



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:22 AM UTC

PDB ID : 1Z0V / pdb_00001z0v
Title : Crystal Structure of A. fulgidus Lon proteolytic domain
Authors : Dauter, Z.; Botos, I.; LaRonde-LeBlanc, N.; Wlodawer, A.
Deposited on : 2005-03-02
Resolution : 3.00 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

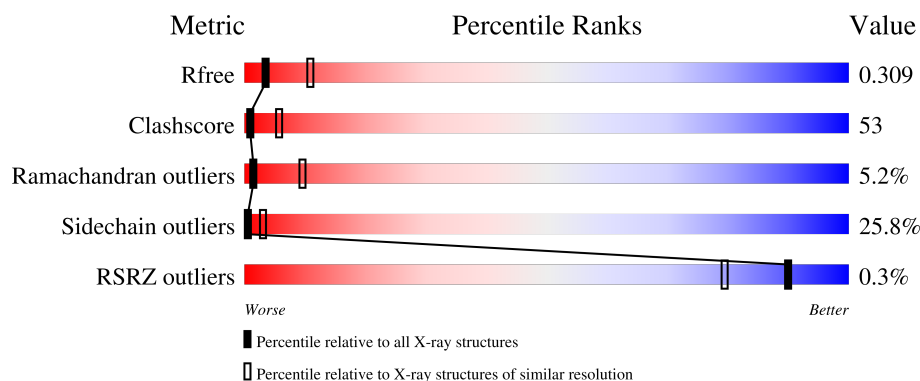
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	205	20% 34% 34% 7% 5%
1	B	205	12% 40% 30% 13% 5%
1	C	205	34% 35% 19% 7% 5%
1	D	205	26% 39% 24% 6% 5%
1	E	205	22% 38% 28% 7% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	205	22% 45% 23% 5% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9236 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 Putative protease La homolog type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1457	921	247	284	5			
1	B	195	Total	C	N	O	S	0	0	0
			1457	921	247	284	5			
1	C	194	Total	C	N	O	S	0	0	0
			1448	915	245	283	5			
1	D	195	Total	C	N	O	S	0	0	0
			1457	921	247	284	5			
1	E	195	Total	C	N	O	S	0	0	0
			1457	921	247	284	5			
1	F	195	Total	C	N	O	S	0	0	0
			1457	921	247	284	5			

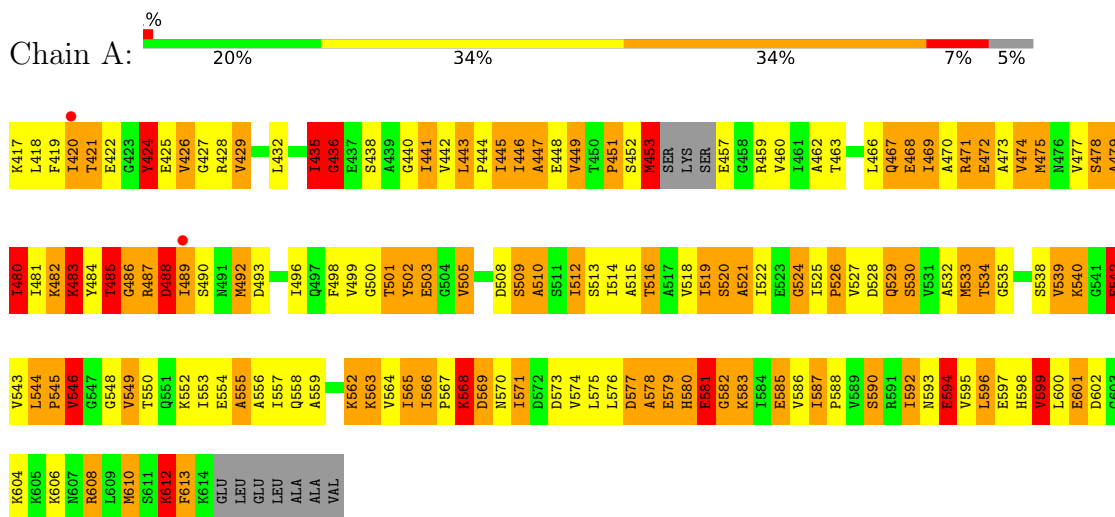
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	78	Total	O	0	0
			78	78		
2	B	74	Total	O	0	0
			74	74		
2	C	104	Total	O	0	0
			104	104		
2	D	99	Total	O	0	0
			99	99		
2	E	69	Total	O	0	0
			69	69		
2	F	79	Total	O	0	0
			79	79		

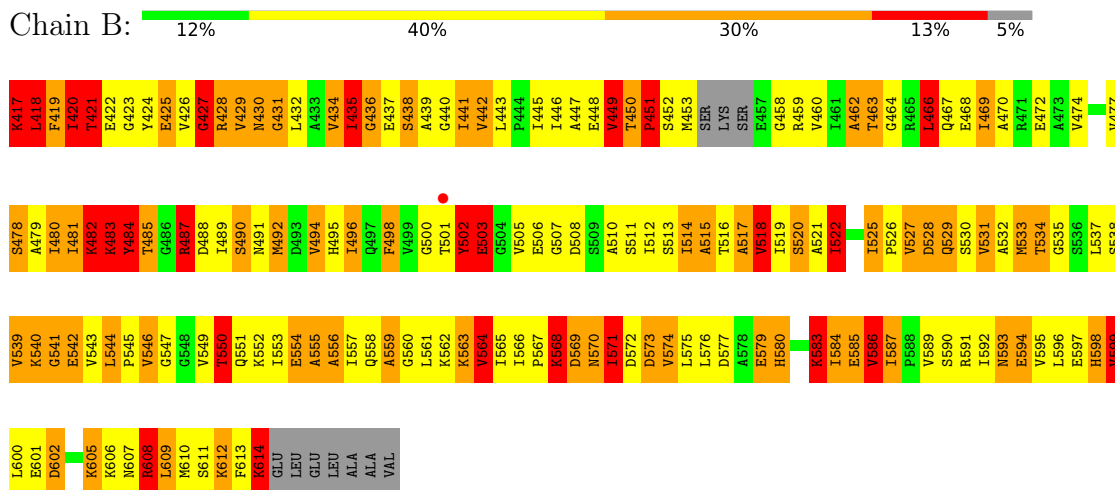
3 Residue-property plots

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

- Molecule 1: Putative protease La homolog type

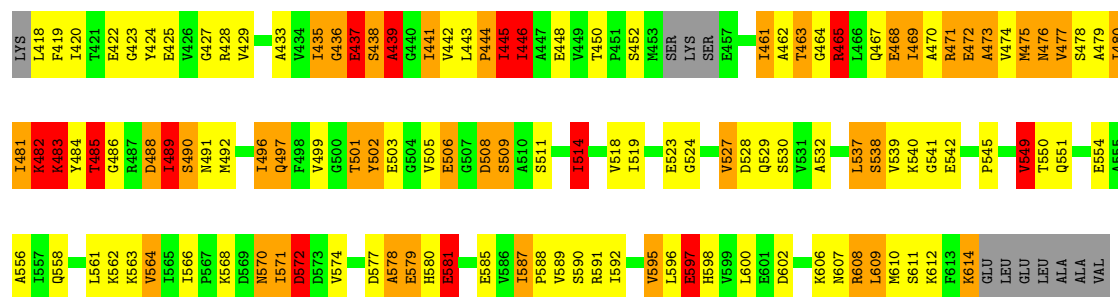


- Molecule 1: Putative protease La homolog type



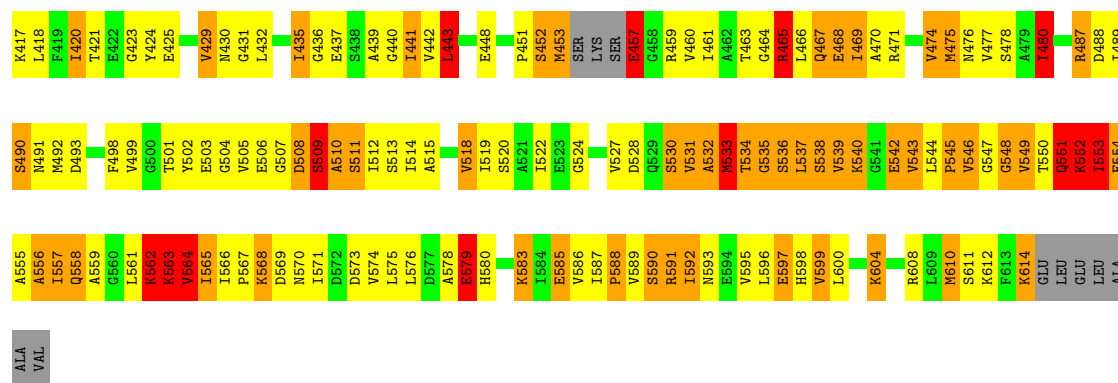
- Molecule 1: Putative protease La homolog type





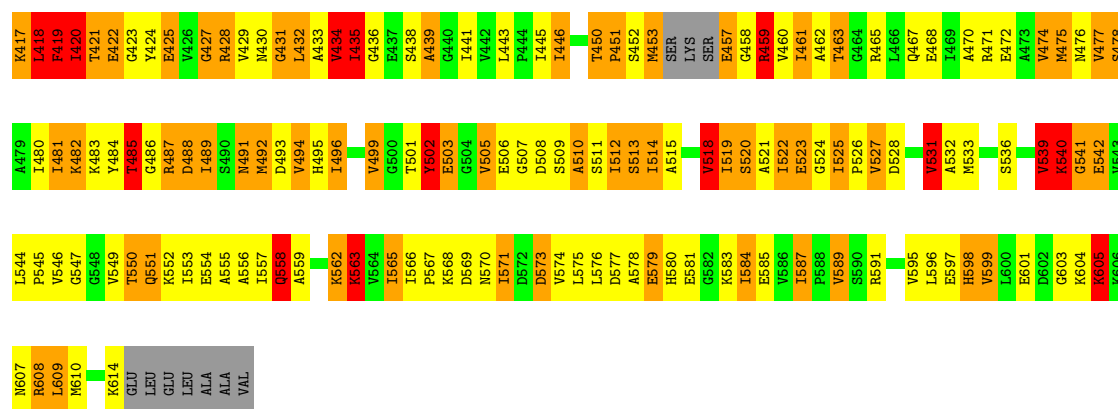
• Molecule 1: Putative protease La homolog type

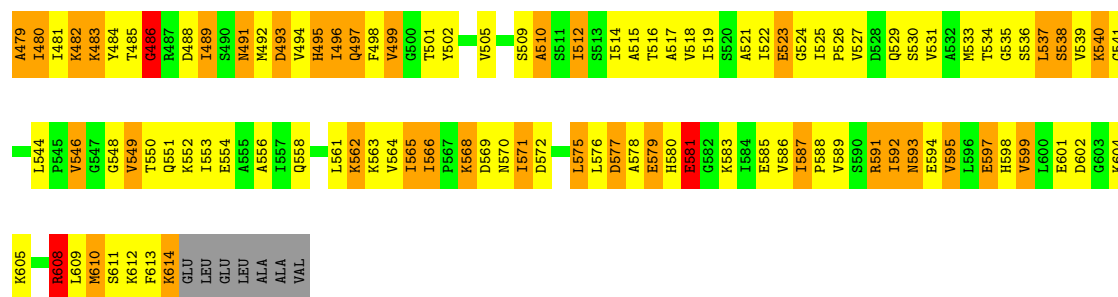
Chain D: 26% 39% 24% 6% 5%



• Molecule 1: Putative protease La homolog type

Chain E: 22% 38% 28% 7% 5%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.45Å 86.28Å 137.97Å 90.00° 92.30° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 15.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (15.00-3.00) 98.2 (15.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.90 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.215 , 0.310 0.215 , 0.309	Depositor DCC
R_{free} test set	1148 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.046 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9236	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4102e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	2.02	32/1470 (2.2%)	2.10	58/1983 (2.9%)
1	B	2.45	69/1470 (4.7%)	2.02	53/1983 (2.7%)
1	C	2.04	27/1461 (1.8%)	1.93	52/1972 (2.6%)
1	D	3.03	73/1470 (5.0%)	2.78	113/1983 (5.7%)
1	E	2.13	41/1470 (2.8%)	1.96	50/1983 (2.5%)
1	F	1.85	17/1470 (1.2%)	1.92	47/1983 (2.4%)
All	All	2.29	259/8811 (2.9%)	2.14	373/11887 (3.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	5
1	C	0	1
1	D	0	5
1	E	0	3
1	F	0	3
All	All	0	18

