67
1:D:223:GLU:HA	1:F:222:MSE:HE2	1.75	0.67
1:A:99:THR:HA	2:A:346:HOH:O	1.95	0.67
1:B:216:ARG:O	1:B:219:THR:HB	1.95	0.67
1:D:61:VAL:HA	1:D:64:ASP:OD2	1.95	0.66
1:D:70:LEU:HD21	1:E:70:LEU:HD22	1.77	0.66
1:D:163:VAL:HG11	1:F:170:GLY:O	1.94	0.66
1:C:172:ARG:HD3	1:C:233:ASP:HA	1.77	0.66
1:E:189:ASP:OD2	1:F:180:THR:HG23	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ASN:O	1:B:106:THR:HG22	1.94	0.66
1:B:173:GLN:NE2	1:C:228:ALA:HB3	2.10	0.66
1:D:125:ARG:HH21	1:F:126:VAL:HG12	1.61	0.66
1:D:153:SER:HG	1:E:158:THR:HB	1.56	0.66
2:E:336:HOH:O	1:F:167:LYS:HE3	1.96	0.66
1:F:222:MSE:O	1:F:226:LEU:HB2	1.95	0.66
1:A:31:TYR:O	1:A:35:VAL:HG23	1.96	0.66
1:A:203:SER:HA	1:A:206:GLN:NE2	2.09	0.66
2:A:342:HOH:O	1:B:77:ILE:HD13	1.96	0.66
1:D:127:THR:HG22	1:E:125:ARG:HH22	1.59	0.66
1:D:150:SER:HB2	1:E:156:ASN:ND2	2.02	0.66
1:F:38:GLN:HG3	2:F:369:HOH:O	1.95	0.66
1:A:143:LYS:HE2	1:C:149:GLN:HG2	1.78	0.66
1:A:153:SER:O	1:C:157:VAL:HG13	1.95	0.66
1:A:202:GLN:NE2	1:B:196:VAL:HG13	2.11	0.66
1:C:62:LYS:O	1:C:66:GLN:HG3	1.96	0.66
1:D:117:THR:O	1:D:120:SER:HB3	1.95	0.66
1:D:31:TYR:O	1:D:35:VAL:HG12	1.96	0.66
1:D:48:LYS:HG2	1:F:10:VAL:HB	1.78	0.66
1:D:24:ARG:O	1:D:26:VAL:HG12	1.96	0.65
1:D:157:VAL:HA	1:F:151:LEU:HD23	1.76	0.65
1:F:169:VAL:CG1	1:F:170:GLY:N	2.53	0.65
1:D:9:PRO:HD2	1:E:48:LYS:NZ	2.12	0.65
1:F:129:ALA:HB3	2:F:398:HOH:O	1.95	0.65
1:C:16:ARG:NH1	1:C:40:THR:HG22	2.11	0.65
1:C:196:VAL:HG22	2:C:240:HOH:O	1.96	0.65
1:F:223:GLU:HG2	1:F:227:ARG:NH2	2.11	0.65
1:A:6:LEU:HB3	1:A:57:TYR:HB2	1.79	0.65
1:A:212:LEU:HD21	2:B:333:HOH:O	1.96	0.65
1:B:156:ASN:HD22	1:B:157:VAL:H	1.45	0.65
1:A:160:SER:HB2	1:A:169:VAL:O	1.97	0.65
1:D:157:VAL:HA	2:F:366:HOH:O	1.97	0.65
1:E:200:TYR:HA	1:E:205:ILE:HD12	1.77	0.65
1:F:168:VAL:O	1:F:168:VAL:CG2	2.45	0.65
1:A:65:GLU:HG2	2:A:264:HOH:O	1.97	0.65
1:B:156:ASN:HD22	1:B:157:VAL:N	1.94	0.65
1:A:54:GLN:HG2	2:A:340:HOH:O	1.95	0.65
1:D:172:ARG:HH12	1:E:166:LYS:CE	2.09	0.65
1:E:229:HIS:HD2	1:F:169:VAL:HG22	1.61	0.65
1:A:1:MSE:SE	1:A:1:MSE:C	2.89	0.65
1:C:212:LEU:HD13	1:C:216:ARG:HD3	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:ALA:HB3	2:E:352:HOH:O	1.97	0.64
1:D:141:VAL:HG13	1:F:141:VAL:HB	1.80	0.64
1:E:102:ASN:HD21	1:F:104:ARG:HH12	1.44	0.64
1:D:165:GLY:H	1:F:156:ASN:ND2	1.96	0.64
1:B:92:THR:O	1:B:96:LYS:HG2	1.97	0.64
1:E:94:ASN:HB2	2:F:383:HOH:O	1.96	0.64
1:A:173:GLN:NE2	1:B:228:ALA:HB3	2.10	0.64
1:B:189:ASP:CG	1:B:192:LEU:HD12	2.22	0.64
1:E:231:LEU:HA	1:F:168:VAL:HG23	1.78	0.64
2:A:333:HOH:O	1:C:157:VAL:C	2.39	0.64
1:D:8:ASN:N	1:D:9:PRO:HD3	2.05	0.64
1:B:203:SER:HA	1:B:206:GLN:HG2	1.79	0.64
1:D:172:ARG:HH12	1:E:166:LYS:HE3	1.62	0.64
1:B:43:GLY:O	1:B:46:ALA:HB3	1.98	0.64
1:B:205:ILE:HG22	2:B:339:HOH:O	1.97	0.64
1:C:50:ASN:HB3	2:C:305:HOH:O	1.98	0.64
1:E:19:ALA:HA	1:E:22:LEU:HD12	1.79	0.64
1:A:69:GLU:HG3	2:B:320:HOH:O	1.98	0.63
1:A:3:ASP:H	1:A:60:GLN:NE2	1.95	0.63
2:A:350:HOH:O	1:C:45:ILE:HD13	1.98	0.63
1:D:179:ALA:HB1	2:F:380:HOH:O	1.97	0.63
1:F:163:VAL:HG23	2:F:306:HOH:O	1.99	0.63
1:C:122:LEU:O	1:C:126:VAL:HG23	1.99	0.63
1:E:200:TYR:HB2	1:F:200:TYR:CD1	2.34	0.63
1:E:215:GLU:HG3	2:E:345:HOH:O	1.99	0.63
1:A:23:PRO:HG3	1:C:27:PHE:HD2	1.63	0.63
1:A:189:ASP:HB2	1:C:180:THR:OG1	1.97	0.63
1:D:102:ASN:HD22	1:E:101:LEU:HD21	1.64	0.63
1:E:16:ARG:HG3	1:E:17:LEU:O	1.99	0.63
1:E:143:LYS:HE3	1:F:140:TYR:O	1.99	0.63
1:C:191:ASP:CA	1:C:192:LEU:HD23	2.29	0.62
1:E:58:ASP:O	1:E:61:VAL:HG13	1.99	0.62
1:E:57:TYR:O	1:E:61:VAL:HG12	1.99	0.62
1:E:87:HIS:O	1:E:91:ILE:HG13	1.99	0.62
1:E:130:GLU:O	1:E:133:ILE:HG23	1.99	0.62
1:E:144:THR:HB	1:F:139:ASP:OD1	1.99	0.62
1:F:35:VAL:HG12	1:F:36:ILE:HD13	1.81	0.62
1:D:116:GLN:HG3	1:E:115:LEU:HD11	1.81	0.62
1:E:208:ILE:HD13	1:E:208:ILE:H	1.63	0.62
1:A:78:LYS:HG3	2:A:292:HOH:O	1.99	0.62
1:C:149:GLN:NE2	2:C:326:HOH:O	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:VAL:O	1:D:158:THR:C	2.42	0.62
1:C:199:THR:O	1:C:200:TYR:HB3	1.99	0.62
1:E:231:LEU:CD1	1:F:168:VAL:HG22	2.20	0.62
1:C:128:THR:HG21	2:C:379:HOH:O	1.99	0.62
1:D:106:THR:O	1:D:109:GLU:HG2	1.99	0.62
1:E:98:ILE:HG23	1:F:101:LEU:HD11	1.81	0.62
1:A:141:VAL:HB	1:C:141:VAL:HB	1.81	0.62
2:A:353:HOH:O	1:B:42:VAL:HG11	1.99	0.62
1:C:199:THR:HG23	1:C:200:TYR:H	1.65	0.61
1:E:61:VAL:HA	1:E:64:ASP:OD2	1.99	0.61
1:D:58:ASP:O	1:D:62:LYS:HG2	2.00	0.61
1:E:158:THR:HG22	1:E:159:THR:N	2.14	0.61
1:F:101:LEU:O	1:F:105:VAL:HG23	2.00	0.61
1:A:222:MSE:HA	1:A:222:MSE:HE3	1.82	0.61
1:C:32:LEU:O	1:C:36:ILE:HG13	2.01	0.61
1:A:156:ASN:HD22	1:B:150:SER:HB3	1.65	0.61
1:D:7:ASN:HA	2:D:255:HOH:O	2.00	0.61
1:D:45:ILE:HG22	1:E:45:ILE:HG21	1.82	0.61
1:D:96:LYS:HB3	2:D:307:HOH:O	2.00	0.61
1:B:195:ALA:O	1:B:204:GLU:HG3	2.01	0.61
1:E:168:VAL:O	1:E:168:VAL:CG1	2.47	0.61
1:E:229:HIS:HB3	1:E:231:LEU:HD22	1.83	0.61
1:D:76:ARG:HB3	1:F:77:ILE:HD13	1.83	0.61
1:D:177:THR:HB	1:F:186:GLY:O	1.99	0.61
1:A:212:LEU:HD13	1:A:216:ARG:HD3	1.82	0.61
1:E:158:THR:HG22	1:E:159:THR:H	1.64	0.61
1:B:157:VAL:HG22	1:C:153:SER:O	2.01	0.61
1:A:38:GLN:HG2	2:C:341:HOH:O	2.00	0.61
1:E:133:ILE:HD12	1:F:136:LEU:HD12	1.83	0.61
1:D:69:GLU:OE2	1:F:70:LEU:HD22	2.00	0.60
1:B:120:SER:O	1:B:123:ASP:HB2	2.00	0.60
1:D:36:ILE:HG23	2:D:257:HOH:O	2.00	0.60
1:F:171:ALA:O	1:F:172:ARG:C	2.43	0.60
1:D:231:LEU:HD23	1:E:168:VAL:HG13	1.82	0.60
1:A:223:GLU:HA	1:B:222:MSE:HE1	1.84	0.60
1:B:201:THR:HB	1:B:204:GLU:HB2	1.82	0.60
1:C:194:PHE:HA	2:C:303:HOH:O	2.00	0.60
1:D:181:GLY:HA3	2:D:297:HOH:O	2.01	0.60
1:F:200:TYR:CE1	1:F:205:ILE:HD13	2.37	0.60
1:A:26:VAL:HG11	1:C:26:VAL:HG23	1.84	0.60
1:A:212:LEU:HD11	2:B:333:HOH:O	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:ASP:OD2	1:F:12:ILE:HB	2.02	0.60
1:E:155:LEU:HD23	1:E:156:ASN:N	2.16	0.60
1:E:208:ILE:HG21	1:F:209:ALA:HB1	1.83	0.60
1:F:140:TYR:HB2	2:F:292:HOH:O	2.01	0.60
1:D:99:THR:HA	1:D:102:ASN:OD1	2.02	0.60
1:E:220:LYS:HE2	1:E:224:ASP:OD1	2.02	0.60
1:F:29:LYS:O	1:F:29:LYS:HG2	2.01	0.60
1:E:67:ASP:HA	1:E:70:LEU:HB2	1.82	0.59
1:D:215:GLU:HG3	1:F:215:GLU:OE1	2.01	0.59
1:B:107:THR:HG23	2:B:349:HOH:O	2.02	0.59
1:E:15:THR:HA	2:E:266:HOH:O	2.03	0.59
1:D:7:ASN:HB2	1:D:57:TYR:HB2	1.84	0.59
1:A:45:ILE:HD11	1:B:46:ALA:HB2	1.85	0.59
1:D:4:PRO:HG2	1:D:64:ASP:OD2	2.02	0.59
1:B:192:LEU:HD13	1:B:192:LEU:N	2.18	0.59
1:D:34:TYR:CE2	1:D:38:GLN:HG3	2.37	0.59
1:D:172:ARG:NH1	1:D:172:ARG:CG	2.61	0.59
1:E:77:ILE:HA	1:E:80:LEU:HD12	1.83	0.59
1:A:141:VAL:HG23	1:B:141:VAL:HB	1.84	0.59
1:E:94:ASN:O	1:E:98:ILE:HG13	2.02	0.59
1:E:183:ALA:HB2	1:E:220:LYS:HD3	1.85	0.59
1:F:202:GLN:H	1:F:202:GLN:NE2	2.00	0.59
2:A:356:HOH:O	1:B:119:VAL:HG11	2.02	0.59
1:A:51:GLU:O	1:A:54:GLN:HB3	2.03	0.59
1:C:14:ALA:HB3	1:D:128:THR:OG1	2.03	0.59
1:A:2:ALA:HA	1:A:60:GLN:HE21	1.68	0.59
1:A:201:THR:O	1:A:205:ILE:HG22	2.02	0.59
1:C:141:VAL:HA	1:C:149:GLN:OE1	2.03	0.59
1:D:109:GLU:HB3	2:D:325:HOH:O	2.01	0.59
1:B:192:LEU:C	1:B:192:LEU:CD2	2.76	0.58