All (259) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	534	THR	C-O	28.45	1.60	1.23
1	D	532	ALA	C-N	25.54	1.66	1.33
1	D	531	VAL	C-N	24.14	1.67	1.33
1	D	532	ALA	C-O	20.76	1.49	1.23
1	D	563	LYS	N-CA	20.30	1.71	1.46
1	D	537	LEU	CA-C	-20.23	1.27	1.52
1	D	552	LYS	CE-NZ	19.70	2.08	1.49
1	D	531	VAL	N-CA	18.26	1.68	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	562	LYS	CA-C	17.90	1.76	1.52
1	D	563	LYS	CE-NZ	17.44	2.01	1.49
1	C	485	THR	CA-C	16.51	1.61	1.52
1	D	535	GLY	CA-C	-16.42	1.35	1.51
1	D	564	VAL	CA-CB	-16.09	1.35	1.54
1	D	532	ALA	N-CA	15.68	1.65	1.45
1	D	531	VAL	CA-CB	-15.34	1.35	1.53
1	D	536	SER	C-N	13.86	1.50	1.33
1	B	435	ILE	CA-CB	12.82	1.72	1.54
1	D	508	ASP	CB-CG	-12.33	1.21	1.52
1	B	418	LEU	CA-C	12.11	1.69	1.52
1	D	563	LYS	C-O	12.03	1.38	1.23
1	D	508	ASP	CA-C	11.92	1.67	1.52
1	B	462	ALA	CA-CB	11.91	1.69	1.53
1	D	534	THR	CA-CB	11.77	1.73	1.53
1	D	537	LEU	C-O	11.31	1.37	1.23
1	B	419	PHE	N-CA	11.23	1.59	1.46
1	D	532	ALA	CA-CB	-10.68	1.36	1.53
1	D	535	GLY	C-O	10.65	1.38	1.23
1	B	501	THR	CA-CB	10.18	1.66	1.53
1	A	453	MET	C-O	9.45	1.42	1.23
1	D	547	GLY	C-O	9.23	1.36	1.23
1	E	420	ILE	CA-CB	9.11	1.66	1.54
1	B	430	ASN	CA-CB	9.04	1.64	1.52
1	B	514	ILE	CA-CB	9.04	1.64	1.54
1	A	601	GLU	CA-C	8.82	1.63	1.52
1	E	522	ILE	CG1-CD1	8.82	1.86	1.51
1	B	525	ILE	CA-C	8.71	1.60	1.53
1	E	555	ALA	N-CA	8.55	1.57	1.46
1	D	530	SER	N-CA	8.41	1.57	1.46
1	B	520	SER	CA-C	8.39	1.63	1.52
1	D	568	LYS	CE-NZ	8.31	1.74	1.49
1	B	518	VAL	CA-CB	8.31	1.65	1.54
1	D	564	VAL	CA-C	-8.29	1.42	1.52
1	A	435	ILE	N-CA	8.27	1.55	1.46
1	A	443	LEU	C-O	8.27	1.34	1.24
1	D	509	SER	C-O	8.20	1.34	1.24
1	E	445	ILE	CA-C	8.18	1.62	1.52
1	B	420	ILE	CA-CB	8.10	1.65	1.54
1	D	533	MET	N-CA	-8.03	1.36	1.46
1	B	587	ILE	CA-CB	7.97	1.62	1.53
1	D	508	ASP	CG-OD1	-7.92	1.10	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	568	LYS	N-CA	7.84	1.56	1.46
1	E	566	ILE	C-O	7.81	1.29	1.24
1	B	484	TYR	CA-C	7.80	1.63	1.52
1	C	473	ALA	CA-C	7.79	1.63	1.52
1	D	551	GLN	C-O	7.77	1.33	1.24
1	E	519	ILE	CA-CB	-7.77	1.45	1.54
1	B	449	VAL	CA-C	7.74	1.61	1.52
1	D	565	ILE	CA-C	-7.73	1.43	1.52
1	D	543	VAL	N-CA	-7.60	1.37	1.46
1	D	562	LYS	C-O	7.58	1.33	1.24
1	D	562	LYS	CE-NZ	7.51	1.71	1.49
1	B	501	THR	C-O	7.47	1.32	1.24
1	D	533	MET	CG-SD	7.41	1.99	1.80
1	A	525	ILE	N-CA	7.38	1.54	1.46
1	C	483	LYS	CB-CG	7.38	1.74	1.52
1	C	469	ILE	CA-CB	7.36	1.65	1.54
1	D	452	SER	N-CA	7.35	1.55	1.46
1	B	612	LYS	CA-C	7.27	1.62	1.52
1	C	485	THR	N-CA	7.26	1.54	1.45
1	A	604	LYS	CD-CE	7.24	1.74	1.52
1	B	421	THR	N-CA	7.23	1.55	1.46
1	E	462	ALA	CA-CB	7.15	1.63	1.53
1	A	587	ILE	CA-CB	-7.14	1.49	1.54
1	B	419	PHE	CA-C	7.14	1.61	1.52
1	E	459	ARG	N-CA	7.10	1.54	1.46
1	E	499	VAL	CA-CB	7.10	1.62	1.54
1	B	450	THR	CA-CB	7.09	1.62	1.52
1	F	473	ALA	CA-C	7.07	1.61	1.52
1	B	574	VAL	C-O	7.04	1.31	1.23
1	C	468	GLU	CD-OE2	7.03	1.38	1.25
1	B	525	ILE	CA-CB	7.01	1.64	1.53
1	D	508	ASP	CG-OD2	6.94	1.38	1.25
1	A	483	LYS	CE-NZ	6.94	1.70	1.49
1	B	436	GLY	N-CA	6.94	1.55	1.45
1	C	445	ILE	CG1-CD1	6.91	1.78	1.51
1	B	576	LEU	CA-C	6.88	1.61	1.52
1	B	438	SER	N-CA	6.87	1.55	1.46
1	C	497	GLN	C-O	6.84	1.32	1.23
1	E	458	GLY	N-CA	6.82	1.52	1.45
1	A	515	ALA	CA-CB	-6.80	1.42	1.53
1	A	577	ASP	N-CA	6.79	1.54	1.46
1	E	467	GLN	CA-C	6.74	1.61	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	461	ILE	CA-CB	-6.72	1.46	1.54
1	F	494	VAL	CA-CB	6.71	1.62	1.54
1	B	527	VAL	CA-C	6.68	1.60	1.52
1	B	429	VAL	CA-C	6.68	1.61	1.52
1	A	480	ILE	CA-CB	6.68	1.61	1.54
1	B	563	LYS	CA-C	6.63	1.60	1.52
1	F	475	MET	SD-CE	6.62	1.96	1.79
1	F	537	LEU	CA-C	-6.58	1.44	1.52
1	A	546	VAL	N-CA	-6.57	1.39	1.46
1	D	599	VAL	N-CA	6.55	1.54	1.46
1	B	539	VAL	CA-CB	6.50	1.62	1.54
1	A	424	TYR	N-CA	6.49	1.54	1.45
1	C	581	GLU	C-O	6.48	1.32	1.24
1	C	443	LEU	N-CA	-6.47	1.40	1.46
1	B	420	ILE	N-CA	6.47	1.54	1.46
1	A	568	LYS	CE-NZ	6.45	1.68	1.49
1	E	587	ILE	CA-C	6.44	1.59	1.52
1	E	418	LEU	CA-C	6.42	1.61	1.52
1	F	445	ILE	CA-C	-6.40	1.47	1.52
1	D	559	ALA	CA-CB	-6.38	1.42	1.53
1	A	460	VAL	CA-CB	6.35	1.63	1.54
1	A	610	MET	CA-C	-6.30	1.44	1.52
1	D	552	LYS	CD-CE	-6.26	1.33	1.52
1	B	418	LEU	N-CA	6.26	1.54	1.46
1	C	468	GLU	CG-CD	6.25	1.67	1.52
1	B	564	VAL	CA-CB	6.25	1.61	1.53
1	D	585	GLU	C-O	6.20	1.31	1.23
1	E	527	VAL	CA-C	6.19	1.60	1.52
1	B	608	ARG	N-CA	6.19	1.54	1.46
1	A	489	ILE	CA-CB	6.16	1.62	1.54
1	D	507	GLY	C-O	6.16	1.29	1.23
1	B	602	ASP	N-CA	6.15	1.53	1.46
1	E	421	THR	CA-C	6.14	1.60	1.52
1	B	482	LYS	CA-C	6.13	1.61	1.52
1	B	458	GLY	N-CA	6.11	1.53	1.45
1	D	480	ILE	CB-CG2	6.03	1.72	1.52
1	B	586	VAL	CA-CB	6.02	1.62	1.54
1	B	485	THR	N-CA	6.01	1.53	1.46
1	E	604	LYS	CA-C	6.01	1.61	1.52
1	F	496	ILE	N-CA	-6.01	1.39	1.46
1	B	605	LYS	CB-CG	6.00	1.70	1.52
1	F	493	ASP	CA-C	6.00	1.59	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	536	SER	CB-OG	5.96	1.54	1.42
1	F	581	GLU	N-CA	5.95	1.53	1.45
1	A	420	ILE	CA-CB	5.94	1.61	1.54
1	B	421	THR	CA-C	5.92	1.60	1.52
1	D	610	MET	CA-C	-5.90	1.45	1.52
1	C	600	LEU	CA-C	5.90	1.60	1.52
1	D	588	PRO	C-N	-5.87	1.25	1.33
1	E	539	VAL	CA-CB	5.87	1.62	1.54
1	E	520	SER	CA-C	5.86	1.60	1.52
1	A	436	GLY	C-O	5.86	1.31	1.23
1	F	592	ILE	CA-C	-5.86	1.45	1.52
1	C	481	ILE	CA-CB	5.84	1.61	1.54
1	D	589	VAL	CA-C	5.83	1.60	1.52
1	B	449	VAL	N-CA	5.82	1.53	1.46
1	B	550	THR	CA-C	5.81	1.59	1.53
1	D	558	GLN	N-CA	5.81	1.53	1.46
1	D	460	VAL	CA-CB	-5.80	1.47	1.54
1	A	462	ALA	CA-CB	-5.80	1.44	1.53
1	B	472	GLU	N-CA	5.76	1.52	1.46
1	E	591	ARG	CZ-NH1	5.75	1.40	1.32
1	D	599	VAL	CA-CB	5.75	1.62	1.54
1	D	451	PRO	CA-C	5.74	1.59	1.52
1	C	562	LYS	CD-CE	5.74	1.69	1.52
1	D	542	GLU	C-O	5.74	1.30	1.23
1	D	545	PRO	C-O	-5.74	1.16	1.23
1	E	605	LYS	N-CA	5.70	1.53	1.46
1	C	591	ARG	N-CA	-5.70	1.38	1.45
1	B	587	ILE	N-CA	5.69	1.50	1.46
1	C	556	ALA	C-O	-5.68	1.17	1.24
1	B	459	ARG	N-CA	5.66	1.52	1.46
1	E	474	VAL	CA-CB	5.65	1.61	1.54
1	D	571	ILE	CA-CB	5.65	1.61	1.54
1	D	553	ILE	CA-CB	-5.65	1.46	1.54
1	F	587	ILE	CA-CB	5.64	1.61	1.54
1	D	540	LYS	CG-CD	5.63	1.69	1.52
1	D	468	GLU	CG-CD	5.62	1.66	1.52
1	E	421	THR	CA-CB	5.62	1.62	1.53
1	C	482	LYS	CG-CD	5.62	1.69	1.52
1	C	484	TYR	CA-C	5.62	1.58	1.52
1	E	495	HIS	CA-CB	-5.61	1.46	1.53
1	E	542	GLU	CB-CG	5.60	1.69	1.52
1	B	542	GLU	N-CA	5.58	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	602	ASP	N-CA	-5.57	1.39	1.46
1	D	591	ARG	N-CA	5.57	1.53	1.45
1	C	537	LEU	CA-C	-5.56	1.45	1.52
1	A	451	PRO	CA-C	5.56	1.60	1.52
1	A	574	VAL	CA-CB	5.55	1.59	1.53
1	A	604	LYS	CE-NZ	5.53	1.66	1.49
1	D	566	ILE	CA-C	5.52	1.58	1.52
1	D	452	SER	CA-C	5.51	1.59	1.52
1	C	595	VAL	C-O	5.51	1.30	1.24
1	E	432	LEU	N-CA	-5.50	1.39	1.45
1	E	604	LYS	N-CA	5.50	1.53	1.46
1	C	483	LYS	N-CA	5.49	1.53	1.46
1	C	598	HIS	N-CA	-5.46	1.38	1.46
1	B	593	ASN	N-CA	5.46	1.53	1.46
1	A	436	GLY	N-CA	5.45	1.53	1.45
1	E	525	ILE	CA-C	5.44	1.57	1.52
1	D	566	ILE	C-O	-5.41	1.20	1.24
1	F	509	SER	CB-OG	5.41	1.52	1.42
1	A	420	ILE	C-O	5.41	1.30	1.24
1	E	562	LYS	CD-CE	5.39	1.68	1.52
1	B	482	LYS	N-CA	5.39	1.53	1.46
1	D	597	GLU	CG-CD	5.38	1.65	1.52
1	F	440	GLY	N-CA	5.38	1.51	1.45
1	B	516	THR	CA-C	5.37	1.59	1.52
1	A	580	HIS	N-CA	5.37	1.53	1.46
1	E	465	ARG	NE-CZ	5.36	1.39	1.33
1	B	608	ARG	CG-CD	5.35	1.68	1.52
1	D	465	ARG	CZ-NH1	5.34	1.40	1.32
1	B	583	LYS	N-CA	5.31	1.53	1.46
1	E	420	ILE	CG1-CD1	5.30	1.72	1.51
1	E	532	ALA	CA-C	-5.30	1.46	1.52
1	E	427	GLY	N-CA	5.29	1.53	1.45
1	A	503	GLU	CA-C	5.29	1.59	1.52
1	B	450	THR	N-CA	5.29	1.51	1.46
1	B	591	ARG	CG-CD	5.27	1.68	1.52
1	D	534	THR	C-N	-5.25	1.26	1.32
1	E	558	GLN	CG-CD	5.25	1.65	1.52
1	B	460	VAL	CA-C	-5.24	1.46	1.52
1	B	563	LYS	N-CA	5.23	1.52	1.46
1	A	526	PRO	C-O	5.23	1.30	1.23
1	A	519	ILE	C-O	-5.22	1.18	1.24
1	F	497	GLN	C-O	5.22	1.30	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	528	ASP	N-CA	5.21	1.53	1.46
1	E	420	ILE	CA-C	5.20	1.59	1.52
1	D	488	ASP	CA-C	5.19	1.59	1.53
1	B	503	GLU	N-CA	-5.19	1.39	1.46
1	D	564	VAL	N-CA	5.18	1.52	1.46
1	A	435	ILE	CA-CB	5.16	1.62	1.55
1	A	581	GLU	C-O	5.16	1.30	1.24
1	D	423	GLY	N-CA	5.15	1.50	1.45
1	C	597	GLU	CA-CB	-5.14	1.45	1.53
1	E	518	VAL	CA-CB	5.14	1.61	1.54
1	A	612	LYS	CA-C	5.14	1.59	1.52
1	B	614	LYS	CE-NZ	5.14	1.64	1.49
1	E	608	ARG	CG-CD	5.14	1.67	1.52
1	D	530	SER	C-O	5.14	1.30	1.24
1	B	483	LYS	CA-C	5.14	1.57	1.52
1	E	531	VAL	C-O	5.13	1.30	1.24
1	E	428	ARG	CA-C	5.11	1.58	1.52
1	F	539	VAL	CA-CB	5.11	1.60	1.54
1	E	419	PHE	N-CA	5.09	1.52	1.46
1	E	429	VAL	CA-C	5.08	1.58	1.52
1	C	475	MET	SD-CE	5.08	1.92	1.79
1	B	449	VAL	CA-CB	5.07	1.62	1.55
1	B	427	GLY	N-CA	5.07	1.52	1.45
1	B	598	HIS	C-O	5.06	1.31	1.24
1	B	591	ARG	NE-CZ	5.06	1.38	1.33
1	B	535	GLY	C-O	5.05	1.29	1.23
1	D	480	ILE	N-CA	-5.05	1.39	1.46
1	D	436	GLY	N-CA	5.04	1.52	1.45
1	E	472	GLU	N-CA	5.04	1.52	1.46
1	C	572	ASP	N-CA	5.04	1.52	1.46
1	D	530	SER	C-N	5.03	1.39	1.33
1	F	517	ALA	N-CA	5.03	1.52	1.46
1	B	522	ILE	CA-CB	5.03	1.60	1.54
1	B	572	ASP	N-CA	5.03	1.52	1.46
1	B	442	VAL	CA-C	5.02	1.58	1.52
1	F	422	GLU	C-O	-5.02	1.17	1.23
1	B	599	VAL	CA-C	5.02	1.59	1.52
1	B	542	GLU	CB-CG	5.01	1.67	1.52
1	F	502	TYR	C-O	5.01	1.29	1.23
1	D	425	GLU	C-O	5.01	1.30	1.23
1	D	511	SER	N-CA	-5.00	1.39	1.46

All (373) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	534	THR	CB-CA-C	-26.27	67.69	109.99
1	D	552	LYS	N-CA-C	23.74	136.78	111.14
1	D	536	SER	O-C-N	-23.02	90.98	122.97
1	A	544	LEU	CA-C-N	21.66	142.09	119.78
1	A	544	LEU	C-N-CA	21.66	142.09	119.78
1	D	563	LYS	O-C-N	-20.27	99.03	123.36
1	D	537	LEU	CA-C-O	19.09	141.94	121.33
1	D	544	LEU	CA-C-N	14.30	134.48	119.89
1	D	544	LEU	C-N-CA	14.30	134.48	119.89
1	D	508	ASP	N-CA-C	-14.18	86.25	109.07
1	D	534	THR	CA-CB-OG1	-13.49	89.37	109.60
1	D	534	THR	CA-CB-CG2	13.37	133.22	110.50
1	D	531	VAL	CA-C-O	13.11	136.57	120.97
1	D	565	ILE	CB-CA-C	-13.10	93.02	110.84
1	B	460	VAL	N-CA-C	-12.99	88.97	107.80
1	D	531	VAL	O-C-N	-12.91	104.64	122.59
1	D	533	MET	N-CA-C	12.79	130.62	108.75
1	D	537	LEU	CD1-CG-CD2	-12.60	83.08	110.80
1	B	422	GLU	N-CA-C	-12.16	91.03	109.14
1	D	531	VAL	N-CA-CB	12.04	126.05	111.60
1	B	593	ASN	N-CA-C	11.80	126.78	112.38
1	E	571	ILE	CB-CA-C	-11.59	96.49	112.14
1	D	564	VAL	CA-C-O	11.51	132.88	120.57
1	D	535	GLY	N-CA-C	11.13	124.21	110.96
1	A	593	ASN	N-CA-C	-11.10	98.84	112.38
1	D	530	SER	N-CA-C	-10.97	99.16	112.54
1	A	480	ILE	CB-CA-C	10.89	125.91	111.87
1	F	483	LYS	N-CA-C	10.86	124.20	111.71
1	C	485	THR	N-CA-C	10.79	125.28	108.12
1	E	563	LYS	N-CA-C	10.73	125.39	109.07
1	D	537	LEU	CB-CA-C	-10.56	87.74	110.45
1	D	534	THR	O-C-N	-10.51	112.42	123.56
1	D	537	LEU	O-C-N	-10.46	111.32	123.25
1	B	449	VAL	N-CA-C	10.40	123.29	108.42
1	D	508	ASP	O-C-N	-10.37	111.05	123.29
1	D	549	VAL	N-CA-C	10.34	121.21	110.36
1	D	535	GLY	CA-C-O	-10.23	111.81	122.05
1	D	452	SER	N-CA-C	10.22	126.27	112.68
1	E	459	ARG	N-CA-C	10.05	124.65	108.76
1	D	566	ILE	CB-CA-C	-9.90	99.20	109.89
1	D	508	ASP	OD1-CG-OD2	9.79	146.38	122.90
1	F	518	VAL	N-CA-C	-9.56	101.55	110.82
1	D	534	THR	CA-C-O	9.46	131.34	120.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	599	VAL	N-CA-C	9.31	119.44	111.90
1	D	511	SER	CB-CA-C	9.26	121.19	109.80
1	B	541	GLY	N-CA-C	9.25	128.31	115.27
1	C	452	SER	N-CA-C	9.05	125.43	113.30
1	D	530	SER	CA-C-O	9.05	130.52	119.38
1	B	520	SER	N-CA-C	9.03	122.04	111.02
1	D	508	ASP	N-CA-CB	9.02	124.72	110.57
1	E	532	ALA	N-CA-C	-8.93	95.84	109.41
1	B	525	ILE	CB-CA-C	8.76	119.09	110.94
1	D	532	ALA	O-C-N	8.59	132.69	123.06
1	D	536	SER	N-CA-CB	8.43	123.26	110.70
1	B	514	ILE	N-CA-C	8.42	118.47	110.30
1	D	587	ILE	CB-CA-C	-8.37	101.23	110.52
1	E	419	PHE	N-CA-C	8.25	122.59	107.99
1	C	566	ILE	CA-C-N	-8.22	111.55	119.85
1	C	566	ILE	C-N-CA	-8.22	111.55	119.85
1	E	604	LYS	N-CA-C	8.22	122.56	112.54
1	F	502	TYR	N-CA-C	8.06	120.11	110.44
1	B	501	THR	CA-C-N	-8.04	110.41	122.47
1	B	501	THR	C-N-CA	-8.04	110.41	122.47
1	D	587	ILE	CA-C-N	-8.04	109.80	119.84
1	D	587	ILE	C-N-CA	-8.04	109.80	119.84
1	D	598	HIS	N-CA-C	-8.04	103.62	113.50
1	D	562	LYS	CA-C-N	7.99	133.54	121.40
1	D	562	LYS	C-N-CA	7.99	133.54	121.40
1	D	564	VAL	N-CA-CB	7.86	120.42	110.99
1	D	551	GLN	CA-C-O	7.86	129.31	120.90
1	C	585	GLU	CA-C-N	-7.84	112.93	123.12
1	C	585	GLU	C-N-CA	-7.84	112.93	123.12
1	A	559	ALA	N-CA-C	7.81	122.07	112.54
1	D	509	SER	CB-CA-C	-7.81	94.89	110.42
1	F	445	ILE	CB-CA-C	-7.80	99.94	112.03
1	D	562	LYS	O-C-N	-7.77	112.71	122.27
1	F	446	ILE	CB-CA-C	-7.77	98.54	111.29
1	D	565	ILE	CA-C-O	7.76	128.87	120.57
1	F	479	ALA	N-CA-C	-7.75	94.30	110.80
1	B	544	LEU	CA-C-N	7.72	129.50	119.84
1	B	544	LEU	C-N-CA	7.72	129.50	119.84
1	E	519	ILE	N-CA-C	-7.70	101.84	110.62
1	B	533	MET	N-CA-C	7.66	120.17	108.52
1	F	435	ILE	N-CA-C	7.66	119.88	108.54
1	C	489	ILE	N-CA-C	7.66	118.43	110.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	602	ASP	N-CA-C	7.66	121.51	110.10
1	D	537	LEU	CB-CG-CD1	7.63	133.60	110.70
1	E	584	ILE	N-CA-C	7.61	117.80	108.06
1	B	462	ALA	N-CA-C	7.58	118.28	108.34
1	B	515	ALA	CA-C-N	-7.55	109.56	120.29
1	B	515	ALA	C-N-CA	-7.55	109.56	120.29
1	D	564	VAL	O-C-N	-7.52	114.69	123.03
1	A	479	ALA	N-CA-C	-7.51	102.13	111.75
1	E	523	GLU	CB-CA-C	7.47	123.73	110.81
1	A	583	LYS	CA-C-N	-7.43	112.00	122.71
1	A	583	LYS	C-N-CA	-7.43	112.00	122.71
1	E	478	SER	N-CA-C	7.43	123.63	111.37
1	E	476	ASN	N-CA-C	-7.38	102.61	111.69
1	D	552	LYS	N-CA-CB	-7.36	99.39	110.07
1	E	566	ILE	N-CA-C	7.35	115.22	109.19
1	A	460	VAL	N-CA-C	-7.34	98.22	108.27
1	E	598	HIS	CB-CA-C	-7.31	98.21	110.56
1	B	574	VAL	CB-CA-C	-7.27	103.38	111.23
1	D	608	ARG	N-CA-C	-7.27	102.75	111.69
1	F	591	ARG	N-CA-C	7.25	121.35	109.24
1	D	531	VAL	CA-CB-CG1	-7.24	98.09	110.40
1	D	548	GLY	N-CA-C	7.24	126.23	115.08
1	D	546	VAL	CA-C-N	-7.24	112.36	120.53
1	D	546	VAL	C-N-CA	-7.24	112.36	120.53
1	D	443	LEU	N-CA-C	-7.22	92.03	108.27
1	F	610	MET	N-CA-C	7.21	119.14	111.28
1	C	471	ARG	N-CA-C	7.19	119.98	111.71
1	B	554	GLU	N-CA-C	7.19	122.44	112.45
1	D	564	VAL	N-CA-C	-7.12	98.18	108.36
1	F	493	ASP	N-CA-C	7.12	120.53	109.07
1	E	462	ALA	N-CA-C	7.12	117.66	108.34
1	F	425	GLU	N-CA-C	7.11	119.73	109.14
1	E	481	ILE	N-CA-CB	7.09	118.85	110.55
1	D	565	ILE	O-C-N	-7.06	115.19	123.03
1	E	424	TYR	N-CA-C	-7.01	97.19	108.55
1	F	571	ILE	N-CA-C	7.01	117.12	110.74
1	C	514	ILE	N-CA-C	-7.00	103.64	110.72
1	D	564	VAL	CB-CA-C	-7.00	101.32	110.84
1	B	459	ARG	N-CA-C	6.98	119.79	108.76
1	D	558	GLN	N-CA-C	6.98	119.78	111.33
1	D	441	ILE	CB-CA-C	-6.98	102.10	111.80
1	D	563	LYS	CD-CE-NZ	-6.97	89.60	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	555	ALA	N-CA-C	6.97	121.04	112.54
1	C	562	LYS	N-CA-C	6.92	118.61	111.14
1	D	532	ALA	N-CA-C	-6.89	99.37	110.32
1	F	512	ILE	CB-CA-C	-6.88	101.11	112.26
1	D	552	LYS	CB-CA-C	-6.87	100.04	110.90
1	B	498	PHE	CA-C-N	-6.87	113.63	123.11
1	B	498	PHE	C-N-CA	-6.87	113.63	123.11
1	E	512	ILE	N-CA-C	6.86	117.56	110.36
1	D	515	ALA	N-CA-C	-6.86	103.81	111.28
1	B	494	VAL	CB-CA-C	6.84	119.94	111.25
1	C	445	ILE	CB-CA-C	-6.82	101.08	110.90
1	C	442	VAL	N-CA-C	-6.82	100.79	109.58
1	C	437	GLU	N-CA-C	6.81	125.31	110.80
1	A	502	TYR	N-CA-C	6.78	118.10	108.54
1	E	527	VAL	N-CA-C	6.77	117.87	108.12
1	B	487	ARG	N-CA-C	6.76	120.90	110.42
1	F	577	ASP	N-CA-C	6.76	118.57	110.19
1	D	536	SER	CB-CA-C	-6.76	98.33	110.36
1	F	434	VAL	N-CA-C	6.75	118.52	108.46
1	D	534	THR	CA-C-N	6.74	132.06	121.62
1	D	534	THR	C-N-CA	6.74	132.06	121.62
1	D	552	LYS	CA-C-O	-6.71	113.79	120.70
1	E	514	ILE	N-CA-C	6.71	117.20	110.23
1	A	601	GLU	N-CA-C	6.69	119.68	110.24
1	E	540	LYS	N-CA-C	-6.68	105.53	113.21
1	A	599	VAL	CB-CA-C	-6.67	104.90	111.30
1	C	445	ILE	N-CA-C	6.64	119.35	108.99
1	F	544	LEU	CA-C-N	-6.63	113.81	120.31
1	F	544	LEU	C-N-CA	-6.63	113.81	120.31
1	A	515	ALA	N-CA-C	-6.62	104.09	111.71
1	D	532	ALA	N-CA-CB	6.62	121.19	110.41
1	E	507	GLY	N-CA-C	-6.58	103.16	112.37
1	D	551	GLN	N-CA-C	-6.57	103.23	111.11
1	D	589	VAL	CB-CA-C	-6.54	100.56	111.29
1	C	538	SER	CA-CB-OG	-6.54	98.02	111.10
1	E	581	GLU	N-CA-C	6.53	120.05	108.24
1	B	428	ARG	N-CA-C	6.52	119.11	108.55
1	E	451	PRO	N-CA-C	-6.52	99.04	112.47
1	D	566	ILE	O-C-N	-6.51	117.16	121.72
1	A	453	MET	CA-C-O	-6.46	109.82	120.80
1	A	488	ASP	N-CA-C	-6.46	98.20	108.73
1	A	472	GLU	N-CA-C	-6.46	103.93	110.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	599	VAL	N-CA-C	6.45	122.75	109.34
1	B	539	VAL	N-CA-C	6.43	116.58	110.53
1	F	523	GLU	N-CA-C	-6.42	103.89	112.94
1	D	508	ASP	CB-CG-OD1	-6.36	103.77	118.40
1	A	555	ALA	CA-C-N	6.36	131.18	120.88
1	A	555	ALA	C-N-CA	6.36	131.18	120.88
1	D	590	SER	CB-CA-C	-6.32	97.84	110.42
1	A	534	THR	N-CA-C	6.31	118.77	108.55
1	D	441	ILE	N-CA-C	6.28	116.55	107.88
1	D	475	MET	CA-C-O	-6.28	114.19	120.90
1	E	541	GLY	N-CA-C	6.26	124.54	114.90
1	E	478	SER	CA-CB-OG	-6.23	98.64	111.10
1	D	502	TYR	N-CA-C	6.21	118.74	108.49
1	C	587	ILE	N-CA-C	6.20	114.80	107.73
1	A	566	ILE	CA-C-N	-6.20	113.38	119.76
1	A	566	ILE	C-N-CA	-6.20	113.38	119.76
1	B	568	LYS	N-CA-CB	6.20	120.96	110.49