1:E:156:ASN:ND2	1:E:157:VAL:H	2.01	0.58
1:F:17:LEU:CD1	1:F:36:ILE:HA	2.33	0.58
1:A:216:ARG:NH2	1:B:192:LEU:CD1	2.66	0.58
1:B:212:LEU:O	1:B:215:GLU:HB3	2.03	0.58
1:F:91:ILE:O	1:F:95:THR:HG22	2.02	0.58
1:C:200:TYR:CE1	1:C:203:SER:HA	2.38	0.58
1:D:11:VAL:O	1:D:12:ILE:HB	2.02	0.58
1:E:133:ILE:HD11	1:F:132:ASN:HB3	1.86	0.58
1:C:226:LEU:CD2	1:C:231:LEU:HD23	2.33	0.58
1:D:188:PHE:HE2	1:E:216:ARG:O	1.86	0.58
1:E:215:GLU:OE2	1:F:216:ARG:HB3	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:ALA:HB2	1:E:45:ILE:CD1	2.33	0.58
1:D:79:GLN:HA	1:D:82:ILE:HG22	1.86	0.58
1:F:72:ASP:O	1:F:76:ARG:HG3	2.04	0.58
1:F:21:ILE:HG13	1:F:21:ILE:O	2.04	0.58
1:F:23:PRO:HB2	1:F:26:VAL:HG11	1.86	0.58
1:F:96:LYS:HD2	2:F:305:HOH:O	2.04	0.58
1:F:119:VAL:O	1:F:122:LEU:HB2	2.04	0.58
1:D:133:ILE:HD11	2:F:418:HOH:O	2.04	0.58
1:E:47:GLY:O	1:E:51:GLU:HG3	2.04	0.58
1:E:111:GLU:O	1:E:115:LEU:HD13	2.03	0.58
1:D:186:GLY:HA2	1:E:177:THR:OG1	2.04	0.57
1:A:9:PRO:HB3	2:A:329:HOH:O	2.02	0.57
1:A:216:ARG:HH21	1:B:192:LEU:CD1	2.17	0.57
1:B:38:GLN:O	1:B:42:VAL:HG23	2.03	0.57
1:D:173:GLN:HB3	2:F:345:HOH:O	2.03	0.57
1:D:150:SER:CB	1:E:156:ASN:HD22	2.07	0.57
1:D:215:GLU:OE2	1:E:215:GLU:HG2	2.04	0.57
1:E:159:THR:HG21	2:E:303:HOH:O	2.04	0.57
1:C:192:LEU:HD23	1:C:192:LEU:N	2.19	0.57
1:D:56:ALA:O	1:D:60:GLN:HG3	2.04	0.57
1:C:13:GLN:O	1:C:13:GLN:HG3	2.04	0.57
1:C:31:TYR:O	1:C:35:VAL:HG22	2.04	0.57
1:C:184:ASN:HD22	1:C:218:ARG:HH11	1.53	0.57
1:D:60:GLN:O	1:D:64:ASP:OD2	2.22	0.57
1:B:31:TYR:CB	1:C:21:ILE:HD12	2.34	0.57
1:F:76:ARG:HD2	2:F:377:HOH:O	2.02	0.57
1:A:192:LEU:N	1:A:192:LEU:HD13	2.20	0.57
1:A:226:LEU:HD12	1:B:222:MSE:CE	2.34	0.57
1:C:197:SER:HB2	1:C:200:TYR:HA	1.86	0.57
1:E:79:GLN:N	1:E:79:GLN:HE21	2.02	0.57
1:C:140:TYR:CZ	1:C:142:SER:HB2	2.40	0.57
1:D:17:LEU:HB3	2:D:257:HOH:O	2.04	0.57
1:E:153:SER:O	1:F:157:VAL:HG22	2.04	0.57
1:A:226:LEU:HD12	1:B:222:MSE:HE3	1.85	0.57
1:B:27:PHE:HB3	1:B:32:LEU:HD13	1.86	0.57
1:D:181:GLY:HA2	1:F:190:ALA:CB	2.34	0.57
1:A:17:LEU:HD13	1:C:34:TYR:CZ	2.40	0.56
1:A:222:MSE:HE3	1:A:222:MSE:CA	2.35	0.56
1:A:75:ALA:HA	1:A:78:LYS:CD	2.35	0.56
1:A:212:LEU:O	1:A:216:ARG:HG2	2.04	0.56
1:D:153:SER:CB	1:D:154:PRO:CA	2.82	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:ILE:HG13	1:F:77:ILE:HD11	1.87	0.56
1:D:223:GLU:HA	1:F:222:MSE:CE	2.36	0.56
1:A:76:ARG:HB3	2:A:321:HOH:O	2.04	0.56
2:B:313:HOH:O	1:C:13:GLN:HG2	2.06	0.56
1:D:79:GLN:HG2	1:D:82:ILE:HG21	1.87	0.56
1:F:205:ILE:O	1:F:208:ILE:HD13	2.06	0.56
1:D:147:THR:O	1:D:148:SER:HB2	2.05	0.56
1:F:77:ILE:O	1:F:80:LEU:HB2	2.06	0.56
1:A:79:GLN:HG3	1:B:81:ARG:HH22	1.71	0.56
1:D:179:ALA:HB2	1:F:218:ARG:NH2	2.21	0.56
1:C:218:ARG:O	1:C:221:ALA:HB3	2.06	0.56
1:F:40:THR:HG22	2:F:352:HOH:O	2.05	0.56
1:C:56:ALA:O	1:C:60:GLN:HG3	2.06	0.56
1:D:106:THR:HG22	1:E:104:ARG:NH1	2.08	0.56
1:E:173:GLN:O	1:E:232:ILE:HG22	2.05	0.56
1:F:24:ARG:HG3	1:F:24:ARG:HH11	1.71	0.56
1:A:33:LEU:HD22	2:A:247:HOH:O	2.06	0.55
1:A:126:VAL:HG11	1:C:125:ARG:HD3	1.88	0.55
1:A:222:MSE:HE1	1:C:226:LEU:HD13	1.88	0.55
1:B:162:SER:OG	1:B:167:LYS:HA	2.06	0.55
1:C:12:ILE:HD13	1:C:46:ALA:HB3	1.86	0.55
1:C:224:ASP:HB3	2:C:311:HOH:O	2.06	0.55
1:D:8:ASN:H	1:D:9:PRO:HD2	1.64	0.55
1:E:229:HIS:O	1:F:169:VAL:N	2.36	0.55
1:F:179:ALA:HB3	2:F:372:HOH:O	2.05	0.55
1:D:57:TYR:O	1:D:61:VAL:HG23	2.07	0.55
1:F:29:LYS:O	1:F:30:SER:HB2	2.05	0.55
1:A:183:ALA:HB2	1:A:220:LYS:CG	2.33	0.55
1:B:18:ASP:OD2	1:B:20:SER:HB2	2.07	0.55
1:E:133:ILE:O	1:E:137:GLN:HG3	2.05	0.55
1:A:62:LYS:O	1:A:66:GLN:HG3	2.06	0.55
1:A:148:SER:HA	1:C:154:PRO:HD2	1.89	0.55
1:D:162:SER:O	1:F:156:ASN:HA	2.06	0.55
1:E:157:VAL:HB	1:F:164:GLY:O	2.07	0.55
1:A:125:ARG:NH2	1:B:126:VAL:HB	2.22	0.55
1:A:212:LEU:HD23	1:C:212:LEU:CD2	2.37	0.55
2:A:333:HOH:O	1:C:157:VAL:HA	2.07	0.55
1:B:81:ARG:HA	1:B:84:VAL:HG22	1.89	0.55
1:D:45:ILE:HD11	1:F:46:ALA:HB2	1.88	0.55
1:F:23:PRO:HB2	1:F:26:VAL:CG1	2.37	0.55
1:F:45:ILE:HB	2:F:378: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:A:155:LEU:HD22	1:A:156:ASN:H	1.71	0.55
1:D:91:ILE:CG1	1:F:91:ILE:HD13	2.33	0.55
1:D:133:ILE:HG23	2:D:306:HOH:O	2.07	0.55
1:B:158:THR:O	1:B:159:THR:HB	2.07	0.55
1:B:194:PHE:HZ	1:B:211:ALA:HB3	1.72	0.55
2:D:322:HOH:O	1:E:166:LYS:HB3	2.06	0.55
1:B:4:PRO:HA	1:B:57:TYR:CE2	2.42	0.55
1:D:17:LEU:HD12	1:D:36:ILE:HG23	1.89	0.55
1:D:176:TRP:CD1	1:F:185:LYS:HZ2	2.24	0.55
1:D:196:VAL:HG21	1:E:206:GLN:HB3	1.89	0.55
1:D:202:GLN:HG3	1:F:198:ASP:HA	1.89	0.55
1:B:62:LYS:NZ	1:B:62:LYS:HB3	2.22	0.54
1:E:133:ILE:O	1:E:136:LEU:HB2	2.06	0.54
1:F:129:ALA:HA	2:F:287:HOH:O	2.07	0.54
1:B:22:LEU:HD13	1:B:32:LEU:HD12	1.89	0.54
1:E:98:ILE:HG23	1:F:101:LEU:CD1	2.37	0.54
1:A:23:PRO:HB2	1:A:26:VAL:HG11	1.90	0.54
1:A:212:LEU:HG	2:B:344:HOH:O	2.06	0.54
1:B:141:VAL:HG21	1:C:141:VAL:HG12	1.89	0.54
1:A:137:GLN:HG2	1:C:136:LEU:HD11	1.88	0.54
1:E:202:GLN:HA	1:E:202:GLN:OE1	2.08	0.54
1:D:156:ASN:O	1:F:151:LEU:HB2	2.07	0.54
1:D:168:VAL:HG23	1:D:169:VAL:HG23	1.89	0.54
1:E:80:LEU:HD13	1:F:80:LEU:HD23	1.88	0.54
1:E:208:ILE:HG21	1:F:209:ALA:CB	2.37	0.54
1:A:111:GLU:HA	1:A:111:GLU:OE1	2.05	0.54
1:E:199:THR:HA	1:F:200:TYR:CZ	2.42	0.54
1:F:151:LEU:CD2	1:F:155:LEU:HD12	2.37	0.54
1:B:192:LEU:HD13	1:B:192:LEU:H	1.73	0.54
1:D:141:VAL:HA	2:D:256:HOH:O	2.08	0.54
1:D:172:ARG:NH1	1:E:166:LYS:HE3	2.21	0.54
1:A:183:ALA:HB1	1:A:221:ALA:HB2	1.89	0.54
1:A:222:MSE:CE	1:C:226:LEU:HD13	2.38	0.54
1:B:7:ASN:ND2	1:B:54:GLN:HA	2.23	0.54
1:C:173:GLN:OE1	1:C:173:GLN:HA	2.07	0.54
1:D:206:GLN:O	1:D:210:ASN:HB2	2.08	0.54
2:D:234:HOH:O	1:F:78:LYS:HD2	2.07	0.54
1:E:98:ILE:CD1	1:F:94:ASN:HB2	2.38	0.54
1:D:152:ALA:HB3	1:F:145:ALA:O	2.08	0.53
1:D:172:ARG:HB3	1:E:168:VAL:HG22	1.91	0.53
1:E:210:ASN:HA	1:E:213:ILE:HD12	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ILE:HD12	1:A:214:THR:N	2.23	0.53
1:A:75:ALA:HA	1:A:78:LYS:HD2	1.90	0.53
1:A:105:VAL:HG21	1:C:101:LEU:HD22	1.90	0.53
1:D:176:TRP:CE2	1:D:232:ILE:HG13	2.44	0.53
1:C:97:ALA:HA	2:C:251:HOH:O	2.08	0.53
1:D:17:LEU:HD23	1:E:34:TYR:CZ	2.44	0.53
1:D:223:GLU:HB2	2:D:300:HOH:O	2.08	0.53
1:F:214:THR:HA	1:F:217:ARG:CD	2.39	0.53
1:C:65:GLU:HA	1:C:68:VAL:HG23	1.91	0.53
1:D:114:SER:O	1:D:117:THR:HB	2.08	0.53
1:E:199:THR:HG23	1:F:200:TYR:CE2	2.43	0.53
1:D:4:PRO:HD3	1:D:64:ASP:OD1	2.09	0.53
1:A:12:ILE:HD11	1:A:46:ALA:CB	2.39	0.53
1:B:94:ASN:O	1:B:98:ILE:HG13	2.08	0.53
1:D:46:ALA:HA	1:E:45:ILE:HG23	1.89	0.53
1:D:153:SER:H	1:E:158:THR:HG21	1.73	0.53
1:D:230:GLY:HA3	1:E:168:VAL:HA	1.89	0.53
1:A:38:GLN:HG3	2:A:353:HOH:O	2.09	0.53
1:A:143:LYS:HA	1:C:151:LEU:HB3	1.90	0.53
1:E:22:LEU:HD21	1:E:35:VAL:HG21	1.90	0.53
1:F:214:THR:O	1:F:217:ARG:HB2	2.09	0.53
1:A:116:GLN:HG3	1:C:115:LEU:HD11	1.90	0.53
1:C:29:LYS:O	1:C:33:LEU:HG	2.09	0.53
1:C:176:TRP:HB2	1:C:233:ASP:OD1	2.09	0.53
1:E:142:SER:HB3	1:E:145:ALA:HB2	1.90	0.53
1:E:157:VAL:CB	1:F:164:GLY:O	2.57	0.53
1:A:150:SER:HB3	1:C:156:ASN:ND2	2.21	0.53