1	D	478	SER	CA-C-N	6.16	128.85	120.54
1	D	478	SER	C-N-CA	6.16	128.85	120.54
1	C	444	PRO	CA-C-O	-6.16	114.35	121.86
1	E	554	GLU	CB-CA-C	6.15	120.95	110.74
1	A	438	SER	N-CA-C	6.11	123.82	110.80
1	A	542	GLU	CA-C-N	-6.11	114.73	122.37
1	A	542	GLU	C-N-CA	-6.11	114.73	122.37
1	D	562	LYS	CA-C-O	6.09	126.98	119.97
1	A	577	ASP	N-CA-C	6.06	119.52	109.46
1	B	488	ASP	N-CA-C	6.06	118.29	107.80
1	B	452	SER	N-CA-C	6.05	118.69	109.62
1	C	474	VAL	CB-CA-C	-6.04	104.23	111.97
1	D	569	ASP	N-CA-C	-5.97	105.95	113.18
1	B	498	PHE	N-CA-C	5.97	119.40	110.14
1	A	574	VAL	CB-CA-C	-5.97	105.47	111.80
1	B	481	ILE	N-CA-C	5.95	116.07	110.30
1	F	438	SER	CA-C-N	5.95	130.28	120.94
1	F	438	SER	C-N-CA	5.95	130.28	120.94
1	C	446	ILE	N-CA-C	-5.94	99.93	108.48
1	A	474	VAL	CB-CA-C	-5.93	104.47	111.94
1	C	502	TYR	N-CA-C	5.93	117.67	109.54
1	A	445	ILE	CB-CA-C	-5.93	101.86	110.63
1	A	530	SER	N-CA-C	-5.92	105.24	112.88
1	C	483	LYS	N-CA-C	5.91	123.39	110.80
1	F	476	ASN	CB-CA-C	5.88	122.11	110.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	524	GLY	CA-C-N	-5.87	116.92	123.02
1	C	524	GLY	C-N-CA	-5.87	116.92	123.02
1	B	585	GLU	N-CA-C	5.86	118.41	109.62
1	F	571	ILE	N-CA-CB	5.85	117.66	110.64
1	C	468	GLU	CB-CA-C	5.85	121.42	109.67
1	E	495	HIS	CA-CB-CG	-5.84	107.95	113.80
1	C	597	GLU	CB-CA-C	-5.84	101.15	110.84
1	C	590	SER	CA-C-N	-5.83	113.65	122.81
1	C	590	SER	C-N-CA	-5.83	113.65	122.81
1	E	565	ILE	N-CA-C	5.81	117.70	108.87
1	D	493	ASP	N-CA-C	-5.81	101.02	110.20
1	E	573	ASP	N-CA-C	-5.80	105.86	113.17
1	D	566	ILE	N-CA-CB	5.80	118.25	111.87
1	A	594	GLU	N-CA-C	5.79	120.19	113.18
1	D	599	VAL	N-CA-C	5.79	121.38	109.34
1	F	439	ALA	N-CA-C	5.79	118.66	110.50
1	C	442	VAL	CA-C-N	-5.77	115.82	122.52
1	C	442	VAL	C-N-CA	-5.77	115.82	122.52
1	A	486	GLY	N-CA-C	5.77	126.86	113.18
1	F	494	VAL	N-CA-C	5.77	116.41	107.99
1	D	574	VAL	CB-CA-C	-5.77	103.60	111.33
1	D	565	ILE	CA-CB-CG1	5.76	120.20	110.40
1	B	525	ILE	N-CA-CB	5.75	116.38	110.23
1	E	430	ASN	N-CA-C	5.74	118.02	108.20
1	B	556	ALA	N-CA-C	5.74	119.54	112.54
1	F	538	SER	CA-CB-OG	-5.73	99.64	111.10
1	B	594	GLU	N-CA-C	-5.73	106.29	113.28
1	E	494	VAL	N-CA-C	5.71	116.84	107.24
1	D	538	SER	CB-CA-C	-5.71	99.51	110.24
1	E	589	VAL	N-CA-C	5.71	116.50	108.17
1	D	474	VAL	CB-CA-C	-5.70	104.55	112.02
1	D	518	VAL	CA-C-O	-5.70	115.13	121.17
1	F	554	GLU	N-CA-C	5.69	118.69	111.69
1	C	496	ILE	CB-CA-C	-5.68	102.37	110.83
1	F	441	ILE	CB-CA-C	-5.67	100.57	110.38
1	F	514	ILE	CA-C-N	-5.67	112.73	120.44
1	F	514	ILE	C-N-CA	-5.67	112.73	120.44
1	A	555	ALA	O-C-N	5.64	128.63	122.20
1	F	569	ASP	N-CA-C	5.64	119.88	112.89
1	C	423	GLY	N-CA-C	-5.64	104.14	111.52
1	A	596	LEU	N-CA-C	-5.63	105.05	111.07
1	B	466	LEU	N-CA-C	5.62	118.92	112.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	450	THR	CA-C-N	5.62	125.60	120.21
1	C	450	THR	C-N-CA	5.62	125.60	120.21
1	F	477	VAL	N-CA-C	5.60	121.00	109.34
1	B	586	VAL	CA-C-N	5.59	126.61	122.59
1	B	586	VAL	C-N-CA	5.59	126.61	122.59
1	D	504	GLY	N-CA-C	-5.58	106.30	114.90
1	D	512	ILE	CA-C-N	-5.56	111.86	120.31
1	D	512	ILE	C-N-CA	-5.56	111.86	120.31
1	B	568	LYS	CA-CB-CG	5.55	125.21	114.10
1	B	527	VAL	N-CA-C	5.54	117.38	108.85
1	C	450	THR	N-CA-C	-5.54	101.63	110.10
1	F	536	SER	CA-C-N	-5.54	114.38	122.19
1	F	536	SER	C-N-CA	-5.54	114.38	122.19
1	D	429	VAL	CA-C-N	-5.53	114.28	122.41
1	D	429	VAL	C-N-CA	-5.53	114.28	122.41
1	B	542	GLU	N-CA-C	5.53	118.83	109.76
1	A	579	GLU	N-CA-CB	5.53	118.25	110.12
1	B	555	ALA	CA-C-N	5.52	129.93	120.72
1	B	555	ALA	C-N-CA	5.52	129.93	120.72
1	F	440	GLY	N-CA-C	5.50	121.52	111.12
1	D	556	ALA	N-CA-C	5.50	117.36	111.36
1	E	522	ILE	CB-CA-C	-5.50	104.87	112.24
1	C	484	TYR	N-CA-C	-5.50	105.68	112.72
1	C	608	ARG	CB-CG-CD	-5.48	98.70	111.30
1	F	467	GLN	CA-CB-CG	5.48	125.06	114.10
1	C	541	GLY	N-CA-C	5.47	123.61	113.76
1	F	608	ARG	N-CA-C	-5.47	106.73	113.41
1	E	608	ARG	N-CA-C	-5.47	105.47	111.82
1	D	604	LYS	CA-C-N	5.46	127.59	120.28
1	D	604	LYS	C-N-CA	5.46	127.59	120.28
1	B	538	SER	CA-C-O	-5.46	115.66	121.94
1	E	522	ILE	CA-C-N	-5.44	113.62	122.65
1	E	522	ILE	C-N-CA	-5.44	113.62	122.65
1	C	468	GLU	CA-CB-CG	5.43	124.96	114.10
1	A	514	ILE	N-CA-C	5.43	115.63	110.53
1	D	536	SER	CA-C-N	-5.42	112.36	121.75
1	D	536	SER	C-N-CA	-5.42	112.36	121.75
1	A	545	PRO	CA-C-N	-5.42	116.04	122.11
1	A	545	PRO	C-N-CA	-5.42	116.04	122.11
1	C	530	SER	CA-C-N	-5.41	115.64	123.11
1	C	530	SER	C-N-CA	-5.41	115.64	123.11
1	E	511	SER	CA-C-N	5.41	127.58	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	511	SER	C-N-CA	5.41	127.58	120.60
1	F	585	GLU	CA-C-N	-5.41	115.61	122.37
1	F	585	GLU	C-N-CA	-5.41	115.61	122.37
1	D	501	THR	CA-C-N	-5.40	115.79	123.03
1	D	501	THR	C-N-CA	-5.40	115.79	123.03
1	A	520	SER	N-CA-C	5.39	117.58	111.11
1	B	485	THR	N-CA-C	5.38	122.26	110.80
1	A	580	HIS	N-CA-C	5.37	119.09	112.54
1	E	502	TYR	N-CA-C	5.37	117.98	109.50
1	F	432	LEU	N-CA-C	-5.37	100.28	108.76
1	F	467	GLN	N-CA-C	5.37	118.93	112.38
1	F	591	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	E	465	ARG	N-CA-C	-5.34	105.62	111.82
1	A	449	VAL	N-CA-C	5.34	115.40	108.35
1	C	537	LEU	CA-C-N	-5.34	113.28	123.32
1	C	537	LEU	C-N-CA	-5.34	113.28	123.32
1	B	431	GLY	N-CA-C	-5.33	106.47	112.33
1	D	598	HIS	CB-CA-C	5.33	118.98	109.29
1	E	571	ILE	N-CA-CB	5.32	117.77	110.54
1	B	517	ALA	O-C-N	5.31	127.75	122.12
1	D	429	VAL	N-CA-C	5.31	116.31	108.45
1	A	587	ILE	CB-CA-C	-5.30	104.98	110.13
1	E	485	THR	CB-CA-C	5.30	118.59	109.15
1	A	447	ALA	N-CA-C	5.30	117.61	109.07
1	D	554	GLU	CA-C-N	5.30	127.33	120.44
1	D	554	GLU	C-N-CA	5.30	127.33	120.44
1	C	589	VAL	N-CA-C	5.29	117.69	108.95
1	C	609	LEU	CB-CG-CD2	-5.29	94.82	110.70
1	A	441	ILE	N-CA-C	5.29	115.80	108.23
1	B	421	THR	N-CA-C	5.29	122.07	110.80
1	D	586	VAL	CB-CA-C	-5.29	104.56	110.96
1	E	550	THR	CA-C-N	5.28	127.36	120.28
1	E	550	THR	C-N-CA	5.28	127.36	120.28
1	E	605	LYS	N-CA-C	-5.28	106.52	113.12
1	D	565	ILE	CG1-CB-CG2	-5.27	94.89	110.70
1	A	608	ARG	N-CA-C	-5.26	104.98	111.40
1	D	467	GLN	N-CA-C	5.26	117.02	111.28
1	F	575	LEU	CA-CB-CG	5.26	134.72	116.30
1	C	529	GLN	N-CA-C	5.26	117.92	111.82
1	F	599	VAL	CB-CA-C	-5.26	102.67	111.29
1	D	430	ASN	CA-C-N	-5.25	115.63	121.83
1	D	430	ASN	C-N-CA	-5.25	115.63	121.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	503	GLU	N-CA-C	5.25	118.50	110.20
1	C	540	LYS	CD-CE-NZ	5.25	128.69	111.90
1	E	431	GLY	N-CA-C	-5.23	105.60	112.82
1	D	553	ILE	CA-CB-CG2	-5.22	101.62	110.50
1	A	463	THR	N-CA-C	-5.22	101.36	109.14
1	E	578	ALA	N-CA-C	-5.22	107.08	113.50
1	A	608	ARG	CG-CD-NE	5.21	123.47	112.00
1	A	565	ILE	CB-CA-C	-5.19	104.41	111.15
1	D	588	PRO	CA-C-O	5.18	130.02	120.60
1	B	535	GLY	CA-C-N	-5.17	114.94	122.65
1	B	535	GLY	C-N-CA	-5.17	114.94	122.65
1	C	523	GLU	N-CA-C	-5.17	106.97	113.28
1	A	524	GLY	CA-C-N	5.16	129.10	123.43
1	A	524	GLY	C-N-CA	5.16	129.10	123.43
1	C	483	LYS	CA-CB-CG	5.15	124.40	114.10
1	F	461	ILE	CB-CA-C	-5.15	101.80	110.71
1	E	503	GLU	N-CA-C	-5.14	100.66	109.24
1	A	521	ALA	N-CA-C	-5.13	105.34	111.03
1	A	512	ILE	CA-C-O	-5.12	115.72	121.05
1	A	586	VAL	CA-C-N	-5.10	118.89	123.33
1	A	586	VAL	C-N-CA	-5.10	118.89	123.33
1	F	568	LYS	N-CA-CB	5.09	117.70	110.06
1	D	537	LEU	N-CA-C	5.08	116.80	109.07
1	A	421	THR	N-CA-C	5.08	119.57	113.17
1	C	540	LYS	N-CA-C	-5.06	106.79	113.17
1	D	465	ARG	NE-CZ-NH2	-5.05	114.66	119.20
1	C	527	VAL	N-CA-C	5.04	116.56	108.89
1	A	575	LEU	N-CA-C	-5.04	101.49	109.96
1	F	568	LYS	N-CA-C	-5.04	105.23	111.33
1	A	505	VAL	N-CA-CB	5.03	116.21	110.72
1	E	501	THR	N-CA-C	5.03	117.33	107.57
1	B	502	TYR	CB-CA-C	5.03	118.37	111.23
1	C	439	ALA	N-CA-C	-5.02	100.11	110.80
1	B	430	ASN	N-CA-CB	5.00	118.16	110.60
1	C	475	MET	N-CA-C	-5.00	105.96	111.71
1	F	491	ASN	CB-CA-C	-5.00	99.77	110.32