1:A:12:ILE:HD11	1:A:46:ALA:HB2	1.90	0.52
1:A:210:ASN:O	1:A:213:ILE:HG13	2.09	0.52
1:D:45:ILE:CD1	1:F:46:ALA:HB2	2.39	0.52
1:D:58:ASP:C	1:D:62:LYS:HE2	2.34	0.52
1:D:198:ASP:OD2	1:E:202:GLN:OE1	2.27	0.52
1:A:140:TYR:HE1	1:C:139:ASP:O	1.92	0.52
1:B:62:LYS:CG	1:C:1:MSE:HE2	2.34	0.52
1:B:73:HIS:O	1:B:77:ILE:HG13	2.10	0.52
1:B:212:LEU:O	1:B:216:ARG:HG2	2.08	0.52
1:C:89:SER:HB2	2:C:318:HOH:O	2.07	0.52
1:D:156:ASN:HB2	1:F:150:SER:CA	2.37	0.52
1:D:208:ILE:O	1:D:211:ALA:HB3	2.09	0.52
1:E:107:THR:HG22	1:E:111:GLU:OE2	2.08	0.52
1:A:27:PHE:HB3	2:A:338:HOH:O	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ASP:OD1	1:B:144:THR:HG23	2.09	0.52
1:B:1:MSE:HE3	2:B:234:HOH:O	2.08	0.52
1:D:155:LEU:O	1:E:162:SER:HB2	2.10	0.52
1:B:90:ARG:HG2	2:B:356:HOH:O	2.08	0.52
1:D:11:VAL:HG23	1:D:12:ILE:H	1.73	0.52
1:E:183:ALA:CB	1:E:220:LYS:HB3	2.37	0.52
1:C:155:LEU:HD13	1:C:161:TYR:HE1	1.75	0.52
1:C:212:LEU:O	1:C:216:ARG:HG2	2.09	0.52
1:E:199:THR:HG23	1:F:200:TYR:CD2	2.45	0.52
1:F:29:LYS:HE3	1:F:29:LYS:N	2.20	0.52
1:A:137:GLN:HB3	2:A:309:HOH:O	2.09	0.52
1:A:141:VAL:CG2	1:B:141:VAL:HB	2.39	0.52
1:B:86:ASP:OD2	1:B:87:HIS:HD2	1.92	0.52
1:B:201:THR:HB	1:B:204:GLU:CB	2.40	0.52
1:C:149:GLN:O	1:C:150:SER:O	2.28	0.52
1:C:176:TRP:HB2	1:C:233:ASP:OD2	2.09	0.52
1:D:193:THR:CG2	1:D:208:ILE:HD13	2.40	0.52
1:A:10:VAL:HG11	1:C:44:ALA:O	2.10	0.52
1:B:76:ARG:HH22	1:C:74:GLU:CD	2.17	0.52
1:B:164:GLY:HA3	2:B:318:HOH:O	2.08	0.52
1:D:62:LYS:HG3	1:F:63:ASN:ND2	2.24	0.52
1:A:155:LEU:CD2	1:A:156:ASN:H	2.22	0.52
1:B:137:GLN:HB3	2:B:244:HOH:O	2.08	0.52
1:A:23:PRO:O	1:A:26:VAL:HG13	2.09	0.52
1:D:160:SER:HB2	1:D:169:VAL:O	2.11	0.52
1:A:223:GLU:HA	1:B:222:MSE:CE	2.39	0.51
1:E:69:GLU:HG3	1:E:69:GLU:O	2.10	0.51
1:B:3:ASP:O	1:B:6:LEU:HB2	2.09	0.51
1:A:195:ALA:O	1:A:204:GLU:HG2	2.11	0.51
1:C:194:PHE:O	1:C:195:ALA:HB2	2.11	0.51
1:D:80:LEU:HD21	1:F:81:ARG:HA	1.93	0.51
1:E:6:LEU:CD2	1:E:56:ALA:HB3	2.41	0.51
1:A:149:GLN:O	1:C:155:LEU:HD23	2.09	0.51
1:B:111:GLU:CD	1:C:116:GLN:HE22	2.18	0.51
1:B:209:ALA:HB2	1:C:208:ILE:HG12	1.92	0.51
1:C:80:LEU:O	1:C:84:VAL:HG23	2.09	0.51
1:D:168:VAL:CG1	1:F:171:ALA:HA	2.40	0.51
2:D:234:HOH:O	1:F:78:LYS:HE3	2.11	0.51
1:A:55:GLY:HA2	2:B:246:HOH:O	2.10	0.51
1:B:4:PRO:HA	1:B:57:TYR:HE2	1.75	0.51
1:B:139:ASP:OD1	1:C:144:THR:HG23	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:VAL:HG12	1:E:125:ARG:NH2	2.24	0.51
1:D:185:LYS:O	1:E:177:THR:OG1	2.29	0.51
1:F:147:THR:O	1:F:149:GLN:HG3	2.10	0.51
1:F:223:GLU:HG2	1:F:227:ARG:HH22	1.73	0.51
1:B:203:SER:HA	1:B:206:GLN:CG	2.40	0.51
1:C:182:THR:O	1:C:217:ARG:HG2	2.11	0.51
1:A:202:GLN:HA	1:A:205:ILE:HG23	1.93	0.51
1:B:28:SER:OG	1:B:30:SER:HB2	2.11	0.51
1:B:105:VAL:O	1:B:109:GLU:HG3	2.10	0.51
1:B:112:ILE:O	1:B:116:GLN:HG3	2.11	0.51
1:D:11:VAL:HG23	1:D:12:ILE:N	2.25	0.51
1:D:81:ARG:HA	1:D:84:VAL:HG12	1.91	0.51
2:D:292:HOH:O	1:F:133:ILE:HD13	2.10	0.51
1:A:148:SER:CA	1:C:154:PRO:HD2	2.41	0.51
1:A:173:GLN:HG2	1:B:229:HIS:HE2	1.76	0.51
1:A:180:THR:HB	1:B:190:ALA:HB2	1.93	0.51
1:A:212:LEU:CD1	1:A:216:ARG:HD3	2.39	0.51
1:B:160:SER:HB3	1:B:167:LYS:HE2	1.92	0.51
1:C:216:ARG:HG3	1:C:216:ARG:HH11	1.76	0.51
1:E:231:LEU:CD1	1:F:168:VAL:CG2	2.83	0.51
1:F:206:GLN:O	1:F:210:ASN:HB2	2.11	0.51
1:A:173:GLN:HG2	1:B:229:HIS:NE2	2.26	0.51
1:D:111:GLU:OE1	1:F:112:ILE:HG21	2.10	0.51
1:D:125:ARG:HH21	1:F:126:VAL:CG1	2.22	0.51
1:F:17:LEU:O	1:F:18:ASP:HB2	2.10	0.51
1:F:94:ASN:H	1:F:94:ASN:HD22	1.59	0.51
1:F:101:LEU:HG	2:F:278:HOH:O	2.11	0.51
1:A:12:ILE:O	1:A:12:ILE:HG22	2.11	0.50
1:C:184:ASN:ND2	1:C:218:ARG:HH11	2.09	0.50
1:D:156:ASN:HB2	1:F:150:SER:HB3	1.93	0.50
1:F:109:GLU:O	1:F:112:ILE:HB	2.11	0.50
1:F:213:ILE:O	1:F:217:ARG:HG3	2.11	0.50
1:B:172:ARG:O	1:B:231:LEU:O	2.29	0.50
1:D:106:THR:HA	1:D:109:GLU:CD	2.36	0.50
1:D:156:ASN:HB2	1:F:150:SER:CB	2.42	0.50
1:D:168:VAL:HG11	1:F:170:GLY:O	2.10	0.50
1:E:204:GLU:O	1:E:207:ALA:HB3	2.11	0.50
1:E:200:TYR:HA	1:E:205:ILE:CD1	2.40	0.50
1:E:212:LEU:O	1:E:212:LEU:HD22	2.12	0.50
1:E:215:GLU:O	1:E:219:THR:OG1	2.29	0.50
1:A:17:LEU:O	1:A:18:ASP:OD2	2.30	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASP:C	1:A:191:ASP:H	2.19	0.50
1:C:23:PRO:HG2	1:C:27:PHE:CZ	2.46	0.50
1:E:173:GLN:HB2	1:E:232:ILE:CG2	2.41	0.50
1:B:125:ARG:NH2	1:C:126:VAL:HG12	2.23	0.50
1:D:31:TYR:HB2	1:F:21:ILE:O	2.12	0.50
1:D:159:THR:O	1:D:160:SER:HB3	2.12	0.50
1:F:116:GLN:O	1:F:119:VAL:HG12	2.11	0.50
1:F:117:THR:O	1:F:120:SER:OG	2.30	0.50
1:F:129:ALA:O	1:F:133:ILE:HG13	2.10	0.50
1:A:45:ILE:HG22	1:C:45:ILE:HG21	1.93	0.50
1:F:94:ASN:H	1:F:94:ASN:ND2	2.09	0.50
1:A:149:GLN:HE21	1:B:143:LYS:HE2	1.76	0.50
1:B:32:LEU:O	1:B:36:ILE:HG12	2.11	0.50
1:C:65:GLU:HG2	2:C:352:HOH:O	2.12	0.50
1:C:101:LEU:O	1:C:105:VAL:HG23	2.12	0.50
1:D:45:ILE:HD11	1:F:12:ILE:HG21	1.94	0.50
1:A:143:LYS:CE	1:C:149:GLN:HG2	2.41	0.50
1:C:204:GLU:O	1:C:206:GLN:HG2	2.11	0.50
1:E:15:THR:O	1:E:15:THR:OG1	2.29	0.50
1:D:79:GLN:HG2	1:D:82:ILE:CG2	2.41	0.50
1:D:98:ILE:HG13	1:D:99:THR:H	1.77	0.50
1:E:81:ARG:HG2	2:F:323:HOH:O	2.12	0.50
1:E:231:LEU:HA	1:F:168:VAL:CG2	2.41	0.50
1:A:11:VAL:HG22	1:A:11:VAL:O	2.10	0.49
1:C:90:ARG:O	1:C:94:ASN:OD1	2.30	0.49
1:C:193:THR:O	1:C:194:PHE:O	2.30	0.49
1:D:204:GLU:OE2	1:D:204:GLU:O	2.29	0.49
1:E:173:GLN:O	1:E:233:ASP:OD2	2.30	0.49
1:E:197:SER:HA	1:F:206:GLN:NE2	2.27	0.49
1:B:194:PHE:CD2	1:B:208:ILE:HG22	2.47	0.49
1:F:168:VAL:C	1:F:169:VAL:HG23	2.28	0.49
1:A:95:THR:HB	1:C:94:ASN:HD21	1.76	0.49
1:A:205:ILE:HD13	1:B:205:ILE:HD11	1.93	0.49
1:A:206:GLN:CG	1:B:196:VAL:HG11	2.41	0.49
2:A:378:HOH:O	1:C:40:THR:HB	2.12	0.49
1:B:177:THR:O	1:B:223:GLU:OE1	2.30	0.49
1:B:223:GLU:HA	1:C:222:MSE:SE	2.62	0.49
1:C:1:MSE:SE	1:C:60:GLN:HB3	2.61	0.49
1:E:101:LEU:HD23	2:E:281:HOH:O	2.11	0.49
1:A:130:GLU:HB3	2:A:371:HOH:O	2.11	0.49
1:A:148:SER:HB2	1:C:154:PRO:CB	2.39	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:ASN:OD1	1:F:54:GLN:OE1	2.30	0.49
1:A:23:PRO:HB2	1:A:26:VAL:CG1	2.43	0.49
1:A:73:HIS:HA	2:A:342:HOH:O	2.13	0.49
1:A:220:LYS:HE3	1:A:224:ASP:CG	2.38	0.49
1:B:190:ALA:O	1:B:191:ASP:OD1	2.30	0.49
1:C:176:TRP:HB2	1:C:233:ASP:CG	2.38	0.49
1:D:9:PRO:HD2	1:E:48:LYS:CE	2.43	0.49
1:B:194:PHE:CE2	1:B:208:ILE:HA	2.47	0.49
1:D:121:ALA:HB1	2:D:318:HOH:O	2.11	0.49
1:D:229:HIS:CE1	1:E:231:LEU:HD12	2.48	0.49
2:A:333:HOH:O	1:C:157:VAL:CA	2.60	0.49
1:B:103:VAL:HA	1:B:106:THR:HG22	1.94	0.49
1:B:172:ARG:O	1:B:232:ILE:HA	2.12	0.49
1:D:58:ASP:O	1:D:62:LYS:HE2	2.12	0.49
1:D:157:VAL:CA	1:F:151:LEU:HD23	2.42	0.49
1:E:194:PHE:HB3	2:E:305:HOH:O	2.12	0.49
1:F:179:ALA:CB	1:F:220:LYS:HB2	2.43	0.49
1:B:197:SER:OG	1:B:204:GLU:OE1	2.30	0.49
2:B:339:HOH:O	1:C:196:VAL:HG12	2.12	0.49
1:C:140:TYR:O	1:C:141:VAL:O	2.30	0.49
1:C:172:ARG:HD3	1:C:233:ASP:CA	2.41	0.49
1:D:4:PRO:HD3	1:D:64:ASP:CG	2.38	0.49
2:D:344:HOH:O	1:F:171:ALA:CB	2.60	0.49
1:F:116:GLN:HA	1:F:119:VAL:HG12	1.95	0.49
1:A:63:ASN:O	1:A:67:ASP:OD2	2.30	0.49
1:D:172:ARG:HE	1:D:233:ASP:N	2.11	0.49
1:E:91:ILE:HG22	1:E:91:ILE:O	2.12	0.49
1:F:62:LYS:HD2	1:F:66:GLN:NE2	2.27	0.49
1:B:151:LEU:HD23	2:B:329:HOH:O	2.13	0.48
1:C:78:LYS:HG2	2:C:283:HOH:O	2.12	0.48
1:D:73:HIS:O	1:D:77:ILE:HG13	2.13	0.48
1:E:60:GLN:O	1:E:64:ASP:OD2	2.30	0.48
1:F:91:ILE:HA	1:F:94:ASN:HD21	1.77	0.48
1:D:157:VAL:O	1:D:158:THR:O	2.30	0.48
1:A:126:VAL:HG11	1:C:125:ARG:HG3	1.95	0.48
1:A:225:ALA:O	1:A:229:HIS:HD2	1.96	0.48
1:B:223:GLU:HB2	1:C:222:MSE:HE1	1.93	0.48
1:D:70:LEU:HD21	1:E:70:LEU:CD2	2.40	0.48
1:A:116:GLN:HE21	1:A:116:GLN:HB2	1.40	0.48
1:C:132:ASN:O	1:C:136:LEU:HD13	2.12	0.48
1:A:150:SER:HA	1:C:156:ASN:O	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:ILE:CG1	1:F:77:ILE:HD11	2.44	0.48
1:E:183:ALA:HB1	1:E:221:ALA:N	2.29	0.48
1:D:212:LEU:O	1:D:213:ILE:HD13	2.13	0.48
1:E:91:ILE:HA	2:F:383:HOH:O	2.13	0.48
1:F:189:ASP:CB	1:F:192:LEU:HB2	2.41	0.48
1:F:200:TYR:O	1:F:201:THR:O	2.29	0.48
1:A:97:ALA:O	1:A:100:ALA:HB3	2.13	0.48
1:A:129:ALA:O	1:A:133:ILE:HB	2.13	0.48
1:A:205:ILE:O	1:A:208:ILE:HB	2.14	0.48
1:B:141:VAL:CG2	1:C:141:VAL:HG12	2.44	0.48
1:D:201:THR:HG22	1:D:203:SER:OG	2.13	0.48
1:F:11:VAL:HA	2:F:334:HOH:O	2.14	0.48
1:A:223:GLU:HG2	2:A:315:HOH:O	2.14	0.48
1:B:104:ARG:HG3	2:B:393:HOH:O	2.13	0.48
1:D:152:ALA:HB3	1:F:146:THR:HA	1.96	0.48
1:F:215:GLU:HG3	1:F:216:ARG:N	2.29	0.48
1:A:98:ILE:CD1	1:C:97:ALA:HB1	2.44	0.48
1:C:9:PRO:HA	1:C:50:ASN:OD1	2.13	0.48
1:C:74:GLU:HG3	1:C:78:LYS:HD3	1.95	0.48
1:F:62:LYS:HD2	1:F:66:GLN:HE21	1.78	0.48
1:F:130:GLU:HG3	2:F:398:HOH:O	2.14	0.48
1:E:199:THR:HA	1:F:200:TYR:CE2	2.49	0.47
1:D:162:SER:O	1:F:161:TYR:OH	2.30	0.47
1:E:229:HIS:NE2	1:F:231:LEU:HB3	2.29	0.47
1:D:95:THR:O	1:D:98:ILE:HG13	2.14	0.47
1:F:227:ARG:HD3	1:F:233:ASP:C	2.39	0.47
1:B:157:VAL:HG21	1:C:155:LEU:HB2	1.96	0.47
1:B:159:THR:O	1:B:160:SER:HB3	2.13	0.47
1:C:192:LEU:N	1:C:192:LEU:CD2	2.77	0.47
1:D:189:ASP:OD2	1:E:216:ARG:HD2	2.15	0.47
1:D:213:ILE:HG22	1:D:216:ARG:HD3	1.97	0.47
1:E:19:ALA:O	1:E:22:LEU:HB2	2.15	0.47
1:A:172:ARG:HG3	1:A:230:GLY:O	2.14	0.47
1:B:59:ALA:HA	1:C:1:MSE:HE1	1.96	0.47
1:C:184:ASN:O	1:C:185:LYS:HD2	2.14	0.47
1:D:163:VAL:HG13	1:F:171:ALA:HA	1.96	0.47
1:D:183:ALA:HB1	1:D:217:ARG:HB3	1.97	0.47
1:F:2:ALA:O	1:F:4:PRO:HD3	2.14	0.47
1:A:75:ALA:O	1:A:78:LYS:HG2	2.15	0.47
1:A:212:LEU:HD23	1:C:212:LEU:HD21	1.97	0.47
1:B:1:MSE:HE2	1:B:64:ASP:CG	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:SER:HB3	1:B:145:ALA:HB2	1.96	0.47
1:D:222:MSE:O	1:D:222:MSE:CE	2.62	0.47
1:D:225:ALA:HB2	1:E:176:TRP:CZ2	2.50	0.47
1:E:60:GLN:HA	1:E:63:ASN:HB2	1.97	0.47
1:F:17:LEU:O	1:F:17:LEU:HD12	2.15	0.47
1:A:143:LYS:HD3	1:C:139:ASP:HA	1.97	0.47
1:B:153:SER:HB2	1:C:147:THR:O	2.14	0.47
1:B:212:LEU:HB2	2:B:344:HOH:O	2.15	0.47
1:D:62:LYS:HE3	1:F:60:GLN:HG2	1.96	0.47
1:D:90:ARG:HB3	1:F:91:ILE:HD11	1.96	0.47
1:D:101:LEU:HD23	2:D:309:HOH:O	2.13	0.47
1:D:222:MSE:SE	1:E:222:MSE:HE1	2.48	0.47
1:F:200:TYR:HE2	1:F:202:GLN:HB3	1.79	0.47
1:D:139:ASP:OD1	1:F:142:SER:OG	2.33	0.47
2:D:344:HOH:O	1:F:171:ALA:HB2	2.14	0.47
1:F:151:LEU:HD23	2:F:366:HOH:O	2.15	0.47
1:A:62:LYS:HB2	1:A:62:LYS:HE2	1.48	0.47
1:D:118:ASN:ND2	2:D:311:HOH:O	2.47	0.47
1:E:193:THR:N	2:E:338:HOH:O	2.48	0.47
1:F:54:GLN:HG3	2:F:330:HOH:O	2.14	0.47
1:D:162:SER:N	1:F:155:LEU:O	2.48	0.47
1:F:171:ALA:O	1:F:172:ARG:O	2.32	0.47
1:A:26:VAL:HG11	1:C:26:VAL:CG2	2.45	0.46
1:A:80:LEU:O	1:A:84:VAL:HG23	2.15	0.46
1:B:96:LYS:HB2	2:B:278:HOH:O	2.14	0.46
1:B:174:THR:HB	1:B:175:GLY:H	1.59	0.46
1:D:91:ILE:CG1	1:E:91:ILE:HG12	2.37	0.46
1:D:220:LYS:HE3	1:D:224:ASP:OD1	2.14	0.46
1:E:156:ASN:HD21	1:E:157:VAL:CG1	2.18	0.46
1:E:160:SER:HB2	1:E:167:LYS:HE2	1.93	0.46
1:F:173:GLN:OE1	1:F:173:GLN:HA	2.15	0.46
1:A:77:ILE:HD11	1:C:77:ILE:HD11	1.96	0.46
1:B:159:THR:O	1:B:159:THR:CG2	2.58	0.46
1:C:74:GLU:HG3	1:C:78:LYS:CD	2.44	0.46
1:D:59:ALA:HA	1:D:62:LYS:CG	2.45	0.46
1:D:202:GLN:O	1:D:202:GLN:NE2	2.48	0.46
1:E:209:ALA:HA	1:E:212:LEU:HB3	1.98	0.46
1:B:7:ASN:HD22	1:B:54:GLN:HB3	1.80	0.46
1:D:9:PRO:HD2	1:E:48:LYS:HE2	1.97	0.46
1:D:183:ALA:O	1:D:217:ARG:NH2	2.48	0.46
1:A:105:VAL:HG12	1:C:104:ARG:NH2	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:O	1:B:143:LYS:O	2.33	0.46
1:A:167:LYS:HE2	1:B:229:HIS:O	2.16	0.46
1:D:34:TYR:CZ	1:F:17:LEU:HG	2.50	0.46
1:E:133:ILE:CD1	1:F:132:ASN:HB3	2.45	0.46
1:F:155:LEU:HB2	2:F:366:HOH:O	2.14	0.46
1:A:14:ALA:HB2	1:C:37:ALA:HB1	1.96	0.46
1:D:133:ILE:HA	2:D:306:HOH:O	2.14	0.46
1:F:214:THR:HA	1:F:217:ARG:HD3	1.96	0.46
1:B:105:VAL:O	1:B:108:ALA:HB3	2.15	0.46
1:C:191:ASP:HB2	1:C:192:LEU:HD23	1.96	0.46
1:E:26:VAL:HG13	1:E:27:PHE:CD1	2.51	0.46
1:F:211:ALA:HA	2:F:361:HOH:O	2.16	0.46
1:B:166:LYS:O	1:B:168:VAL:HG22	2.16	0.46
1:D:70:LEU:HD22	1:E:69:GLU:CG	2.45	0.46
1:D:185:LYS:HD2	1:E:176:TRP:CA	2.44	0.46
1:A:34:TYR:CZ	1:B:17:LEU:HG	2.51	0.46
1:A:96:LYS:HG2	2:A:248:HOH:O	2.15	0.46
1:D:97:ALA:HB1	1:F:98:ILE:HG21	1.98	0.46
1:E:205:ILE:HG12	1:F:205:ILE:CG2	2.42	0.46
1:A:62:LYS:HG2	1:B:63:ASN:CG	2.41	0.46
1:A:92:THR:HG22	1:A:96:LYS:HD2	1.98	0.46
1:C:8:ASN:HD22	1:C:9:PRO:HD2	1.80	0.46
1:F:176:TRP:HZ3	1:F:223:GLU:OE2	1.97	0.46
1:A:10:VAL:HG22	1:C:48:LYS:HD2	1.97	0.46
1:A:226:LEU:HD22	1:A:231:LEU:CD1	2.38	0.46
1:C:122:LEU:HA	1:C:125:ARG:HG2	1.97	0.46
1:D:80:LEU:HG	1:F:81:ARG:HH21	1.81	0.46
1:D:165:GLY:C	1:D:166:LYS:HZ3	2.24	0.46
1:D:176:TRP:H	1:F:185:LYS:CD	2.17	0.46
1:D:220:LYS:HE3	1:D:224:ASP:CG	2.41	0.46
1:E:189:ASP:HA	1:F:180:THR:CG2	2.46	0.46
1:A:32:LEU:N	2:A:338:HOH:O	2.49	0.45
1:A:140:TYR:CE1	1:A:142:SER:HB2	2.51	0.45
1:C:140:TYR:OH	1:C:142:SER:HB2	2.16	0.45
1:D:8:ASN:N	1:D:9:PRO:HD2	2.26	0.45
1:F:3:ASP:O	1:F:6:LEU:HG	2.16	0.45
1:A:125:ARG:NH1	1:B:130:GLU:OE2	2.50	0.45
1:B:1:MSE:N	2:B:288:HOH:O	2.48	0.45
1:D:171:ALA:O	1:D:173:GLN:NE2	2.49	0.45
1:D:220:LYS:O	1:D:224:ASP:N	2.50	0.45
1:E:66:GLN:NE2	1:F:66:GLN:OE1	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:ASN:ND2	2:E:325:HOH:O	2.50	0.45
1:A:24:ARG:HE	1:A:24:ARG:HB3	1.49	0.45
1:A:95:THR:CG2	1:C:94:ASN:HD21	2.30	0.45
1:A:195:ALA:HB2	2:A:374:HOH:O	2.15	0.45
1:A:212:LEU:HD12	1:B:194:PHE:HE1	1.81	0.45
1:A:213:ILE:O	1:A:217:ARG:HG3	2.17	0.45
1:B:162:SER:HA	1:B:168:VAL:CG2	2.46	0.45
1:D:20:SER:N	2:D:291:HOH:O	2.49	0.45
1:D:63:ASN:O	1:D:66:GLN:N	2.50	0.45
1:E:130:GLU:OE1	1:F:125:ARG:NH2	2.49	0.45
1:E:183:ALA:HB2	1:E:220:LYS:CD	2.46	0.45
1:F:94:ASN:HD22	1:F:94:ASN:N	2.13	0.45
1:A:1:MSE:HE3	1:A:2:ALA:O	2.16	0.45
1:A:17:LEU:HD13	1:C:34:TYR:CE1	2.51	0.45
1:A:172:ARG:NH2	1:C:166:LYS:HG2	2.31	0.45
1:B:183:ALA:HB2	1:B:220:LYS:CG	2.46	0.45
1:C:1:MSE:HB3	1:C:2:ALA:H	1.55	0.45
1:C:22:LEU:O	1:C:23:PRO:O	2.34	0.45
1:C:139:ASP:OD1	1:C:139:ASP:N	2.49	0.45
1:C:216:ARG:NH1	2:C:236:HOH:O	2.49	0.45
1:E:81:ARG:NH1	1:E:85:ASP:OD2	2.49	0.45
1:E:145:ALA:O	1:F:153:SER:HB3	2.16	0.45
1:E:185:LYS:C	1:F:177:THR:HG1	2.24	0.45
1:E:209:ALA:O	1:E:213:ILE:N	2.49	0.45