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	485	THR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	B	417	LYS	Peptide
1	B	441	ILE	Peptide
1	B	451	PRO	Peptide
1	B	462	ALA	Peptide
1	B	585	GLU	Peptide
1	C	437	GLU	Peptide
1	D	457	GLU	Peptide
1	D	536	SER	Mainchain
1	D	552	LYS	Mainchain
1	D	563	LYS	Mainchain
1	D	580	HIS	Peptide
1	E	417	LYS	Peptide
1	E	434	VAL	Peptide
1	E	502	TYR	Peptide
1	F	484	TYR	Peptide
1	F	486	GLY	Peptide
1	F	577	ASP	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	1457	0	1523	169	0
1	B	1457	0	1523	236	0
1	C	1448	0	1510	142	0
1	D	1457	0	1523	137	0
1	E	1457	0	1523	159	0
1	F	1457	0	1523	156	1
2	A	78	0	0	12	0
2	B	74	0	0	13	0
2	C	104	0	0	6	0
2	D	99	0	0	10	0
2	E	69	0	0	13	0
2	F	79	0	0	11	0
All	All	9236	0	9125	946	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 53.

All (946) 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:562:LYS:C	1:D:562:LYS:CA	1.76	1.56
1:C:445:ILE:CD1	1:C:445:ILE:CG1	1.78	1.56
1:A:483:LYS:CE	1:A:483:LYS:NZ	1.70	1.55
1:D:531:VAL:N	1:D:531:VAL:CA	1.68	1.55
1:A:568:LYS:CE	1:A:568:LYS:NZ	1.68	1.55
1:C:483:LYS:CG	1:C:483:LYS:CB	1.74	1.55
1:D:563:LYS:N	1:D:563:LYS:CA	1.71	1.52
1:D:568:LYS:NZ	1:D:568:LYS:CE	1.74	1.51
1:D:531:VAL:C	1:D:532:ALA:N	1.67	1.50
1:D:562:LYS:CE	1:D:562:LYS:NZ	1.71	1.50
1:E:522:ILE:CD1	1:E:522:ILE:CG1	1.86	1.49
1:C:446:ILE:HD11	1:C:499:VAL:CG2	1.60	1.29
1:D:563:LYS:CE	1:D:563:LYS:NZ	2.01	1.24
1:B:481:ILE:HG23	1:B:485:THR:OG1	1.41	1.19
1:D:552:LYS:CE	1:D:552:LYS:NZ	2.08	1.17
1:F:428:ARG:HD2	1:F:446:ILE:HG23	1.28	1.13
1:A:487:ARG:HG3	1:A:487:ARG:HH11	1.07	1.12
1:B:563:LYS:HD3	1:B:587:ILE:HD11	1.31	1.12
1:B:449:VAL:HG13	1:B:521:ALA:HB1	1.15	1.11
1:A:540:LYS:HD2	2:A:689:HOH:O	1.51	1.10
1:B:492:MET:CE	1:B:522:ILE:HD11	1.81	1.10
1:A:544:LEU:HB3	1:A:545:PRO:HD2	1.33	1.10
1:B:492:MET:HE3	1:B:522:ILE:HD11	1.10	1.10
1:B:431:GLY:HA2	1:B:533:MET:O	1.52	1.09
1:F:492:MET:HE1	1:F:522:ILE:HG12	1.26	1.09
1:B:487:ARG:HH11	1:B:487:ARG:CG	1.65	1.09
1:B:487:ARG:HH11	1:B:487:ARG:HG3	0.91	1.06
1:A:428:ARG:HA	1:A:445:ILE:O	1.54	1.06
1:B:531:VAL:HG21	1:B:599:VAL:HG12	1.33	1.06
1:B:492:MET:HE3	1:B:522:ILE:CD1	1.86	1.05
1:D:537:LEU:HG	1:D:538:SER:N	1.49	1.05
1:A:535:GLY:HA2	1:A:546:VAL:HG11	1.37	1.05
1:C:578:ALA:HA	1:C:581:GLU:OE2	1.57	1.04
1:B:424:TYR:HA	1:B:527:VAL:O	1.57	1.04
1:C:446:ILE:HD11	1:C:499:VAL:HG23	1.05	1.03
1:B:487:ARG:HG3	1:B:487:ARG:NH1	1.63	1.03
1:E:453:MET:HG2	1:F:482:LYS:HD3	1.40	1.02
1:A:568:LYS:HB2	1:A:588:PRO:HB3	1.37	1.02
1:B:481:ILE:HG22	1:B:487:ARG:HB2	1.42	1.02
1:B:526:PRO:HG2	1:B:601:GLU:HB3	1.43	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:563:LYS:HB3	1:E:585:GLU:HB3	1.43	1.00
1:A:595:VAL:O	1:A:599:VAL:HG13	1.58	1.00
1:F:446:ILE:HD12	1:F:497:GLN:HB2	1.44	1.00
1:A:452:SER:O	1:A:453:MET:HB2	1.58	0.99
1:D:487:ARG:HG3	1:D:487:ARG:HH11	1.21	0.99
1:A:481:ILE:HD12	1:A:489:ILE:HD11	1.04	0.99
1:B:449:VAL:HG13	1:B:521:ALA:CB	1.92	0.99
1:E:478:SER:OG	1:E:489:ILE:HD11	1.63	0.98
1:B:489:ILE:HA	1:B:492:MET:HE1	1.45	0.98
1:F:435:ILE:HG22	1:F:505:VAL:HG22	1.45	0.98
1:E:450:THR:HG22	1:E:493:ASP:HB2	1.44	0.97
1:B:419:PHE:CZ	1:B:559:ALA:HA	1.98	0.97
1:A:481:ILE:HD12	1:A:489:ILE:CD1	1.93	0.97
1:A:487:ARG:HG3	1:A:487:ARG:NH1	1.75	0.96
1:E:494:VAL:CG1	1:E:496:ILE:HD11	1.96	0.96
1:F:435:ILE:HG13	1:F:439:ALA:HB3	1.46	0.95
1:E:435:ILE:CG2	1:E:441:ILE:HG23	1.97	0.95
1:E:453:MET:HG2	1:F:482:LYS:CD	1.96	0.95
1:C:446:ILE:CD1	1:C:499:VAL:HG23	1.96	0.95
1:F:478:SER:HA	1:F:481:ILE:HB	1.47	0.95
1:E:453:MET:CG	1:F:482:LYS:HD3	1.97	0.94
1:E:568:LYS:O	1:E:571:ILE:HG13	1.65	0.94
1:C:465:ARG:HD3	1:C:503:GLU:OE2	1.66	0.94
1:E:494:VAL:HG12	1:E:496:ILE:HD11	1.48	0.94
1:C:465:ARG:HB3	1:C:465:ARG:CZ	1.95	0.94
1:D:537:LEU:HG	1:D:538:SER:H	1.29	0.94
1:F:537:LEU:HG	1:F:538:SER:O	1.69	0.93
1:C:578:ALA:HA	1:C:581:GLU:CD	1.93	0.93
1:F:489:ILE:H	1:F:489:ILE:CD1	1.81	0.93
1:E:522:ILE:HG22	1:E:523:GLU:HG2	1.51	0.92
1:A:467:GLN:HG3	1:A:471:ARG:NH1	1.85	0.92
1:F:568:LYS:O	1:F:571:ILE:HG12	1.68	0.92
1:C:472:GLU:HG3	1:C:473:ALA:H	1.30	0.92
1:C:501:THR:HG21	2:D:666:HOH:O	1.67	0.92
1:E:491:ASN:HB3	1:E:492:MET:HE3	1.50	0.92
1:E:551:GLN:CD	1:E:551:GLN:H	1.75	0.91
1:C:446:ILE:CD1	1:C:499:VAL:CG2	2.47	0.91
1:D:424:TYR:CE1	1:D:528:ASP:HB2	2.06	0.90
1:D:542:GLU:OE2	1:D:591:ARG:HG3	1.72	0.90
1:E:577:ASP:OD1	1:E:580:HIS:N	2.05	0.89
1:F:553:ILE:O	1:F:556:ALA:HB3	1.72	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:489:ILE:H	1:F:489:ILE:HD13	1.36	0.88
1:A:481:ILE:CD1	1:A:489:ILE:HD11	1.98	0.88
1:D:542:GLU:OE2	1:D:591:ARG:CG	2.22	0.88
1:E:585:GLU:HG3	1:E:587:ILE:HD11	1.54	0.87
1:D:578:ALA:O	1:D:579:GLU:HB3	1.73	0.87
1:E:597:GLU:HG2	1:E:610:MET:CE	2.04	0.87
1:B:463:THR:HG22	2:B:643:HOH:O	1.74	0.87
1:A:418:LEU:HD13	1:A:500:GLY:HA3	1.56	0.87
1:D:461:ILE:HD13	1:E:475:MET:SD	2.14	0.86
1:B:553:ILE:HG23	1:B:564:VAL:HG11	1.56	0.86
1:F:476:ASN:O	1:F:478:SER:N	2.06	0.86
1:A:568:LYS:CB	1:A:588:PRO:HB3	2.06	0.86
1:C:463:THR:HG22	2:D:648:HOH:O	1.74	0.86
1:E:435:ILE:HG21	1:E:441:ILE:HG23	1.54	0.86
1:B:474:VAL:HA	1:B:477:VAL:HG12	1.58	0.85
1:C:608:ARG:C	1:C:608:ARG:HD3	2.00	0.85
1:A:554:GLU:HG3	2:A:673:HOH:O	1.77	0.84
1:B:419:PHE:HZ	1:B:559:ALA:HA	1.36	0.84
1:D:550:THR:O	1:D:554:GLU:HB2	1.76	0.84
1:E:417:LYS:HB3	1:E:419:PHE:H	1.41	0.84
1:E:487:ARG:HH11	1:E:487:ARG:HB3	1.43	0.84
1:D:465:ARG:H	1:D:465:ARG:HD2	1.42	0.84
1:D:534:THR:O	1:D:534:THR:HG23	1.77	0.83
1:D:562:LYS:NZ	1:D:562:LYS:CG	2.41	0.83
1:C:472:GLU:HG3	1:C:473:ALA:N	1.93	0.83
1:B:502:TYR:HB2	1:B:505:VAL:CG2	2.09	0.82
1:B:449:VAL:CG1	1:B:521:ALA:HB1	2.06	0.82
1:B:568:LYS:HG3	1:B:590:SER:HB2	1.62	0.82
1:F:492:MET:CE	1:F:522:ILE:HG12	2.09	0.82
1:F:446:ILE:CD1	1:F:497:GLN:HB2	2.09	0.82
1:A:418:LEU:HD13	1:A:500:GLY:CA	2.10	0.81
1:A:577:ASP:HB3	2:A:682:HOH:O	1.80	0.81
1:B:418:LEU:HD22	1:C:545:PRO:HG2	1.62	0.81
1:B:481:ILE:CG2	1:B:485:THR:OG1	2.27	0.81
1:B:425:GLU:HB2	1:B:529:GLN:NE2	1.96	0.80
1:A:449:VAL:H	1:B:540:LYS:HZ1	1.28	0.80
1:C:489:ILE:C	1:C:491:ASN:H	1.88	0.80
1:B:577:ASP:CG	1:B:580:HIS:HE1	1.90	0.80
1:A:581:GLU:O	1:A:583:LYS:N	2.15	0.79
1:A:558:GLN:HB2	2:A:693:HOH:O	1.82	0.79
1:A:470:ALA:O	1:A:474:VAL:HG23	1.83	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:MET:SD	1:A:522:ILE:HD11	2.23	0.79
1:B:525:ILE:HG23	1:B:526:PRO:HD2	1.62	0.79
1:D:551:GLN:HG3	2:D:702:HOH:O	1.82	0.79
1:E:597:GLU:HG2	1:E:610:MET:HE2	1.64	0.79
1:F:565:ILE:HA	1:F:587:ILE:O	1.82	0.79
1:A:542:GLU:OE2	1:A:542:GLU:HA	1.83	0.78
1:A:535:GLY:HA2	1:A:546:VAL:CG1	2.13	0.78
1:A:553:ILE:HG21	1:A:576:LEU:HD11	1.66	0.78
1:A:563:LYS:HG2	1:A:585:GLU:HB2	1.66	0.78
1:D:487:ARG:HH11	1:D:487:ARG:CG	1.96	0.78
1:F:434:VAL:O	1:F:505:VAL:HA	1.83	0.78
1:F:435:ILE:HG13	1:F:439:ALA:CB	2.13	0.78
1:A:528:ASP:OD1	1:A:530:SER:OG	2.02	0.78
1:A:534:THR:O	1:A:567:PRO:HD3	1.84	0.78
1:B:502:TYR:HB2	1:B:505:VAL:HG23	1.64	0.78
1:D:562:LYS:NZ	1:D:562:LYS:CD	2.45	0.77
1:D:489:ILE:HG21	1:D:522:ILE:CD1	2.14	0.77
1:A:519:ILE:HD13	1:A:596:LEU:HD11	1.66	0.77
1:C:465:ARG:CD	1:C:503:GLU:OE2	2.32	0.77
1:B:489:ILE:HA	1:B:492:MET:CE	2.15	0.77
1:B:449:VAL:CG1	1:B:521:ALA:CB	2.63	0.76
1:B:563:LYS:HD3	1:B:587:ILE:CD1	2.13	0.76
1:E:459:ARG:HG3	1:E:459:ARG:HH11	1.49	0.76
1:A:449:VAL:H	1:B:540:LYS:NZ	1.83	0.76
1:C:489:ILE:HD12	1:C:492:MET:HE2	1.67	0.76
1:E:482:LYS:HD3	2:E:675:HOH:O	1.84	0.76
1:A:487:ARG:HH11	1:A:487:ARG:CG	1.92	0.76
1:D:534:THR:OG1	1:D:535:GLY:N	2.12	0.76
1:C:608:ARG:HD3	1:C:608:ARG:O	1.85	0.76
1:B:577:ASP:OD2	1:B:580:HIS:HE1	1.69	0.76
1:F:579:GLU:O	1:F:580:HIS:HB2	1.86	0.76
1:B:494:VAL:CG1	1:B:496:ILE:HD11	2.15	0.76
1:F:431:GLY:O	1:F:432:LEU:HD23	1.86	0.76
1:C:428:ARG:CD	1:C:446:ILE:HG23	2.16	0.75
1:A:467:GLN:HG3	1:A:471:ARG:HH12	1.47	0.75
1:A:568:LYS:HB2	1:A:588:PRO:CB	2.15	0.75
1:C:448:GLU:OE2	1:D:539:VAL:HG13	1.87	0.75
1:C:437:GLU:OE1	1:C:437:GLU:HA	1.85	0.75
1:B:531:VAL:CG2	1:B:599:VAL:HG12	2.13	0.75
1:F:435:ILE:HG22	1:F:505:VAL:CG2	2.17	0.75
1:E:478:SER:OG	1:E:489:ILE:CD1	2.33	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:GLU:H	1:B:529:GLN:HE21	1.35	0.74
1:F:587:ILE:HG21	1:F:598:HIS:CD2	2.22	0.74
1:E:435:ILE:HD12	2:E:642:HOH:O	1.85	0.74
1:E:435:ILE:HG22	1:E:441:ILE:HG23	1.69	0.74
1:F:473:ALA:HA	1:F:510:ALA:HA	1.69	0.74
1:F:566:ILE:HD13	1:F:586:VAL:CG1	2.17	0.74
1:B:592:ILE:O	1:B:595:VAL:HB	1.87	0.74
1:C:475:MET:HB2	2:C:675:HOH:O	1.88	0.74