1:F:24:ARG:NH1	1:F:25:ASN:OD1	2.50	0.45
1:F:182:THR:O	1:F:217:ARG:NH1	2.50	0.45
1:F:227:ARG:HD3	1:F:233:ASP:O	2.16	0.45
1:A:95:THR:CB	1:C:94:ASN:HD21	2.29	0.45
1:C:114:SER:HB2	2:C:347:HOH:O	2.17	0.45
1:C:133:ILE:HG22	1:C:137:GLN:NE2	2.31	0.45
1:A:78:LYS:HB3	1:A:78:LYS:HE3	1.29	0.45
1:A:92:THR:O	1:A:96:LYS:HD2	2.16	0.45
1:A:105:VAL:HG21	1:C:101:LEU:CD2	2.46	0.45
1:A:156:ASN:ND2	2:A:322:HOH:O	2.50	0.45
1:A:194:PHE:HB3	1:A:195:ALA:H	1.55	0.45
1:C:29:LYS:HG2	1:C:30:SER:N	2.31	0.45
1:C:213:ILE:CG2	1:C:217:ARG:HD2	2.47	0.45
1:D:18:ASP:O	1:D:21:ILE:HG12	2.17	0.45
1:D:102:ASN:O	1:D:106:THR:HG23	2.16	0.45
1:D:173:GLN:NE2	2:D:330:HOH:O	2.50	0.45
1:F:17:LEU:HD13	1:F:36:ILE:HA	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:PRO:C	1:A:26:VAL:HG13	2.42	0.45
1:A:73:HIS:HE1	1:B:74:GLU:HG2	1.81	0.45
1:B:163:VAL:CG1	1:B:168:VAL:HG21	2.41	0.45
1:C:199:THR:HG23	1:C:200:TYR:N	2.29	0.45
1:D:17:LEU:HD23	1:E:34:TYR:CE1	2.52	0.45
1:D:63:ASN:OD1	1:E:66:GLN:NE2	2.49	0.45
1:D:76:ARG:NH1	2:D:315:HOH:O	2.50	0.45
1:D:213:ILE:N	1:D:216:ARG:HD3	2.30	0.45
1:A:125:ARG:HD2	1:B:130:GLU:OE1	2.17	0.45
1:B:203:SER:HA	1:B:206:GLN:CD	2.42	0.45
1:C:22:LEU:HD12	1:C:22:LEU:HA	1.81	0.45
1:D:88:GLU:OE2	1:E:90:ARG:NH1	2.50	0.45
1:E:95:THR:HA	2:F:364:HOH:O	2.17	0.45
1:F:24:ARG:HG3	1:F:24:ARG:NH1	2.31	0.45
1:A:151:LEU:O	1:A:152:ALA:HB3	2.17	0.45
1:A:189:ASP:OD1	1:A:190:ALA:N	2.50	0.45
2:A:234:HOH:O	1:C:63:ASN:ND2	2.49	0.45
1:B:180:THR:OG1	1:C:189:ASP:OD1	2.33	0.45
1:D:98:ILE:O	1:D:102:ASN:ND2	2.50	0.45
1:D:109:GLU:OE1	1:E:104:ARG:NH1	2.50	0.45
1:D:153:SER:H	1:E:158:THR:CG2	2.30	0.45
1:D:208:ILE:O	1:D:211:ALA:O	2.35	0.45
1:F:128:THR:HA	1:F:131:ASN:HB2	1.98	0.45
1:F:148:SER:O	1:F:149:GLN:HB2	2.17	0.45
1:A:185:LYS:HE2	1:C:176:TRP:CD1	2.52	0.45
1:A:217:ARG:NH2	1:B:191:ASP:OD2	2.50	0.45
1:A:219:THR:HG21	1:B:215:GLU:OE2	2.17	0.45
1:E:84:VAL:O	1:F:87:HIS:HE1	2.00	0.45
1:A:3:ASP:OD1	1:A:4:PRO:HD2	2.17	0.44
1:B:12:ILE:HD13	2:B:258:HOH:O	2.17	0.44
1:B:74:GLU:O	1:B:78:LYS:HB2	2.17	0.44
1:C:8:ASN:HD22	1:C:9:PRO:CD	2.30	0.44
1:C:196:VAL:HB	1:C:197:SER:C	2.42	0.44
1:E:95:THR:HG22	1:E:96:LYS:N	2.32	0.44
1:F:48:LYS:HB2	1:F:48:LYS:HE3	1.78	0.44
1:F:172:ARG:HA	1:F:231:LEU:O	2.17	0.44
1:F:206:GLN:O	1:F:210:ASN:N	2.50	0.44
1:A:140:TYR:CZ	1:A:142:SER:HB2	2.51	0.44
1:A:202:GLN:HA	1:A:205:ILE:CG2	2.47	0.44
1:D:162:SER:HB3	1:F:156:ASN:CB	2.43	0.44
1:D:222:MSE:O	1:D:222:MSE:HE2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:194:PHE:CG	1:F:208:ILE:HG22	2.52	0.44
1:B:133:ILE:HG13	1:B:134:SER:N	2.33	0.44
1:B:223:GLU:CB	1:C:222:MSE:HE1	2.48	0.44
1:D:94:ASN:ND2	1:F:91:ILE:HD12	2.32	0.44
1:E:38:GLN:O	1:E:42:VAL:HG23	2.18	0.44
1:E:92:THR:HG22	2:E:301:HOH:O	2.16	0.44
1:F:46:ALA:N	2:F:378:HOH:O	2.50	0.44
1:F:76:ARG:NE	2:F:395:HOH:O	2.50	0.44
1:F:151:LEU:O	1:F:152:ALA:HB3	2.18	0.44
1:D:136:LEU:HB3	1:E:136:LEU:HD11	2.00	0.44
1:D:216:ARG:HG2	1:F:215:GLU:HB2	1.99	0.44
1:D:230:GLY:HA3	1:E:167:LYS:O	2.18	0.44
1:E:100:ALA:HA	2:E:283:HOH:O	2.18	0.44
1:B:36:ILE:HD13	1:B:36:ILE:N	2.32	0.44
1:B:115:LEU:HD22	1:C:119:VAL:HG21	1.98	0.44
1:C:185:LYS:NZ	1:C:185:LYS:HA	2.33	0.44
1:E:172:ARG:HG3	1:E:230:GLY:O	2.17	0.44
1:F:91:ILE:O	1:F:94:ASN:ND2	2.50	0.44
1:F:119:VAL:HB	2:F:358:HOH:O	2.16	0.44
1:B:76:ARG:HD2	2:B:289:HOH:O	2.16	0.44
1:B:90:ARG:NH2	2:B:356:HOH:O	2.50	0.44
1:B:184:ASN:OD1	1:B:186:GLY:N	2.50	0.44
1:C:96:LYS:HD3	2:C:371:HOH:O	2.18	0.44
1:C:149:GLN:HE21	1:C:149:GLN:HB2	1.50	0.44
1:C:216:ARG:HG2	1:C:216:ARG:H	1.59	0.44
1:D:95:THR:HA	1:D:98:ILE:HG12	1.98	0.44
2:D:234:HOH:O	1:F:78:LYS:HA	2.18	0.44
1:E:29:LYS:O	1:E:29:LYS:HG3	2.16	0.44
1:A:141:VAL:O	1:A:149:GLN:NE2	2.50	0.44
1:B:115:LEU:CD2	1:C:119:VAL:HG21	2.48	0.44
1:C:37:ALA:HA	1:C:40:THR:OG1	2.18	0.44
1:D:26:VAL:O	1:F:23:PRO:HG3	2.18	0.44
1:D:173:GLN:HB2	1:D:232:ILE:HD12	1.99	0.44
1:E:23:PRO:HB2	1:E:26:VAL:CG1	2.48	0.44
1:E:157:VAL:HG23	1:F:164:GLY:H	1.78	0.44
1:F:127:THR:O	1:F:131:ASN:OD1	2.35	0.44
1:A:185:LYS:HA	1:A:218:ARG:NH1	2.33	0.44
1:B:108:ALA:O	1:B:112:ILE:HD12	2.18	0.44
1:B:147:THR:HA	2:B:328:HOH:O	2.18	0.44
1:B:231:LEU:O	1:C:229:HIS:HE1	2.01	0.44
1:D:185:LYS:O	1:D:185:LYS:HG3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:LEU:CD1	1:F:222:MSE:HE3	2.38	0.44
2:E:314:HOH:O	1:F:181:GLY:HA2	2.18	0.44
1:C:18:ASP:C	1:C:22:LEU:HD22	2.43	0.44
1:C:157:VAL:HG13	1:C:158:THR:N	2.08	0.44
1:D:172:ARG:HE	1:D:232:ILE:C	2.25	0.44
1:D:176:TRP:CA	1:F:185:LYS:HG2	2.42	0.44
1:F:6:LEU:HD12	1:F:57:TYR:HA	1.99	0.44
1:A:85:ASP:OD1	1:A:85:ASP:N	2.50	0.43
1:B:174:THR:HA	1:B:233:ASP:HB2	1.99	0.43
1:D:176:TRP:N	1:F:185:LYS:HD3	2.16	0.43
1:A:212:LEU:HD23	1:C:212:LEU:HD23	1.98	0.43
1:D:79:GLN:O	1:D:82:ILE:HG23	2.18	0.43
1:B:178:ALA:HA	1:B:223:GLU:OE1	2.19	0.43
1:E:78:LYS:HG3	1:F:76:ARG:HH12	1.82	0.43
1:F:6:LEU:HD11	1:F:60:GLN:OE1	2.18	0.43
1:C:81:ARG:HD3	1:C:85:ASP:OD1	2.17	0.43
1:B:171:ALA:O	1:C:229:HIS:NE2	2.50	0.43
1:C:71:ALA:HB2	2:C:256:HOH:O	2.18	0.43
1:D:31:TYR:CE2	1:F:22:LEU:HD23	2.53	0.43
1:D:80:LEU:O	1:D:83:ASP:HB2	2.18	0.43
1:D:147:THR:HG22	1:D:148:SER:N	2.33	0.43
1:E:194:PHE:O	1:E:195:ALA:HB2	2.16	0.43
1:F:41:ASP:O	1:F:45:ILE:HD12	2.19	0.43
1:D:123:ASP:HA	1:E:122:LEU:HD11	2.01	0.43
1:D:203:SER:O	1:D:206:GLN:N	2.50	0.43
1:E:32:LEU:O	1:E:36:ILE:HG12	2.18	0.43
1:A:100:ALA:O	1:A:103:VAL:HG22	2.18	0.43
1:A:215:GLU:O	1:A:218:ARG:HB3	2.19	0.43
1:B:132:ASN:ND2	2:B:245:HOH:O	2.50	0.43
1:D:59:ALA:HA	1:D:62:LYS:CE	2.49	0.43
1:D:90:ARG:NH2	1:F:88:GLU:OE2	2.50	0.43
1:E:140:TYR:CE1	1:F:136:LEU:HD21	2.53	0.43
1:F:94:ASN:HB3	2:F:364:HOH:O	2.18	0.43
1:B:186:GLY:O	1:B:218:ARG:NH1	2.51	0.43
1:C:37:ALA:O	1:C:40:THR:N	2.51	0.43
1:C:204:GLU:O	1:C:205:ILE:HG22	2.18	0.43
1:D:48:LYS:HA	1:D:48:LYS:HD3	1.46	0.43
1:D:117:THR:HG22	1:D:118:ASN:N	2.33	0.43
1:D:152:ALA:HA	1:E:158:THR:OG1	2.19	0.43
1:F:174:THR:HA	1:F:233:ASP:HB2	2.01	0.43
1:A:21:ILE:HD12	1:C:31:TYR:HD1	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLU:OE1	1:A:215:GLU:HA	2.18	0.43
1:A:222:MSE:O	1:A:225:ALA:HB3	2.19	0.43
1:B:222:MSE:HB3	1:C:222:MSE:HE3	1.99	0.43
1:C:22:LEU:HD23	1:C:32:LEU:HD11	2.01	0.43
1:C:143:LYS:HE3	1:C:143:LYS:HB2	1.52	0.43
1:D:150:SER:HB2	1:E:156:ASN:HB3	2.00	0.43
1:D:189:ASP:OD2	1:E:216:ARG:CB	2.65	0.43
1:F:188:PHE:CZ	1:F:215:GLU:HA	2.43	0.43
1:A:6:LEU:HD22	1:A:53:GLY:HA2	2.00	0.43
1:A:159:THR:O	1:A:160:SER:HB3	2.18	0.43
1:D:122:LEU:HD12	1:D:122:LEU:HA	1.81	0.43
1:E:23:PRO:HA	2:E:253:HOH:O	2.18	0.43
1:E:31:TYR:O	1:E:35:VAL:HG13	2.19	0.43
1:E:167:LYS:O	1:E:168:VAL:HG23	2.18	0.43
1:E:218:ARG:HH21	1:F:179:ALA:HB2	1.83	0.43
1:F:155:LEU:HD23	1:F:156:ASN:N	2.34	0.43
1:F:207:ALA:HA	1:F:210:ASN:HB2	2.01	0.43
1:C:218:ARG:HG3	1:C:218:ARG:NH1	2.34	0.42
1:D:29:LYS:HA	1:D:32:LEU:HD12	2.00	0.42
1:D:91:ILE:HA	1:D:94:ASN:HB2	2.01	0.42
1:D:197:SER:OG	1:D:198:ASP:N	2.50	0.42
1:F:118:ASN:O	1:F:122:LEU:HD22	2.19	0.42
1:F:201:THR:HG22	1:F:203:SER:HB3	2.00	0.42
1:A:26:VAL:HG21	1:C:26:VAL:CG2	2.45	0.42
1:A:111:GLU:O	1:A:114:SER:HB2	2.19	0.42
1:C:191:ASP:HB2	1:C:192:LEU:CD2	2.49	0.42
1:D:48:LYS:HG2	1:F:10:VAL:CB	2.48	0.42
1:D:174:THR:HA	1:D:233:ASP:CB	2.38	0.42
1:D:213:ILE:CA	1:D:216:ARG:HD3	2.49	0.42
2:D:327:HOH:O	1:F:143:LYS:NZ	2.49	0.42
1:E:172:ARG:HG3	1:E:232:ILE:HA	2.02	0.42
1:F:143:LYS:HB3	2:F:389:HOH:O	2.18	0.42
1:B:223:GLU:O	1:B:223:GLU:HG3	2.20	0.42
1:C:205:ILE:HA	2:C:234:HOH:O	2.19	0.42
1:D:68:VAL:HG13	1:D:69:GLU:H	1.83	0.42
1:E:63:ASN:OD1	1:E:66:GLN:NE2	2.52	0.42
1:E:82:ILE:HD13	1:E:82:ILE:HA	1.84	0.42
1:F:226:LEU:HB3	1:F:232:ILE:HG12	2.01	0.42
1:A:98:ILE:HG21	2:C:290:HOH:O	2.19	0.42
1:B:32:LEU:HD12	1:B:32:LEU:HA	1.78	0.42
1:C:207:ALA:HB3	2:C:234:HOH:O	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:ASN:O	1:D:66:GLN:HB2	2.20	0.42
1:E:91:ILE:HG23	2:F:383:HOH:O	2.19	0.42
1:A:88:GLU:OE2	1:C:90:ARG:NH1	2.50	0.42
1:B:81:ARG:O	1:B:84:VAL:HG22	2.19	0.42
1:B:194:PHE:O	1:B:195:ALA:HB3	2.19	0.42
1:C:29:LYS:O	1:C:32:LEU:HB3	2.19	0.42
1:D:92:THR:HA	2:D:277:HOH:O	2.18	0.42
1:F:189:ASP:CG	1:F:192:LEU:HB2	2.45	0.42
1:A:75:ALA:HA	1:A:78:LYS:CG	2.49	0.42
1:B:16:ARG:NE	2:B:290:HOH:O	2.52	0.42
1:B:96:LYS:HZ2	1:B:96:LYS:N	2.17	0.42
1:B:213:ILE:HG12	1:C:192:LEU:HB3	2.01	0.42
1:B:220:LYS:O	1:B:224:ASP:OD2	2.38	0.42
1:C:35:VAL:HG23	1:C:36:ILE:N	2.34	0.42
1:D:75:ALA:HB2	2:D:265:HOH:O	2.20	0.42
1:D:208:ILE:O	1:D:211:ALA:N	2.52	0.42
1:E:70:LEU:HD13	1:E:70:LEU:HA	1.83	0.42
1:E:102:ASN:HB2	2:E:358:HOH:O	2.19	0.42
1:F:179:ALA:HB3	1:F:220:LYS:HB2	2.00	0.42
1:A:89:SER:HB3	2:A:305:HOH:O	2.19	0.42
1:A:95:THR:HG22	1:C:94:ASN:HD21	1.85	0.42
1:C:26:VAL:HG13	1:C:27:PHE:N	2.34	0.42
1:F:86:ASP:HB2	2:F:424:HOH:O	2.19	0.42
1:A:29:LYS:HA	1:A:29:LYS:HD2	1.74	0.42
1:A:212:LEU:HD12	1:B:194:PHE:CE1	2.55	0.42
1:A:218:ARG:NH2	1:C:223:GLU:OE2	2.51	0.42
1:C:149:GLN:CD	2:C:326:HOH:O	2.62	0.42
1:D:184:ASN:O	1:D:185:LYS:HB3	2.19	0.42
1:E:99:THR:O	1:E:103:VAL:HG23	2.20	0.42
1:A:180:THR:C	1:B:190:ALA:HA	2.45	0.42
1:B:122:LEU:O	1:B:126:VAL:HG23	2.20	0.42
1:B:172:ARG:O	1:B:172:ARG:HG3	2.16	0.42
1:D:173:GLN:HG3	2:F:345:HOH:O	2.20	0.42
1:F:81:ARG:HE	1:F:81:ARG:HB2	1.67	0.42
1:A:81:ARG:O	1:A:85:ASP:OD1	2.37	0.42
1:B:76:ARG:NH1	2:B:237:HOH:O	2.50	0.42
1:B:84:VAL:HG23	1:B:85:ASP:N	2.35	0.42
1:B:181:GLY:O	1:B:220:LYS:HE2	2.19	0.42
1:D:188:PHE:CE2	1:E:216:ARG:HB3	2.54	0.42
1:D:193:THR:HB	1:D:208:ILE:HD13	2.02	0.42
1:A:194:PHE:CE2	1:C:209:ALA:HB3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLN:O	1:A:205:ILE:HG23	2.20	0.41
1:D:8:ASN:OD1	1:D:54:GLN:OE1	2.38	0.41
1:E:189:ASP:HA	1:F:180:THR:HG22	2.02	0.41
1:E:229:HIS:CD2	1:F:231:LEU:HD22	2.54	0.41
1:A:92:THR:HG23	2:A:324:HOH:O	2.19	0.41
1:C:13:GLN:HE21	1:C:13:GLN:HB2	1.60	0.41
1:C:111:GLU:O	1:C:115:LEU:HD13	2.20	0.41
1:E:197:SER:H	1:F:206:GLN:HE22	1.67	0.41
1:A:66:GLN:NE2	2:A:234:HOH:O	2.50	0.41
1:A:115:LEU:HD21	2:B:350:HOH:O	2.20	0.41
1:C:35:VAL:HG23	1:C:36:ILE:H	1.85	0.41
1:C:212:LEU:CD1	1:C:216:ARG:HD3	2.49	0.41
1:D:27:PHE:HB2	1:D:32:LEU:HD21	2.02	0.41
1:D:98:ILE:HG13	1:D:99:THR:N	2.36	0.41
1:D:154:PRO:CA	1:E:160:SER:O	2.67	0.41
1:D:183:ALA:HB1	1:D:217:ARG:O	2.21	0.41
1:D:218:ARG:HA	1:D:218:ARG:HD2	1.29	0.41
1:E:66:GLN:O	1:E:70:LEU:HD23	2.21	0.41
1:A:91:ILE:HG13	1:B:91:ILE:HD13	2.02	0.41
1:B:7:ASN:ND2	2:B:304:HOH:O	2.53	0.41
1:E:156:ASN:HA	1:F:162:SER:HB2	2.02	0.41
1:A:95:THR:HA	1:A:98:ILE:CG2	2.49	0.41
1:A:115:LEU:HD21	1:B:116:GLN:HG2	2.02	0.41
1:A:148:SER:HB2	1:C:154:PRO:CG	2.51	0.41
1:B:157:VAL:HG22	1:B:158:THR:H	1.86	0.41
1:B:183:ALA:HB1	1:B:221:ALA:HA	2.02	0.41
1:C:12:ILE:HD13	1:C:46:ALA:CB	2.50	0.41
1:C:35:VAL:O	1:C:38:GLN:HB2	2.20	0.41
1:E:151:LEU:HD23	1:E:153:SER:HB3	2.03	0.41
1:F:115:LEU:HD23	1:F:115:LEU:HA	1.90	0.41
1:B:220:LYS:HG3	1:B:224:ASP:OD2	2.20	0.41
1:C:8:ASN:HA	1:C:9:PRO:HD3	1.85	0.41
1:C:17:LEU:HB3	1:C:18:ASP:H	1.57	0.41
1:C:141:VAL:HG13	1:C:149:GLN:OE1	2.20	0.41
1:D:116:GLN:CG	1:E:115:LEU:HD11	2.49	0.41
1:D:125:ARG:HE	1:D:125:ARG:HB3	1.65	0.41
1:E:147:THR:O	1:E:147:THR:HG23	2.20	0.41
1:E:194:PHE:HE1	1:E:211:ALA:HB3	1.85	0.41
1:D:37:ALA:HA	1:D:40:THR:HG23	2.03	0.41
1:D:90:ARG:HG2	2:D:269:HOH:O	2.20	0.41
1:D:229:HIS:NE2	1:E:172:ARG:HA	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:213:ILE:HG22	1:F:214:THR:N	2.36	0.41
1:A:140:TYR:CD1	1:C:140:TYR:HA	2.55	0.41
1:B:159:THR:O	1:B:160:SER:CB	2.69	0.41
1:D:32:LEU:HA	1:D:35:VAL:CG1	2.51	0.41
1:D:91:ILE:CD1	1:F:91:ILE:HD13	2.50	0.41
1:E:174:THR:HA	1:E:233:ASP:OD1	2.19	0.41
1:A:136:LEU:HD12	1:C:136:LEU:HD23	2.03	0.41
1:B:92:THR:HB	2:B:327:HOH:O	2.20	0.41
1:B:183:ALA:HB2	1:B:220:LYS:HG3	2.03	0.41
1:B:183:ALA:HB1	1:B:221:ALA:CA	2.51	0.41
1:D:81:ARG:HA	1:D:84:VAL:CG1	2.51	0.41
1:D:127:THR:HG22	1:E:125:ARG:NH2	2.30	0.41
1:D:188:PHE:CE1	1:E:216:ARG:HD3	2.52	0.41
1:F:69:GLU:O	1:F:73:HIS:ND1	2.54	0.41
1:F:131:ASN:O	1:F:134:SER:HB2	2.21	0.41
1:F:194:PHE:CD2	1:F:208:ILE:HG22	2.56	0.41
1:A:32:LEU:HD13	1:A:32:LEU:HA	1.90	0.41
1:B:206:GLN:O	1:B:210:ASN:HB2	2.21	0.41
1:C:194:PHE:O	1:C:195:ALA:CB	2.69	0.41
1:C:217:ARG:NH2	2:C:320:HOH:O	2.54	0.41
1:D:45:ILE:HG21	2:F:378:HOH:O	2.21	0.41
1:D:226:LEU:HD22	1:D:226:LEU:HA	1.83	0.41
1:E:68:VAL:O	1:E:71:ALA:HB3	2.20	0.41
1:E:74:GLU:OE2	1:E:78:LYS:HE3	2.21	0.41
1:F:6:LEU:CD1	1:F:57:TYR:HA	2.51	0.41
1:F:202:GLN:H	1:F:202:GLN:CD	2.28	0.41
1:A:98:ILE:HD11	1:C:97:ALA:HB1	2.03	0.40
1:A:126:VAL:HG11	1:C:125:ARG:CD	2.51	0.40
1:A:151:LEU:N	2:A:333:HOH:O	2.50	0.40
1:B:81:ARG:HH11	1:B:84:VAL:HG21	1.85	0.40
1:C:185:LYS:HA	1:C:185:LYS:CE	2.47	0.40
1:D:118:ASN:ND2	2:D:304:HOH:O	2.49	0.40
1:D:150:SER:O	1:F:143:LYS:HB3	2.21	0.40
1:D:216:ARG:HG2	1:F:215:GLU:OE1	2.20	0.40
1:E:79:GLN:HE21	1:E:79:GLN:CA	2.33	0.40
1:E:142:SER:OG	1:E:145:ALA:N	2.54	0.40
1:F:73:HIS:HD2	2:F:276:HOH:O	2.04	0.40
1:A:23:PRO:CB	1:C:27:PHE:HB3	2.49	0.40
1:B:81:ARG:C	1:B:84:VAL:HG22	2.45	0.40
1:B:88:GLU:HA	2:B:326:HOH:O	2.22	0.40
1:C:184:ASN:C	1:C:185:LYS:HD2	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ASP:OD1	1:A:76:ARG:NH1	2.54	0.40
1:B:215:GLU:HB2	2:B:333:HOH:O	2.21	0.40
1:C:16:ARG:HH11	1:C:40:THR:HG22	1.83	0.40
1:D:29:LYS:N	2:D:254:HOH:O	2.54	0.40
1:E:41:ASP:O	1:E:44:ALA:HB3	2.21	0.40
1:F:35:VAL:HG12	1:F:36:ILE:N	2.35	0.40
1:A:7:ASN:HB2	1:A:57:TYR:CD1	2.55	0.40
1:B:103:VAL:HA	1:B:106:THR:CG2	2.51	0.40
1:C:62:LYS:HE3	1:C:65:GLU:OE2	2.21	0.40
1:C:196:VAL:HB	1:C:197:SER:CA	2.49	0.40
1:D:140:TYR:HB3	2:D:263:HOH:O	2.20	0.40
1:D:208:ILE:HD12	1:E:209:ALA:HB2	2.03	0.40
1:E:63:ASN:HA	1:E:66:GLN:HE21	1.86	0.40
1:E:131:ASN:HD22	1:E:131:ASN:HA	1.63	0.40
1:E:176:TRP:CE2	1:E:232:ILE:HG21	2.56	0.40
1:A:36:ILE:HD13	1:A:36:ILE:HA	1.90	0.40
1:C:200:TYR:HE1	1:C:203:SER:HA	1.85	0.40
1:D:196:VAL:HG11	1:E:206:GLN:NE2	2.36	0.40
1:D:209:ALA:O	1:D:211:ALA:O	2.39	0.40
1:D:216:ARG:O	1:D:219:THR:OG1	2.40	0.40

There are no symmetry-related clashes.