1:E:512:ILE:O	1:E:513:SER:C	2.31	0.74
1:F:428:ARG:HD2	1:F:446:ILE:CG2	2.15	0.74
1:E:453:MET:HG2	1:F:482:LYS:CE	2.17	0.73
1:B:469:ILE:HD12	1:B:507:GLY:HA3	1.68	0.73
1:C:532:ALA:HB2	1:C:561:LEU:HD13	1.70	0.73
1:A:475:MET:SD	1:F:461:ILE:HD13	2.28	0.73
1:E:531:VAL:HA	1:E:563:LYS:O	1.88	0.73
1:A:544:LEU:CB	1:A:545:PRO:HD2	1.92	0.73
1:F:608:ARG:O	1:F:612:LYS:HG3	1.89	0.73
1:B:480:ILE:HD13	1:B:592:ILE:HG21	1.70	0.73
1:E:435:ILE:HG13	1:E:436:GLY:N	2.03	0.73
1:B:558:GLN:C	1:B:560:GLY:N	2.46	0.73
1:E:453:MET:CG	1:F:482:LYS:HE2	2.19	0.73
1:F:538:SER:OG	1:F:541:GLY:N	2.22	0.73
1:A:478:SER:HA	1:A:489:ILE:HD12	1.70	0.73
1:B:521:ALA:HA	2:B:645:HOH:O	1.88	0.73
1:A:452:SER:O	1:A:453:MET:CB	2.36	0.72
1:C:578:ALA:CA	1:C:581:GLU:OE2	2.37	0.72
1:A:542:GLU:HG3	2:A:649:HOH:O	1.89	0.72
1:D:534:THR:O	1:D:534:THR:CG2	2.35	0.72
1:E:450:THR:CG2	1:E:493:ASP:HB2	2.19	0.72
1:E:563:LYS:CB	1:E:585:GLU:HB3	2.18	0.72
1:B:537:LEU:HD11	1:B:592:ILE:HB	1.71	0.72
1:F:566:ILE:HD13	1:F:586:VAL:HG11	1.70	0.72
1:A:520:SER:O	1:A:524:GLY:N	2.22	0.72
1:B:482:LYS:HG2	2:B:667:HOH:O	1.88	0.72
1:C:446:ILE:N	1:C:446:ILE:HD13	2.05	0.72
1:C:428:ARG:HD3	1:C:446:ILE:HG23	1.71	0.72
1:A:440:GLY:C	1:A:555:ALA:HB2	2.15	0.71
1:B:551:GLN:CD	1:B:551:GLN:H	1.98	0.71
1:F:442:VAL:HG12	1:F:444:PRO:HD3	1.71	0.71
1:E:587:ILE:HG22	1:E:589:VAL:CG1	2.19	0.71
1:B:438:SER:OG	1:B:551:GLN:HG2	1.89	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:ASP:CG	1:B:580:HIS:CE1	2.68	0.71
1:D:562:LYS:NZ	1:D:562:LYS:HG3	2.04	0.71
1:B:595:VAL:O	1:B:599:VAL:HG22	1.91	0.71
1:F:435:ILE:CG1	1:F:439:ALA:HB3	2.20	0.71
1:A:478:SER:CA	1:A:489:ILE:HD12	2.21	0.71
1:E:452:SER:N	1:E:491:ASN:O	2.23	0.71
1:D:489:ILE:HG21	1:D:522:ILE:HD11	1.72	0.71
1:D:520:SER:O	1:D:524:GLY:N	2.24	0.70
1:B:531:VAL:CG1	1:B:565:ILE:HG13	2.22	0.70
1:E:505:VAL:HG12	1:E:506:GLU:H	1.55	0.70
1:D:563:LYS:HG2	1:D:585:GLU:HB3	1.74	0.70
1:D:431:GLY:HA2	1:D:533:MET:O	1.91	0.70
1:D:487:ARG:HG3	1:D:487:ARG:NH1	2.02	0.70
1:F:480:ILE:CD1	1:F:592:ILE:HG21	2.22	0.70
1:E:431:GLY:HA2	1:E:513:SER:OG	1.92	0.70
1:F:591:ARG:O	1:F:594:GLU:HB2	1.92	0.69
1:E:551:GLN:CD	1:E:551:GLN:N	2.49	0.69
1:D:542:GLU:OE2	1:D:591:ARG:HG2	1.93	0.69
1:B:544:LEU:HB3	1:B:545:PRO:CD	2.22	0.69
1:B:508:ASP:HB2	1:B:511:SER:HB2	1.73	0.69
1:E:450:THR:O	1:E:492:MET:HA	1.92	0.69
1:A:445:ILE:HD11	2:A:637:HOH:O	1.92	0.69
1:C:489:ILE:C	1:C:491:ASN:N	2.51	0.69
1:B:525:ILE:CG2	1:B:526:PRO:HD2	2.23	0.69
1:A:420:ILE:HD11	1:A:428:ARG:NH2	2.07	0.68
1:A:417:LYS:HB3	2:A:690:HOH:O	1.91	0.68
1:E:553:ILE:CD1	1:E:574:VAL:HG13	2.22	0.68
1:A:440:GLY:HA3	1:A:555:ALA:HB2	1.74	0.68
1:D:549:VAL:O	1:D:553:ILE:HG13	1.94	0.68
1:B:435:ILE:CG2	1:B:503:GLU:O	2.42	0.68
1:E:553:ILE:HD12	1:E:574:VAL:HG13	1.76	0.68
1:A:581:GLU:C	1:A:583:LYS:H	2.01	0.67
1:B:470:ALA:HA	1:B:514:ILE:HD13	1.75	0.67
1:A:485:THR:HG23	1:A:485:THR:O	1.94	0.67
1:B:418:LEU:HD13	1:C:545:PRO:O	1.93	0.67
1:C:463:THR:CG2	1:D:469:ILE:HD11	2.25	0.67
1:E:481:ILE:HB	2:E:675:HOH:O	1.94	0.67
1:F:434:VAL:HB	1:F:439:ALA:O	1.95	0.67
1:D:429:VAL:HG22	1:D:527:VAL:HG11	1.76	0.67
1:D:435:ILE:HD11	1:D:439:ALA:HB3	1.77	0.67
1:A:532:ALA:O	1:A:564:VAL:HA	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:422:GLU:OE1	1:E:423:GLY:N	2.27	0.67
1:A:549:VAL:O	1:A:550:THR:C	2.37	0.67
1:D:514:ILE:CG2	2:D:714:HOH:O	2.42	0.67
1:C:472:GLU:OE1	1:C:509:SER:HB3	1.95	0.67
1:E:460:VAL:HB	1:E:471:ARG:HG2	1.76	0.67
1:E:571:ILE:O	1:E:574:VAL:HG23	1.95	0.67
1:A:545:PRO:HG2	1:F:499:VAL:HG13	1.74	0.66
1:F:432:LEU:HB3	1:F:552:LYS:HG2	1.77	0.66
1:B:479:ALA:HA	1:B:482:LYS:HE3	1.76	0.66
1:D:551:GLN:H	1:D:551:GLN:CD	2.03	0.66
1:F:462:ALA:HB2	1:F:496:ILE:HB	1.77	0.66
1:C:578:ALA:O	1:C:579:GLU:HB3	1.94	0.66
1:D:421:THR:HG22	1:D:561:LEU:HD21	1.77	0.66
1:D:532:ALA:O	1:D:565:ILE:N	2.24	0.66
1:C:482:LYS:HD3	1:C:488:ASP:HB2	1.78	0.66
1:A:581:GLU:O	1:A:583:LYS:HG3	1.96	0.66
1:D:563:LYS:NZ	1:D:563:LYS:CD	2.59	0.66
1:E:453:MET:HG3	1:F:482:LYS:HE2	1.76	0.66
1:B:435:ILE:HD11	1:B:441:ILE:CG2	2.26	0.66
1:D:461:ILE:HG21	1:E:475:MET:HE3	1.78	0.66
1:F:535:GLY:HA2	1:F:546:VAL:HG11	1.76	0.66
1:A:478:SER:CB	1:A:489:ILE:HD12	2.26	0.66
1:B:568:LYS:HD2	1:B:569:ASP:H	1.61	0.66
1:B:596:LEU:HD13	1:B:609:LEU:HD21	1.78	0.66
1:C:445:ILE:CD1	1:C:445:ILE:CB	2.71	0.66
1:F:437:GLU:HA	1:F:437:GLU:OE2	1.94	0.66
1:C:424:TYR:HA	1:C:527:VAL:O	1.96	0.65
1:D:519:ILE:HD13	1:D:596:LEU:HD11	1.79	0.65
1:E:491:ASN:HB3	1:E:492:MET:CE	2.26	0.65
1:F:489:ILE:HD13	1:F:489:ILE:N	2.10	0.65
1:F:566:ILE:CD1	1:F:586:VAL:HG11	2.26	0.65
1:B:577:ASP:OD1	1:B:580:HIS:CE1	2.48	0.65
1:B:557:ILE:O	1:B:560:GLY:HA2	1.97	0.65
1:C:418:LEU:HD12	1:D:545:PRO:HB2	1.78	0.65
1:E:605:LYS:O	1:E:609:LEU:N	2.27	0.65
1:F:530:SER:HB2	1:F:562:LYS:HG3	1.77	0.65
1:B:545:PRO:HA	1:B:567:PRO:HG2	1.77	0.65
1:C:597:GLU:HG2	1:C:610:MET:HE2	1.79	0.65
1:B:487:ARG:CG	1:B:487:ARG:NH1	2.34	0.65
1:D:467:GLN:HG3	1:D:471:ARG:NH2	2.12	0.65
1:F:467:GLN:CD	1:F:471:ARG:HH22	2.04	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:THR:O	1:A:485:THR:CG2	2.43	0.64
1:E:433:ALA:HB3	1:E:441:ILE:CG1	2.26	0.64
1:B:464:GLY:O	1:B:467:GLN:HG2	1.98	0.64
1:B:556:ALA:HA	1:B:559:ALA:HB3	1.77	0.64
1:B:478:SER:HB2	1:B:489:ILE:HG12	1.80	0.64
1:B:593:ASN:HB2	1:B:610:MET:HE1	1.80	0.64
1:F:477:VAL:CG2	1:F:515:ALA:HB1	2.27	0.64
1:A:566:ILE:HD11	1:A:571:ILE:HD12	1.80	0.64
1:D:424:TYR:HA	1:D:527:VAL:O	1.97	0.64
1:B:597:GLU:HG2	1:B:610:MET:HE2	1.80	0.64
1:D:465:ARG:HD2	1:D:465:ARG:N	2.10	0.64
1:F:477:VAL:HG13	1:F:481:ILE:HD12	1.80	0.64
1:A:440:GLY:CA	1:A:555:ALA:HB2	2.28	0.63
1:D:548:GLY:O	1:D:552:LYS:HG3	1.98	0.63
1:B:477:VAL:HG21	1:B:515:ALA:HB1	1.78	0.63
1:B:558:GLN:C	1:B:560:GLY:H	2.05	0.63
1:C:537:LEU:HD12	1:C:542:GLU:O	1.98	0.63
1:D:568:LYS:HE3	2:D:669:HOH:O	1.97	0.63
1:E:489:ILE:HG22	1:E:492:MET:SD	2.39	0.63
1:B:580:HIS:O	1:B:583:LYS:HB2	1.99	0.63
1:B:431:GLY:CA	1:B:513:SER:HB3	2.28	0.63
1:F:488:ASP:HB3	1:F:491:ASN:ND2	2.14	0.63
1:B:539:VAL:C	1:B:541:GLY:H	2.07	0.63
1:B:483:LYS:HG3	1:B:484:TYR:N	2.15	0.62
1:D:514:ILE:HG23	2:D:714:HOH:O	1.97	0.62
1:E:461:ILE:HG23	1:F:475:MET:HE2	1.79	0.62
1:D:552:LYS:C	1:D:554:GLU:N	2.57	0.62
1:F:593:ASN:O	1:F:610:MET:HE1	1.99	0.62
1:C:446:ILE:HD11	1:C:499:VAL:HG21	1.72	0.62
1:C:463:THR:CG2	1:C:464:GLY:N	2.61	0.62
1:D:531:VAL:N	1:D:531:VAL:HA	2.01	0.62
1:C:438:SER:OG	1:C:551:GLN:CD	2.43	0.62
1:C:445:ILE:C	1:C:446:ILE:HD13	2.24	0.62
1:D:465:ARG:NE	1:D:503:GLU:OE2	2.32	0.62
1:B:477:VAL:O	1:B:481:ILE:HD12	2.00	0.62
1:C:550:THR:O	1:C:554:GLU:HG3	1.99	0.62
1:C:606:LYS:C	1:C:608:ARG:N	2.55	0.62
1:D:562:LYS:HG3	1:D:562:LYS:HZ3	1.63	0.62
1:B:492:MET:CE	1:B:522:ILE:CD1	2.63	0.62
1:A:577:ASP:O	1:A:580:HIS:N	2.33	0.62
1:B:467:GLN:HG3	2:B:629:HOH:O	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:HIS:HA	1:B:583:LYS:HB2	1.80	0.61
1:E:451:PRO:O	1:E:452:SER:C	2.43	0.61
1:B:432:LEU:HB2	1:B:552:LYS:HD3	1.83	0.61
1:B:480:ILE:CD1	1:B:592:ILE:HG21	2.31	0.61
1:C:578:ALA:HA	1:C:581:GLU:OE1	2.01	0.61
1:E:523:GLU:O	1:E:525:ILE:HG13	2.00	0.61
1:F:588:PRO:C	1:F:589:VAL:HG13	2.26	0.61
1:A:474:VAL:HA	1:A:477:VAL:HG12	1.81	0.61
1:C:514:ILE:O	1:C:518:VAL:HG23	2.01	0.61
1:B:445:ILE:HD11	2:B:626:HOH:O	2.00	0.61
1:A:532:ALA:HB3	1:A:564:VAL:HB	1.83	0.61
1:B:553:ILE:O	1:B:556:ALA:HB3	2.00	0.61
1:F:435:ILE:CG2	1:F:505:VAL:HG22	2.27	0.61
1:F:588:PRO:C	1:F:589:VAL:CG1	2.74	0.61
1:A:548:GLY:O	1:A:552:LYS:HG3	2.00	0.60
1:E:420:ILE:H	1:E:428:ARG:HH21	1.49	0.60
1:B:503:GLU:OE1	1:B:503:GLU:HA	2.00	0.60
1:B:557:ILE:HD13	1:B:583:LYS:HB3	1.82	0.60
1:E:435:ILE:HB	2:E:642:HOH:O	2.00	0.60
1:E:435:ILE:HG23	1:E:439:ALA:O	2.01	0.60
1:A:425:GLU:H	1:A:527:VAL:H	1.48	0.60
1:C:467:GLN:O	1:C:470:ALA:HB3	2.01	0.60
1:A:428:ARG:HB2	1:A:529:GLN:OE1	2.00	0.60
1:C:608:ARG:C	1:C:608:ARG:CD	2.75	0.60
1:A:539:VAL:HG13	1:F:448:GLU:CD	2.27	0.60
1:E:494:VAL:HG12	1:E:496:ILE:CD1	2.29	0.60
1:E:597:GLU:CG	1:E:610:MET:HE2	2.31	0.60
1:B:448:GLU:HB3	1:C:539:VAL:HG23	1.83	0.60
1:A:449:VAL:N	1:B:540:LYS:HZ1	1.99	0.59
1:B:431:GLY:HA3	1:B:513:SER:CB	2.31	0.59
1:C:433:ALA:HB3	1:C:441:ILE:HD11	1.84	0.59
1:C:485:THR:OG1	1:C:486:GLY:N	2.35	0.59
1:B:557:ILE:HD12	1:B:580:HIS:HB3	1.84	0.59
1:C:461:ILE:HG21	1:D:475:MET:HE3	1.84	0.59
1:C:578:ALA:O	1:C:579:GLU:CB	2.50	0.59
1:D:578:ALA:O	1:D:579:GLU:CB	2.48	0.59
1:A:512:ILE:HG12	1:A:535:GLY:N	2.16	0.59
1:B:438:SER:O	1:B:551:GLN:HG2	2.02	0.59