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	231/233 (99%)	199 (86%)	19 (8%)	13 (6%)	1 0
1	B	231/233 (99%)	211 (91%)	14 (6%)	6 (3%)	4 1
1	C	231/233 (99%)	199 (86%)	18 (8%)	14 (6%)	1 0
1	D	231/233 (99%)	176 (76%)	36 (16%)	19 (8%)	0 0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	231/233 (99%)	204 (88%)	17 (7%)	10 (4%)	2	0
1	F	231/233 (99%)	200 (87%)	16 (7%)	15 (6%)	1	0
All	All	1386/1398 (99%)	1189 (86%)	120 (9%)	77 (6%)	1	0

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	190	ALA
1	A	191	ASP
1	A	194	PHE
1	A	200	TYR
1	C	23	PRO
1	C	150	SER
1	C	187	VAL
1	C	192	LEU
1	C	194	PHE
1	C	195	ALA
1	C	200	TYR
1	C	201	THR
1	C	204	GLU
1	C	205	ILE
1	D	2	ALA
1	D	8	ASN
1	D	9	PRO
1	D	26	VAL
1	D	148	SER
1	D	154	PRO
1	D	158	THR
1	D	183	ALA
1	D	185	LYS
1	E	18	ASP
1	E	157	VAL
1	E	158	THR
1	E	168	VAL
1	E	169	VAL
1	E	195	ALA
1	F	7	ASN
1	F	18	ASP
1	F	148	SER
1	F	169	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	172	ARG
1	F	186	GLY
1	F	195	ALA
1	F	205	ILE
1	A	11	VAL
1	A	145	ALA
1	B	198	ASP
1	D	10	VAL
1	D	17	LEU
1	D	184	ASN
1	E	176	TRP
1	F	30	SER
1	F	149	GLN
1	F	201	THR
1	A	14	ALA
1	A	16	ARG
1	A	142	SER
1	B	173	GLN
1	B	192	LEU
1	B	200	TYR
1	C	141	VAL
1	E	204	GLU
1	F	29	LYS
1	A	10	VAL
1	A	13	GLN
1	A	19	ALA
1	B	201	THR
1	D	76	ARG
1	D	157	VAL
1	D	178	ALA
1	D	213	ILE
1	D	230	GLY
1	F	164	GLY
1	B	190	ALA
1	C	2	ALA
1	D	179	ALA
1	E	20	SER
1	E	200	TYR
1	D	12	ILE
1	F	165	GLY
1	F	26	VAL
1	C	26	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	157	VAL

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	184/182 (101%)	130 (71%)	54 (29%)	0	0
1	B	184/182 (101%)	127 (69%)	57 (31%)	0	0
1	C	184/182 (101%)	127 (69%)	57 (31%)	0	0
1	D	177/182 (97%)	112 (63%)	65 (37%)	0	0
1	E	178/182 (98%)	111 (62%)	67 (38%)	0	0
1	F	183/182 (100%)	118 (64%)	65 (36%)	0	0
All	All	1090/1092 (100%)	725 (66%)	365 (34%)	0	0

All (365) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	5	SER
1	A	8	ASN
1	A	10	VAL
1	A	11	VAL
1	A	12	ILE
1	A	16	ARG
1	A	24	ARG
1	A	25	ASN
1	A	26	VAL
1	A	32	LEU
1	A	38	GLN
1	A	42	VAL
1	A	45	ILE
1	A	48	LYS
1	A	60	GLN
1	A	62	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	65	GLU
1	A	78	LYS
1	A	95	THR
1	A	98	ILE
1	A	104	ARG
1	A	119	VAL
1	A	123	ASP
1	A	132	ASN
1	A	133	ILE
1	A	136	LEU
1	A	142	SER
1	A	143	LYS
1	A	150	SER
1	A	151	LEU
1	A	155	LEU
1	A	158	THR
1	A	162	SER
1	A	168	VAL
1	A	174	THR
1	A	180	THR
1	A	182	THR
1	A	185	LYS
1	A	189	ASP
1	A	192	LEU
1	A	194	PHE
1	A	196	VAL
1	A	202	GLN
1	A	203	SER
1	A	204	GLU
1	A	205	ILE
1	A	212	LEU
1	A	216	ARG
1	A	219	THR
1	A	220	LYS
1	A	223	GLU
1	A	227	ARG
1	A	232	ILE
1	B	6	LEU
1	B	12	ILE
1	B	13	GLN
1	B	21	ILE
1	B	24	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	26	VAL
1	B	28	SER
1	B	32	LEU
1	B	33	LEU
1	B	36	ILE
1	B	40	THR
1	B	51	GLU
1	B	54	GLN
1	B	62	LYS
1	B	65	GLU
1	B	69	GLU
1	B	78	LYS
1	B	79	GLN
1	B	81	ARG
1	B	86	ASP
1	B	88	GLU
1	B	89	SER
1	B	90	ARG
1	B	96	LYS
1	B	99	THR
1	B	102	ASN
1	B	104	ARG
1	B	106	THR
1	B	107	THR
1	B	114	SER
1	B	118	ASN
1	B	120	SER
1	B	122	LEU
1	B	133	ILE
1	B	136	LEU
1	B	137	GLN
1	B	147	THR
1	B	148	SER
1	B	150	SER
1	B	155	LEU
1	B	157	VAL
1	B	163	VAL
1	B	167	LYS
1	B	168	VAL
1	B	172	ARG
1	B	174	THR
1	B	180	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	184	ASN
1	B	187	VAL
1	B	192	LEU
1	B	196	VAL
1	B	197	SER
1	B	201	THR
1	B	205	ILE
1	B	208	ILE
1	B	216	ARG
1	B	222	MSE
1	C	1	MSE
1	C	12	ILE
1	C	13	GLN
1	C	15	THR
1	C	20	SER
1	C	22	LEU
1	C	24	ARG
1	C	25	ASN
1	C	27	PHE
1	C	29	LYS
1	C	32	LEU
1	C	33	LEU
1	C	36	ILE
1	C	38	GLN
1	C	40	THR
1	C	48	LYS
1	C	61	VAL
1	C	62	LYS
1	C	65	GLU
1	C	68	VAL
1	C	77	ILE
1	C	78	LYS
1	C	82	ILE
1	C	96	LYS
1	C	105	VAL
1	C	114	SER
1	C	115	LEU
1	C	120	SER
1	C	122	LEU
1	C	123	ASP
1	C	125	ARG
1	C	128	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	142	SER
1	C	143	LYS
1	C	146	THR
1	C	147	THR
1	C	149	GLN
1	C	151	LEU
1	C	155	LEU
1	C	157	VAL
1	C	162	SER
1	C	163	VAL
1	C	182	THR
1	C	185	LYS
1	C	187	VAL
1	C	192	LEU
1	C	197	SER
1	C	200	TYR
1	C	201	THR
1	C	203	SER
1	C	204	GLU
1	C	206	GLN
1	C	210	ASN
1	C	212	LEU
1	C	216	ARG
1	C	231	LEU
1	C	233	ASP
1	D	8	ASN
1	D	13	GLN
1	D	15	THR
1	D	16	ARG
1	D	17	LEU
1	D	24	ARG
1	D	28	SER
1	D	35	VAL
1	D	38	GLN
1	D	40	THR
1	D	48	LYS
1	D	62	LYS
1	D	68	VAL
1	D	69	GLU
1	D	76	ARG
1	D	78	LYS
1	D	79	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	80	LEU
1	D	82	ILE
1	D	83	ASP
1	D	89	SER
1	D	96	LYS
1	D	99	THR
1	D	102	ASN
1	D	104	ARG
1	D	112	ILE
1	D	115	LEU
1	D	117	THR
1	D	122	LEU
1	D	125	ARG
1	D	126	VAL
1	D	130	GLU
1	D	141	VAL
1	D	144	THR
1	D	147	THR
1	D	151	LEU
1	D	153	SER
1	D	162	SER
1	D	163	VAL
1	D	166	LYS
1	D	169	VAL
1	D	172	ARG
1	D	173	GLN
1	D	174	THR
1	D	180	THR
1	D	184	ASN
1	D	185	LYS
1	D	187	VAL
1	D	189	ASP
1	D	192	LEU
1	D	193	THR
1	D	194	PHE
1	D	202	GLN
1	D	203	SER
1	D	204	GLU
1	D	205	ILE
1	D	213	ILE
1	D	214	THR
1	D	215	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	218	ARG
1	D	220	LYS
1	D	222	MSE
1	D	226	LEU
1	D	227	ARG
1	D	232	ILE
1	E	1	MSE
1	E	6	LEU
1	E	10	VAL
1	E	12	ILE
1	E	13	GLN
1	E	15	THR
1	E	16	ARG
1	E	17	LEU
1	E	21	ILE
1	E	24	ARG
1	E	25	ASN
1	E	29	LYS
1	E	33	LEU
1	E	35	VAL
1	E	36	ILE
1	E	38	GLN
1	E	61	VAL
1	E	62	LYS
1	E	66	GLN
1	E	69	GLU
1	E	70	LEU
1	E	79	GLN
1	E	81	ARG
1	E	82	ILE
1	E	83	ASP
1	E	90	ARG
1	E	92	THR
1	E	95	THR
1	E	101	LEU
1	E	106	THR
1	E	107	THR
1	E	114	SER
1	E	117	THR
1	E	120	SER
1	E	122	LEU
1	E	127	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	133	ILE
1	E	134	SER
1	E	136	LEU
1	E	143	LYS
1	E	144	THR
1	E	146	THR
1	E	148	SER
1	E	151	LEU
1	E	155	LEU
1	E	157	VAL
1	E	159	THR
1	E	172	ARG
1	E	174	THR
1	E	177	THR
1	E	182	THR
1	E	185	LYS
1	E	193	THR
1	E	194	PHE
1	E	196	VAL
1	E	201	THR
1	E	206	GLN
1	E	208	ILE
1	E	212	LEU
1	E	214	THR
1	E	217	ARG
1	E	218	ARG
1	E	219	THR
1	E	222	MSE
1	E	226	LEU
1	E	231	LEU
1	E	232	ILE
1	F	1	MSE
1	F	8	ASN
1	F	10	VAL
1	F	16	ARG
1	F	17	LEU
1	F	20	SER
1	F	21	ILE
1	F	22	LEU
1	F	24	ARG
1	F	27	PHE
1	F	28	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	29	LYS
1	F	30	SER
1	F	35	VAL
1	F	36	ILE
1	F	48	LYS
1	F	62	LYS
1	F	65	GLU
1	F	68	VAL
1	F	77	ILE
1	F	78	LYS
1	F	80	LEU
1	F	81	ARG
1	F	82	ILE
1	F	86	ASP
1	F	94	ASN
1	F	95	THR
1	F	96	LYS
1	F	99	THR
1	F	109	GLU
1	F	122	LEU
1	F	128	THR
1	F	134	SER
1	F	146	THR
1	F	147	THR
1	F	150	SER
1	F	151	LEU
1	F	153	SER
1	F	155	LEU
1	F	157	VAL
1	F	166	LYS
1	F	167	LYS
1	F	182	THR
1	F	185	LYS
1	F	187	VAL
1	F	191	ASP
1	F	193	THR
1	F	196	VAL
1	F	197	SER
1	F	198	ASP
1	F	199	THR
1	F	201	THR
1	F	202	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	203	SER
1	F	204	GLU
1	F	205	ILE
1	F	208	ILE
1	F	212	LEU
1	F	213	ILE
1	F	215	GLU
1	F	217	ARG
1	F	218	ARG
1	F	220	LYS
1	F	226	LEU
1	F	232	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	8	ASN
1	A	38	GLN
1	A	60	GLN
1	A	66	GLN
1	A	73	HIS
1	A	79	GLN
1	A	94	ASN
1	A	149	GLN
1	A	156	ASN
1	A	173	GLN
1	A	202	GLN
1	A	206	GLN
1	A	210	ASN
1	B	7	ASN
1	B	8	ASN
1	B	38	GLN
1	B	79	GLN
1	B	87	HIS
1	B	102	ASN
1	B	132	ASN
1	B	137	GLN
1	B	202	GLN
1	C	8	ASN
1	C	13	GLN
1	C	38	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	60	GLN
1	C	66	GLN
1	C	79	GLN
1	C	94	ASN
1	C	116	GLN
1	C	118	ASN
1	C	137	GLN
1	C	184	ASN
1	C	210	ASN
1	D	38	GLN
1	D	118	ASN
1	D	132	ASN
1	D	137	GLN
1	D	173	GLN
1	D	206	GLN
1	D	210	ASN
1	E	8	ASN
1	E	25	ASN
1	E	50	ASN
1	E	54	GLN
1	E	66	GLN
1	E	79	GLN
1	E	87	HIS
1	E	102	ASN
1	E	118	ASN
1	E	131	ASN
1	E	149	GLN
1	E	156	ASN
1	E	229	HIS
1	F	8	ASN
1	F	54	GLN
1	F	66	GLN
1	F	94	ASN
1	F	102	ASN
1	F	131	ASN
1	F	149	GLN
1	F	156	ASN
1	F	202	GLN
1	F	206	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

There are no ligands in this entry.

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	227/233 (97%)	1.31	43 (18%) 3 3	2, 14, 36, 48	0
1	B	229/233 (98%)	1.00	27 (11%) 9 9	2, 16, 29, 38	0
1	C	229/233 (98%)	1.56	51 (22%) 2 2	3, 15, 55, 75	0
1	D	231/233 (99%)	1.85	80 (34%) 1 1	5, 21, 56, 75	0
1	E	228/233 (97%)	1.51	64 (28%) 1 1	4, 18, 59, 77	0
1	F	229/233 (98%)	1.49	60 (26%) 1 1	3, 17, 43, 56	0
All	All	1373/1398 (98%)	1.45	325 (23%) 2 2	2, 17, 48, 77	0

All (325) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	193	THR	12.8
1	C	195	ALA	11.2
1	D	195	ALA	8.8
1	D	199	THR	8.1
1	D	213	ILE	8.0
1	C	198	ASP	8.0
1	F	190	ALA	7.8
1	D	196	VAL	7.8
1	C	202	GLN	7.6
1	D	188	PHE	7.5
1	F	194	PHE	7.4
1	D	157	VAL	7.1
1	C	192	LEU	7.0
1	C	197	SER	7.0
1	F	170	GLY	6.9
1	D	10	VAL	6.8
1	C	196	VAL	6.8
1	F	196	VAL	6.7
1	C	194	PHE	6.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	18	ASP	6.5
1	F	164	GLY	6.4
1	D	178	ALA	6.3
1	F	167	LYS	6.3
1	E	158	THR	6.3
1	A	195	ALA	6.2
1	E	193	THR	6.2
1	E	192	LEU	6.1
1	F	195	ALA	6.1
1	C	19	ALA	6.0
1	C	199	THR	6.0
1	C	205	ILE	6.0
1	D	190	ALA	5.9
1	E	157	VAL	5.9
1	D	11	VAL	5.8
1	A	110	GLY	5.7
1	E	208	ILE	5.6
1	D	211	ALA	5.5
1	F	18	ASP	5.5
1	A	182	THR	5.4
1	A	183	ALA	5.4
1	C	189	ASP	5.4
1	E	205	ILE	5.4
1	D	204	GLU	5.3
1	A	194	PHE	5.3
1	C	17	LEU	5.3
1	D	197	SER	5.3
1	C	149	GLN	5.3
1	C	201	THR	5.2
1	D	2	ALA	5.1
1	D	192	LEU	5.1
1	D	189	ASP	5.1
1	F	91	ILE	5.0
1	D	201	THR	5.0
1	C	200	TYR	5.0
1	F	171	ALA	5.0
1	A	192	LEU	5.0
1	E	200	TYR	5.0
1	D	179	ALA	4.9
1	D	200	TYR	4.9
1	F	168	VAL	4.8
1	E	198	ASP	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	208	ILE	4.7
1	E	167	LYS	4.7
1	F	205	ILE	4.7
1	E	156	ASN	4.6
1	A	178	ALA	4.6
1	A	32	LEU	4.6
1	F	151	LEU	4.5
1	D	202	GLN	4.5
1	D	8	ASN	4.5
1	A	179	ALA	4.5
1	E	202	GLN	4.5
1	F	163	VAL	4.4
1	E	233	ASP	4.4
1	D	198	ASP	4.3
1	E	199	THR	4.3
1	A	98	ILE	4.3
1	D	15	THR	4.2
1	C	108	ALA	4.2
1	F	193	THR	4.1
1	C	204	GLU	4.1
1	E	18	ASP	4.1
1	D	102	ASN	4.1
1	F	166	LYS	4.0
1	A	101	LEU	3.9
1	F	169	VAL	3.9
1	D	9	PRO	3.9
1	E	175	GLY	3.8
1	C	16	ARG	3.8
1	B	189	ASP	3.8
1	A	13	GLN	3.8
1	E	206	GLN	3.8
1	B	194	PHE	3.7
1	F	200	TYR	3.7
1	B	84	VAL	3.7
1	B	123	ASP	3.7
1	E	176	TRP	3.6
1	E	147	THR	3.6
1	E	181	GLY	3.6
1	D	153	SER	3.6
1	E	17	LEU	3.6
1	A	15	THR	3.5
1	E	219	THR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	223	GLU	3.5
1	A	25	ASN	3.5
1	A	158	THR	3.5
1	C	26	VAL	3.5
1	E	168	VAL	3.5
1	C	184	ASN	3.5
1	A	212	LEU	3.5
1	C	191	ASP	3.4
1	F	204	GLU	3.4
1	D	180	THR	3.4
1	A	196	VAL	3.4
1	A	18	ASP	3.4
1	E	217	ARG	3.4
1	E	194	PHE	3.4
1	A	17	LEU	3.4
1	C	203	SER	3.3
1	F	24	ARG	3.3
1	B	15	THR	3.3
1	E	170	GLY	3.3
1	B	215	GLU	3.3
1	E	182	THR	3.3
1	D	187	VAL	3.3
1	D	182	THR	3.2
1	E	203	SER	3.2
1	F	17	LEU	3.2
1	C	139	ASP	3.2
1	F	202	GLN	3.2
1	E	195	ALA	3.2
1	F	94	ASN	3.2
1	E	215	GLU	3.2
1	D	84	VAL	3.2
1	C	233	ASP	3.2
1	D	193	THR	3.2
1	E	166	LYS	3.2
1	F	183	ALA	3.1
1	E	123	ASP	3.1
1	B	176	TRP	3.1
1	B	200	TYR	3.1
1	C	159	THR	3.1
1	D	194	PHE	3.1
1	A	24	ARG	3.1
1	D	191	ASP	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	11	VAL	3.1
1	A	111	GLU	3.1
1	E	207	ALA	3.1
1	E	133	ILE	3.1
1	D	214	THR	3.1
1	E	24	ARG	3.1
1	D	109	GLU	3.1
1	E	183	ALA	3.1
1	B	177	THR	3.0
1	F	108	ALA	3.0
1	F	36	ILE	3.0
1	A	200	TYR	3.0
1	A	6	LEU	3.0
1	E	214	THR	3.0
1	F	215	GLU	2.9
1	B	175	GLY	2.9
1	C	23	PRO	2.9
1	E	216	ARG	2.9
1	F	203	SER	2.9
1	E	196	VAL	2.9
1	D	184	ASN	2.9
1	B	209	ALA	2.9
1	B	191	ASP	2.9
1	D	98	ILE	2.9
1	E	209	ALA	2.9
1	A	198	ASP	2.8
1	D	152	ALA	2.8
1	E	53	GLY	2.8
1	A	36	ILE	2.8
1	B	192	LEU	2.8
1	C	157	VAL	2.8
1	D	26	VAL	2.8
1	B	118	ASN	2.8
1	F	207	ALA	2.8
1	F	122	LEU	2.8
1	D	158	THR	2.8
1	B	178	ALA	2.7
1	D	212	LEU	2.7
1	E	122	LEU	2.7
1	D	156	ASN	2.7
1	E	178	ALA	2.7
1	E	228	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	211	ALA	2.7
1	D	226	LEU	2.7
1	F	65	GLU	2.7
1	C	24	ARG	2.7
1	C	117	THR	2.7
1	E	197	SER	2.7
1	E	67	ASP	2.7
1	A	193	THR	2.6
1	A	23	PRO	2.6
1	D	7	ASN	2.6
1	E	191	ASP	2.6
1	F	209	ALA	2.6
1	F	199	THR	2.6
1	F	212	LEU	2.6
1	D	55	GLY	2.6
1	E	171	ALA	2.6
1	E	201	THR	2.6
1	F	174	THR	2.6
1	C	151	LEU	2.6
1	C	28	SER	2.6
1	F	27	PHE	2.6
1	B	196	VAL	2.6
1	B	206	GLN	2.6
1	C	169	VAL	2.6
1	E	151	LEU	2.6
1	F	115	LEU	2.6
1	F	10	VAL	2.5
1	D	229	HIS	2.5
1	C	96	LYS	2.5
1	A	199	THR	2.5
1	C	97	ALA	2.5
1	A	205	ILE	2.5
1	D	87	HIS	2.5
1	D	14	ALA	2.5
1	E	179	ALA	2.5
1	F	22	LEU	2.5
1	D	12	ILE	2.5
1	F	82	ILE	2.5
1	D	89	SER	2.5
1	B	56	ALA	2.5
1	D	4	PRO	2.5
1	E	154	PRO	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	27	PHE	2.5
1	F	8	ASN	2.5
1	F	26	VAL	2.4
1	B	129	ALA	2.4
1	C	145	ALA	2.4
1	D	228	ALA	2.4
1	B	91	ILE	2.4
1	B	114	SER	2.4
1	C	100	ALA	2.4
1	E	16	ARG	2.4
1	F	78	LYS	2.4
1	A	184	ASN	2.4
1	C	8	ASN	2.4
1	C	187	VAL	2.4
1	F	112	ILE	2.4
1	A	16	ARG	2.4
1	A	140	TYR	2.4
1	F	117	THR	2.4
1	E	226	LEU	2.4
1	D	3	ASP	2.4
1	E	169	VAL	2.4
1	D	73	HIS	2.4
1	D	71	ALA	2.3
1	D	6	LEU	2.3
1	A	71	ALA	2.3
1	F	192	LEU	2.3
1	B	24	ARG	2.3
1	C	185	LYS	2.3
1	A	27	PHE	2.3
1	A	188	PHE	2.3
1	C	188	PHE	2.3
1	C	119	VAL	2.3
1	D	68	VAL	2.3
1	D	154	PRO	2.3
1	B	225	ALA	2.3
1	E	224	ASP	2.3
1	F	6	LEU	2.3
1	F	191	ASP	2.3
1	C	20	SER	2.3
1	E	54	GLN	2.3
1	D	169	VAL	2.3
1	F	105	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	102	ASN	2.3
1	A	14	ALA	2.3
1	D	224	ASP	2.3
1	D	176	TRP	2.3
1	F	197	SER	2.2
1	A	213	ILE	2.2
1	F	187	VAL	2.2
1	D	62	LYS	2.2
1	E	19	ALA	2.2
1	C	150	SER	2.2
1	A	10	VAL	2.2
1	D	166	LYS	2.2
1	D	185	LYS	2.2
1	E	213	ILE	2.2
1	F	107	THR	2.2
1	B	171	ALA	2.2
1	D	25	ASN	2.2
1	F	198	ASP	2.2
1	E	135	ALA	2.2
1	F	19	ALA	2.2
1	A	203	SER	2.2
1	B	197	SER	2.2
1	D	210	ASN	2.2
1	D	77	ILE	2.1
1	A	37	ALA	2.1
1	C	190	ALA	2.1
1	D	46	ALA	2.1
1	D	209	ALA	2.1
1	F	145	ALA	2.1
1	C	134	SER	2.1
1	B	102	ASN	2.1
1	D	106	THR	2.1
1	A	173	GLN	2.1
1	D	36	ILE	2.1
1	E	164	GLY	2.1
1	C	93	ALA	2.1
1	D	121	ALA	2.1
1	A	142	SER	2.1
1	D	203	SER	2.1
1	E	172	ARG	2.1
1	E	150	SER	2.1
1	F	148	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	205	ILE	2.1
1	B	103	VAL	2.1
1	D	119	VAL	2.1
1	F	20	SER	2.1
1	D	217	ARG	2.0
1	F	172	ARG	2.0
1	D	174	THR	2.0
1	C	186	GLY	2.0
1	D	181	GLY	2.0
1	D	134	SER	2.0
1	E	89	SER	2.0
1	D	145	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.