1:B:495:HIS:CD2	1:C:479:ALA:HB2	2.38	0.59
1:A:477:VAL:HG22	1:A:477:VAL:O	2.02	0.59
1:B:481:ILE:HG22	1:B:487:ARG:CB	2.24	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:489:ILE:HG21	1:D:522:ILE:HD13	1.84	0.59
1:E:451:PRO:HA	1:E:492:MET:HG3	1.85	0.59
1:C:554:GLU:HB3	2:C:706:HOH:O	2.01	0.59
1:E:432:LEU:HB2	1:E:552:LYS:HD3	1.84	0.59
1:F:477:VAL:HG23	1:F:515:ALA:HB1	1.85	0.59
1:A:427:GLY:O	1:A:446:ILE:HA	2.03	0.59
1:C:497:GLN:OE1	1:D:509:SER:HB3	2.02	0.59
1:E:453:MET:CG	1:F:482:LYS:CD	2.70	0.59
1:B:580:HIS:C	1:B:583:LYS:HB2	2.27	0.59
1:D:457:GLU:HG3	1:D:490:SER:O	2.03	0.59
1:F:535:GLY:HA2	1:F:546:VAL:CG1	2.33	0.58
1:B:418:LEU:HD12	2:B:693:HOH:O	2.03	0.58
1:B:445:ILE:HD12	1:B:498:PHE:CD1	2.38	0.58
1:B:564:VAL:HG12	1:B:584:ILE:HG12	1.83	0.58
1:C:549:VAL:HG21	1:C:570:ASN:HB3	1.84	0.58
1:A:472:GLU:HG2	1:A:510:ALA:HB2	1.85	0.58
1:B:580:HIS:CA	1:B:583:LYS:HB2	2.34	0.58
1:C:445:ILE:CD1	1:C:445:ILE:CG2	2.81	0.58
1:F:591:ARG:HD2	2:F:691:HOH:O	2.01	0.58
1:C:463:THR:HG21	1:D:469:ILE:HD11	1.85	0.58
1:C:571:ILE:HD11	1:C:588:PRO:HG3	1.85	0.58
1:E:518:VAL:O	1:E:519:ILE:C	2.44	0.58
1:F:597:GLU:HG3	1:F:610:MET:HE2	1.85	0.58
1:D:530:SER:C	1:D:531:VAL:CA	2.69	0.58
1:E:453:MET:CG	1:F:482:LYS:CE	2.78	0.58
1:B:481:ILE:CG2	1:B:487:ARG:HB2	2.27	0.58
1:C:489:ILE:O	1:C:491:ASN:N	2.36	0.58
1:E:487:ARG:HB3	1:E:487:ARG:NH1	2.16	0.58
1:C:446:ILE:CD1	1:C:499:VAL:HG21	2.30	0.58
1:B:429:VAL:HG11	1:B:513:SER:HA	1.84	0.58
1:B:478:SER:O	1:B:482:LYS:HG3	2.03	0.58
1:F:435:ILE:CG1	1:F:439:ALA:CB	2.79	0.58
1:A:512:ILE:HG12	1:A:535:GLY:H	1.70	0.57
1:C:549:VAL:CG1	1:C:574:VAL:HG22	2.34	0.57
1:D:543:VAL:HB	1:D:590:SER:HA	1.85	0.57
1:F:427:GLY:O	1:F:446:ILE:HA	2.04	0.57
1:A:538:SER:OG	1:A:542:GLU:HB2	2.03	0.57
1:E:450:THR:O	1:E:493:ASP:N	2.34	0.57
1:B:512:ILE:O	1:B:513:SER:C	2.46	0.57
1:D:531:VAL:O	1:D:532:ALA:N	2.32	0.57
1:F:611:SER:O	1:F:614:LYS:HB3	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:LYS:CB	1:A:588:PRO:CB	2.78	0.57
1:B:494:VAL:HG12	1:B:496:ILE:HD11	1.84	0.57
1:D:452:SER:O	1:D:453:MET:SD	2.62	0.57
1:F:473:ALA:HB2	2:F:657:HOH:O	2.04	0.57
1:D:537:LEU:CG	1:D:538:SER:H	2.13	0.57
1:E:595:VAL:O	1:E:599:VAL:HG22	2.05	0.57
1:B:445:ILE:HD12	1:B:498:PHE:HD1	1.68	0.57
1:B:555:ALA:O	1:B:559:ALA:HB2	2.04	0.57
1:B:558:GLN:O	1:B:559:ALA:C	2.48	0.57
1:A:485:THR:HG22	1:A:487:ARG:H	1.69	0.57
1:B:451:PRO:HA	1:B:491:ASN:O	2.05	0.57
1:E:459:ARG:HH11	1:E:459:ARG:CG	2.16	0.56
1:C:549:VAL:HG12	1:C:550:THR:N	2.20	0.56
1:C:608:ARG:NH2	1:C:612:LYS:HE3	2.20	0.56
1:E:420:ILE:H	1:E:428:ARG:NH2	2.03	0.56
1:B:431:GLY:HA3	1:B:513:SER:OG	2.04	0.56
1:B:593:ASN:O	1:B:597:GLU:HB2	2.05	0.56
1:D:487:ARG:CG	1:D:487:ARG:NH1	2.62	0.56
1:A:420:ILE:HD11	1:A:428:ARG:CZ	2.35	0.56
1:A:568:LYS:O	1:A:571:ILE:HG12	2.04	0.56
1:D:489:ILE:HG22	1:D:492:MET:SD	2.46	0.56
1:E:520:SER:O	1:E:521:ALA:C	2.46	0.56
1:A:418:LEU:HD13	1:A:500:GLY:HA2	1.88	0.56
1:A:557:ILE:HG21	1:A:580:HIS:HD2	1.70	0.56
1:D:470:ALA:O	1:D:474:VAL:HG23	2.05	0.56
1:E:457:GLU:HG3	2:E:672:HOH:O	2.06	0.56
1:E:470:ALA:HA	1:E:514:ILE:HD13	1.87	0.56
1:A:441:ILE:HA	1:A:555:ALA:HB1	1.87	0.56
1:D:591:ARG:HB3	1:D:593:ASN:OD1	2.06	0.56
1:F:485:THR:OG1	1:F:609:LEU:HD11	2.05	0.56
1:A:446:ILE:O	1:A:446:ILE:HD13	2.06	0.56
1:A:566:ILE:HD11	1:A:571:ILE:CD1	2.35	0.56
1:B:428:ARG:HG3	1:B:445:ILE:O	2.06	0.56
1:C:480:ILE:HG21	2:C:707:HOH:O	2.06	0.56
1:D:563:LYS:NZ	1:D:563:LYS:HD3	2.21	0.56
1:B:500:GLY:HA2	2:B:693:HOH:O	2.06	0.56
1:D:570:ASN:ND2	1:D:573:ASP:OD2	2.34	0.56
1:E:597:GLU:HG2	1:E:610:MET:HE1	1.87	0.56
1:A:419:PHE:HB3	1:A:444:PRO:HG3	1.88	0.55
1:A:577:ASP:O	1:A:578:ALA:C	2.48	0.55
1:B:495:HIS:NE2	1:C:479:ALA:HB2	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:610:MET:HE3	1:C:610:MET:HA	1.88	0.55
1:E:478:SER:HG	1:E:489:ILE:HD11	1.70	0.55
1:E:563:LYS:HD3	1:E:587:ILE:HD11	1.87	0.55
1:C:572:ASP:OD1	1:C:572:ASP:N	2.38	0.55
1:E:433:ALA:HB3	1:E:441:ILE:HG13	1.89	0.55
1:F:417:LYS:HD2	1:F:419:PHE:CE1	2.42	0.55
1:F:578:ALA:HA	1:F:581:GLU:OE1	2.06	0.55
1:B:431:GLY:CA	1:B:513:SER:CB	2.83	0.55
1:A:526:PRO:HD2	1:A:601:GLU:HB3	1.89	0.55
1:F:478:SER:O	1:F:479:ALA:C	2.46	0.55
1:C:606:LYS:C	1:C:608:ARG:H	2.13	0.55
1:D:435:ILE:CG2	1:D:505:VAL:HG22	2.37	0.55
1:D:508:ASP:HB3	1:D:546:VAL:HG11	1.88	0.55
1:F:477:VAL:HG22	1:F:481:ILE:HG13	1.89	0.55
1:B:563:LYS:CD	1:B:587:ILE:HD11	2.22	0.55
1:C:446:ILE:CD1	1:C:446:ILE:N	2.67	0.55
1:C:611:SER:O	1:C:614:LYS:HE2	2.07	0.55
1:E:485:THR:HG21	1:E:523:GLU:OE2	2.07	0.55
1:E:545:PRO:HG3	1:E:569:ASP:HB2	1.89	0.55
1:A:568:LYS:HD3	1:A:569:ASP:N	2.23	0.54
1:D:533:MET:HG3	1:D:534:THR:N	2.20	0.54
1:E:558:GLN:NE2	1:E:580:HIS:HE1	2.05	0.54
1:F:452:SER:HA	1:F:493:ASP:OD2	2.07	0.54
1:E:491:ASN:CB	1:E:492:MET:HE3	2.31	0.54
1:A:448:GLU:CD	1:B:539:VAL:HG22	2.32	0.54
1:E:433:ALA:HB3	1:E:441:ILE:HG12	1.88	0.54
1:E:587:ILE:HG22	1:E:589:VAL:HG13	1.88	0.54
1:A:470:ALA:O	1:A:473:ALA:HB3	2.08	0.54
1:A:475:MET:HE2	1:F:459:ARG:HH22	1.72	0.54
1:A:545:PRO:HG2	1:F:499:VAL:CG1	2.38	0.54
1:B:525:ILE:HD13	1:B:600:LEU:HD13	1.88	0.54
1:E:491:ASN:C	1:E:492:MET:HE3	2.32	0.54
1:E:492:MET:HG2	2:E:654:HOH:O	2.07	0.54
1:B:537:LEU:CD1	1:B:592:ILE:HB	2.36	0.54
1:D:421:THR:HG22	1:D:561:LEU:CD2	2.37	0.54
1:D:551:GLN:CD	1:D:551:GLN:N	2.66	0.54
1:C:472:GLU:O	1:C:476:ASN:N	2.41	0.54
1:B:418:LEU:HD23	1:B:418:LEU:N	2.23	0.54
1:B:614:LYS:HD3	1:B:614:LYS:C	2.32	0.54
1:C:438:SER:HA	1:C:551:GLN:OE1	2.07	0.54
1:B:558:GLN:O	1:B:560:GLY:N	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:ILE:O	1:B:589:VAL:HG22	2.08	0.54
1:D:474:VAL:HA	1:D:477:VAL:HG12	1.89	0.54
1:E:463:THR:HG21	1:F:472:GLU:HB2	1.90	0.54
1:F:424:TYR:C	1:F:425:GLU:HG2	2.26	0.54
1:A:544:LEU:HB3	1:A:545:PRO:CD	2.22	0.53
1:B:544:LEU:CB	1:B:545:PRO:CD	2.85	0.53
1:C:489:ILE:HD12	1:C:492:MET:CE	2.35	0.53
1:A:596:LEU:HB3	1:A:600:LEU:CD1	2.39	0.53
1:B:432:LEU:HD23	1:B:442:VAL:HG22	1.89	0.53
1:B:448:GLU:OE2	1:B:449:VAL:N	2.42	0.53
1:B:528:ASP:C	1:B:530:SER:H	2.17	0.53
1:B:531:VAL:HG11	1:B:565:ILE:CD1	2.38	0.53
1:D:421:THR:O	1:D:530:SER:HA	2.09	0.53
1:B:427:GLY:O	1:B:446:ILE:HA	2.08	0.53
1:B:566:ILE:HD13	1:B:586:VAL:HG13	1.91	0.53
1:D:489:ILE:HD13	1:D:522:ILE:HD11	1.90	0.53
1:F:428:ARG:O	1:F:529:GLN:NE2	2.32	0.53
1:B:453:MET:HB2	1:C:482:LYS:HE2	1.90	0.53
1:B:589:VAL:HB	1:B:594:GLU:HB2	1.90	0.53
1:B:478:SER:HA	1:B:489:ILE:HG21	1.90	0.53
1:C:427:GLY:O	1:C:446:ILE:HA	2.08	0.53
1:F:579:GLU:O	1:F:580:HIS:CB	2.54	0.53
1:B:423:GLY:O	1:B:529:GLN:HG2	2.07	0.53
1:C:465:ARG:HB3	1:C:465:ARG:NH1	2.23	0.53
1:D:562:LYS:CG	1:D:562:LYS:HZ2	2.22	0.53
1:D:463:THR:HA	1:D:467:GLN:NE2	2.24	0.52
1:D:508:ASP:HB3	1:D:546:VAL:CG1	2.39	0.52
1:E:526:PRO:HG2	1:E:601:GLU:OE1	2.09	0.52
1:B:424:TYR:CD1	1:B:601:GLU:HB2	2.44	0.52
1:A:544:LEU:CB	1:A:545:PRO:CD	2.76	0.52
1:F:523:GLU:O	1:F:525:ILE:HG13	2.09	0.52
1:B:481:ILE:HG23	1:B:485:THR:HG1	1.69	0.52
1:C:433:ALA:HB3	1:C:441:ILE:CD1	2.40	0.52
1:D:564:VAL:CG2	1:D:565:ILE:N	2.67	0.52
1:E:482:LYS:HG3	1:E:488:ASP:HB2	1.91	0.52
1:A:565:ILE:HA	1:A:587:ILE:O	2.10	0.52
1:C:479:ALA:O	1:C:483:LYS:N	2.36	0.52
1:B:608:ARG:O	1:B:612:LYS:HE2	2.09	0.52
1:A:446:ILE:HD11	1:A:448:GLU:OE1	2.10	0.52
1:C:501:THR:HG22	2:D:638:HOH:O	2.09	0.52
1:F:418:LEU:O	1:F:499:VAL:HG11	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:428:ARG:CD	1:F:446:ILE:HG23	2.19	0.52
1:F:578:ALA:C	1:F:579:GLU:O	2.52	0.52
1:B:429:VAL:HG21	1:B:517:ALA:N	2.24	0.52
1:C:532:ALA:O	1:C:564:VAL:HA	2.09	0.52
1:A:568:LYS:HD3	1:A:568:LYS:C	2.35	0.51
1:B:563:LYS:HB3	1:B:587:ILE:HD12	1.91	0.51
1:D:480:ILE:HD13	1:D:592:ILE:HG21	1.91	0.51
1:A:498:PHE:N	1:A:498:PHE:CD2	2.78	0.51
1:B:435:ILE:HD11	1:B:441:ILE:HG21	1.91	0.51
1:D:435:ILE:HG22	1:D:505:VAL:HG22	1.92	0.51
1:D:489:ILE:C	1:D:491:ASN:H	2.19	0.51
1:E:478:SER:HB3	1:E:482:LYS:HE3	1.92	0.51
1:E:518:VAL:C	1:E:520:SER:N	2.63	0.51
1:A:570:ASN:HA	1:A:573:ASP:OD2	2.11	0.51
1:B:577:ASP:OD1	1:B:579:GLU:N	2.44	0.51
1:C:445:ILE:CD1	1:C:445:ILE:HG21	2.40	0.51
1:B:556:ALA:HA	1:B:559:ALA:CB	2.41	0.51
1:C:472:GLU:CG	1:C:473:ALA:N	2.71	0.51
1:F:488:ASP:OD1	1:F:489:ILE:HD13	2.11	0.51
1:F:523:GLU:O	1:F:524:GLY:C	2.53	0.51
1:A:467:GLN:CG	1:A:471:ARG:HH12	2.21	0.51
1:A:501:THR:HG23	2:A:634:HOH:O	2.09	0.51
1:A:543:VAL:N	1:A:590:SER:O	2.24	0.51
1:D:532:ALA:O	1:D:564:VAL:HA	2.11	0.51
1:D:534:THR:HG23	1:D:567:PRO:HD3	1.92	0.51
1:F:604:LYS:HD3	2:F:689:HOH:O	2.11	0.51
1:A:475:MET:SD	1:F:461:ILE:CD1	2.99	0.51
1:A:573:ASP:OD2	1:F:417:LYS:N	2.44	0.51
1:A:596:LEU:HB3	1:A:600:LEU:HG	1.92	0.51
1:B:557:ILE:CD1	1:B:580:HIS:HB3	2.41	0.51
1:A:563:LYS:HG2	1:A:585:GLU:CB	2.36	0.51
1:D:518:VAL:HG23	2:D:714:HOH:O	2.10	0.51
1:E:563:LYS:HD3	1:E:587:ILE:CD1	2.40	0.51
1:D:420:ILE:CG2	1:D:421:THR:N	2.74	0.51
1:C:428:ARG:HD2	1:C:446:ILE:HG23	1.93	0.51
1:E:459:ARG:CG	1:E:459:ARG:NH1	2.73	0.51
1:B:480:ILE:HD12	1:B:613:PHE:HE1	1.76	0.50
1:C:435:ILE:O	1:C:436:GLY:C	2.54	0.50
1:E:585:GLU:HG3	1:E:587:ILE:CD1	2.35	0.50
1:F:597:GLU:HB3	2:F:686:HOH:O	2.11	0.50
1:D:514:ILE:HG22	2:D:714:HOH:O	2.07	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:GLU:C	1:A:556:ALA:N	2.68	0.50
1:B:425:GLU:O	1:B:527:VAL:HB	2.11	0.50
1:B:474:VAL:HG22	1:B:518:VAL:HG21	1.92	0.50
1:B:531:VAL:HG11	1:B:565:ILE:HG13	1.93	0.50
1:F:485:THR:OG1	1:F:486:GLY:N	2.43	0.50
1:B:479:ALA:HA	1:B:482:LYS:CE	2.41	0.50
1:B:601:GLU:HG3	2:B:659:HOH:O	2.11	0.50
1:D:563:LYS:HG2	1:D:585:GLU:CB	2.40	0.50
1:F:447:ALA:HA	1:F:495:HIS:O	2.11	0.50
1:B:434:VAL:HG12	1:B:439:ALA:O	2.11	0.50
1:C:477:VAL:HG22	1:C:481:ILE:HG13	1.93	0.50
1:D:435:ILE:CD1	1:D:439:ALA:HB3	2.42	0.50
1:D:595:VAL:O	1:D:599:VAL:HG22	2.11	0.50
1:A:475:MET:CE	1:F:459:ARG:HH22	2.25	0.50
1:B:451:PRO:HD3	1:B:492:MET:HG2	1.94	0.50
1:A:592:ILE:HG13	1:A:592:ILE:O	2.11	0.50
1:B:544:LEU:HB3	1:B:545:PRO:HD2	1.94	0.50
1:C:469:ILE:CG2	1:C:508:ASP:O	2.60	0.50
1:C:473:ALA:O	1:C:477:VAL:HG12	2.12	0.50
1:C:483:LYS:CB	1:C:483:LYS:CD	2.82	0.50
1:D:480:ILE:CD1	1:D:592:ILE:HG21	2.42	0.50
1:B:510:ALA:O	1:B:511:SER:C	2.55	0.49
1:B:534:THR:OG1	1:B:546:VAL:HG21	2.12	0.49
1:B:609:LEU:HD11	1:B:613:PHE:HE2	1.77	0.49
1:C:499:VAL:HG13	1:D:545:PRO:HG2	1.92	0.49
1:E:432:LEU:CB	1:E:552:LYS:HD3	2.42	0.49
1:B:550:THR:OG1	1:B:573:ASP:O	2.29	0.49
1:E:425:GLU:H	1:E:527:VAL:H	1.59	0.49
1:B:478:SER:CB	1:B:489:ILE:HG12	2.42	0.49
1:B:520:SER:OG	1:B:527:VAL:CG2	2.60	0.49
1:C:435:ILE:HG13	1:C:439:ALA:HB3	1.95	0.49
1:C:489:ILE:HG22	1:C:490:SER:N	2.27	0.49
1:D:568:LYS:CB	1:D:588:PRO:HB2	2.42	0.49
1:E:486:GLY:HA2	2:E:644:HOH:O	2.12	0.49
1:E:579:GLU:O	1:E:583:LYS:NZ	2.32	0.49
1:F:566:ILE:O	1:F:588:PRO:HA	2.12	0.49
1:A:417:LYS:NZ	1:A:421:THR:HG23	2.26	0.49
1:A:484:TYR:O	1:A:612:LYS:HB3	2.12	0.49
1:B:417:LYS:HZ3	1:B:421:THR:CG2	2.26	0.49
1:B:489:ILE:HG13	1:B:490:SER:N	2.27	0.49
1:B:554:GLU:C	1:B:556:ALA:N	2.69	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:ILE:HG23	1:C:505:VAL:HG22	1.93	0.49
1:E:542:GLU:HB2	2:E:660:HOH:O	2.13	0.49
1:A:518:VAL:O	1:A:519:ILE:C	2.56	0.49
1:B:502:TYR:C	1:B:503:GLU:O	2.55	0.49
1:B:571:ILE:O	1:B:574:VAL:HG23	2.13	0.49
1:E:434:VAL:HA	1:E:439:ALA:O	2.12	0.49
1:F:477:VAL:HG21	1:F:515:ALA:HB1	1.94	0.49
1:F:568:LYS:N	1:F:589:VAL:O	2.42	0.49
1:F:488:ASP:HB3	1:F:491:ASN:HD21	1.77	0.49
1:B:480:ILE:HD12	1:B:613:PHE:CE1	2.47	0.49
1:B:551:GLN:H	1:B:551:GLN:NE2	2.09	0.49
1:A:580:HIS:C	1:A:581:GLU:O	2.55	0.49
1:F:467:GLN:HG3	1:F:471:ARG:NH2	2.28	0.49
1:A:435:ILE:HG23	1:A:505:VAL:HG22	1.95	0.48
1:B:420:ILE:O	1:B:421:THR:HG22	2.13	0.48
1:B:425:GLU:CB	1:B:529:GLN:NE2	2.72	0.48
1:E:419:PHE:HE1	1:E:559:ALA:HB1	1.78	0.48
1:E:475:MET:O	1:E:478:SER:HB2	2.13	0.48
1:F:516:THR:OG1	1:F:595:VAL:HG11	2.12	0.48
1:F:595:VAL:O	1:F:599:VAL:HG22	2.13	0.48
1:B:544:LEU:HB3	1:B:545:PRO:HD3	1.95	0.48
1:F:461:ILE:HD12	1:F:495:HIS:ND1	2.28	0.48
1:F:587:ILE:HG21	1:F:598:HIS:NE2	2.27	0.48
1:B:514:ILE:O	1:B:517:ALA:HB3	2.13	0.48
1:D:533:MET:HB2	1:D:565:ILE:HB	1.96	0.48
1:C:445:ILE:HD12	1:C:514:ILE:HA	1.95	0.48
1:C:578:ALA:N	1:C:581:GLU:OE2	2.47	0.48
1:F:485:THR:HB	1:F:613:PHE:CE2	2.48	0.48
1:F:581:GLU:CD	1:F:581:GLU:H	2.21	0.48
1:B:482:LYS:CG	2:B:667:HOH:O	2.56	0.48
1:E:418:LEU:HD22	1:E:499:VAL:HG13	1.95	0.48
1:A:482:LYS:O	1:A:484:TYR:N	2.46	0.48
1:D:420:ILE:HG22	1:D:421:THR:N	2.29	0.48
1:E:450:THR:O	1:E:492:MET:CA	2.61	0.48
1:F:538:SER:HB2	2:F:630:HOH:O	2.14	0.48
1:A:468:GLU:O	1:A:469:ILE:C	2.54	0.48
1:F:571:ILE:HD11	1:F:588:PRO:HB2	1.95	0.48
1:A:443:LEU:HD21	1:A:466:LEU:HD13	1.96	0.48
1:A:487:ARG:HD3	1:A:492:MET:HE1	1.94	0.48
1:C:463:THR:HG23	1:D:469:ILE:HD11	1.92	0.48
1:F:478:SER:O	1:F:479:ALA:O	2.32	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:531:VAL:HA	1:F:563:LYS:O	2.13	0.48
1:F:562:LYS:CG	2:F:626:HOH:O	2.61	0.48
1:C:419:PHE:HB3	1:C:444:PRO:HG3	1.95	0.48
1:B:448:GLU:C	1:B:448:GLU:CD	2.81	0.48
1:B:601:GLU:HG2	1:B:602:ASP:N	2.28	0.48
1:F:608:ARG:C	1:F:612:LYS:HZ2	2.21	0.48
1:A:549:VAL:O	1:A:552:LYS:N	2.47	0.47
1:F:432:LEU:HB2	1:F:534:THR:HB	1.95	0.47
1:D:531:VAL:N	1:D:531:VAL:C	2.62	0.47
1:A:429:VAL:HG21	1:A:513:SER:O	2.13	0.47
1:B:478:SER:OG	1:B:482:LYS:HD3	2.14	0.47
1:F:512:ILE:HG13	1:F:533:MET:HG3	1.96	0.47
1:A:428:ARG:CB	1:A:529:GLN:OE1	2.62	0.47
1:A:557:ILE:HG21	1:A:580:HIS:CD2	2.49	0.47
1:B:419:PHE:CE1	1:B:559:ALA:HA	2.48	0.47
1:B:424:TYR:CA	1:B:527:VAL:O	2.47	0.47
1:B:553:ILE:HG23	1:B:564:VAL:CG1	2.35	0.47
1:C:435:ILE:HG13	1:C:439:ALA:O	2.15	0.47
1:D:614:LYS:HE2	1:D:614:LYS:HB3	1.64	0.47
1:E:577:ASP:OD1	1:E:580:HIS:HB2	2.14	0.47
1:F:466:LEU:HB2	1:F:498:PHE:CD2	2.50	0.47
1:A:487:ARG:CD	1:A:492:MET:HE1	2.44	0.47
1:B:480:ILE:CD1	1:B:613:PHE:CE1	2.98	0.47
1:E:539:VAL:C	1:E:541:GLY:H	2.22	0.47
1:E:546:VAL:HG22	1:E:567:PRO:HG2	1.97	0.47
1:E:549:VAL:HG21	1:E:570:ASN:CG	2.40	0.47
1:A:441:ILE:HD11	1:A:505:VAL:HG21	1.97	0.47
1:A:592:ILE:C	1:A:594:GLU:N	2.64	0.47
1:B:417:LYS:HE2	1:B:417:LYS:HB2	1.38	0.47
1:B:577:ASP:OD1	1:B:577:ASP:C	2.58	0.47
1:C:502:TYR:HD2	1:C:505:VAL:HG21	1.80	0.47
1:F:435:ILE:N	1:F:439:ALA:O	2.48	0.47
1:F:489:ILE:CD1	1:F:489:ILE:N	2.58	0.47
1:A:420:ILE:O	1:A:529:GLN:HB3	2.15	0.47
1:B:492:MET:HB2	1:B:492:MET:HE2	1.39	0.47
1:B:568:LYS:HE2	1:B:590:SER:OG	2.15	0.47
1:E:438:SER:O	1:E:439:ALA:C	2.58	0.47
1:A:435:ILE:HG23	1:A:505:VAL:CG2	2.45	0.46
1:A:440:GLY:C	1:A:555:ALA:CB	2.87	0.46
1:B:480:ILE:CD1	1:B:613:PHE:HE1	2.27	0.46
1:B:543:VAL:N	1:B:590:SER:O	2.43	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:513:SER:CB	2:D:657:HOH:O	2.63	0.46
1:B:468:GLU:HG2	2:B:629:HOH:O	2.15	0.46
1:A:447:ALA:O	1:A:521:ALA:HB2	2.14	0.46
1:C:571:ILE:HD13	1:C:571:ILE:HA	1.81	0.46
1:E:453:MET:SD	1:F:482:LYS:HD3	2.54	0.46
1:E:547:GLY:O	1:E:552:LYS:NZ	2.48	0.46
1:E:571:ILE:HG23	2:E:688:HOH:O	2.15	0.46
1:B:440:GLY:C	1:B:555:ALA:HB2	2.40	0.46
1:D:533:MET:CG	1:D:534:THR:N	2.70	0.46
1:E:417:LYS:HB3	1:E:419:PHE:N	2.22	0.46
1:F:571:ILE:HD11	1:F:588:PRO:CB	2.45	0.46
1:E:563:LYS:HB3	1:E:585:GLU:CB	2.30	0.46
1:F:419:PHE:CD2	1:F:419:PHE:N	2.84	0.46
1:A:417:LYS:HD3	2:A:690:HOH:O	2.15	0.46
1:B:570:ASN:O	1:B:571:ILE:C	2.57	0.46
1:E:576:LEU:HA	2:E:671:HOH:O	2.16	0.46
1:B:463:THR:HB	2:B:627:HOH:O	2.16	0.46
1:B:598:HIS:O	1:B:599:VAL:CG1	2.64	0.46
1:C:610:MET:HA	1:C:610:MET:CE	2.45	0.46
1:E:450:THR:CG2	1:F:482:LYS:NZ	2.79	0.46
1:A:444:PRO:HD2	1:A:502:TYR:OH	2.16	0.45
1:A:546:VAL:HG13	1:A:567:PRO:HG2	1.98	0.45
1:C:463:THR:HG23	1:C:464:GLY:H	1.79	0.45
1:F:609:LEU:HA	1:F:609:LEU:HD12	1.43	0.45
1:A:478:SER:O	1:A:479:ALA:C	2.58	0.45
1:D:563:LYS:N	1:D:563:LYS:C	2.65	0.45
1:F:420:ILE:HD13	1:F:425:GLU:OE2	2.16	0.45
1:A:444:PRO:HB2	1:A:499:VAL:HB	1.99	0.45
1:A:482:LYS:O	1:A:483:LYS:C	2.59	0.45
1:B:512:ILE:C	1:B:514:ILE:N	2.75	0.45
1:E:457:GLU:N	2:E:676:HOH:O	2.49	0.45
1:E:477:VAL:HG23	1:E:515:ALA:HB1	1.97	0.45
1:A:424:TYR:CD1	1:A:528:ASP:N	2.84	0.45
1:A:597:GLU:HG3	1:A:610:MET:HE2	1.97	0.45
1:A:599:VAL:CG2	1:A:600:LEU:N	2.79	0.45
1:B:518:VAL:O	1:B:519:ILE:C	2.60	0.45
1:C:476:ASN:O	1:C:476:ASN:CG	2.58	0.45
1:E:573:ASP:O	1:E:575:LEU:HD12	2.15	0.45
1:B:426:VAL:CG1	1:B:427:GLY:H	2.29	0.45
1:B:428:ARG:C	1:B:429:VAL:HG23	2.41	0.45
1:C:478:SER:N	2:C:629:HOH:O	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:435:ILE:H	1:D:435:ILE:HG13	1.50	0.45
1:A:420:ILE:CD1	1:A:428:ARG:NH2	2.76	0.45
1:A:513:SER:HA	1:A:533:MET:SD	2.57	0.45
1:F:482:LYS:HD2	2:F:700:HOH:O	2.16	0.45
1:F:525:ILE:HA	1:F:526:PRO:HD3	1.81	0.45
1:A:501:THR:HB	2:B:653:HOH:O	2.16	0.45
1:B:418:LEU:HD23	1:B:418:LEU:H	1.81	0.45
1:B:420:ILE:C	1:B:421:THR:CG2	2.90	0.45
1:C:592:ILE:O	1:C:595:VAL:HB	2.17	0.45
1:B:449:VAL:HG21	1:B:522:ILE:HD12	1.99	0.45
1:A:571:ILE:HD11	1:A:588:PRO:HG3	1.98	0.45
1:A:581:GLU:C	1:A:583:LYS:N	2.65	0.45
1:B:531:VAL:HG13	1:B:563:LYS:HB2	1.98	0.45
1:C:418:LEU:CD1	1:D:545:PRO:HB2	2.46	0.45
1:C:463:THR:HG23	1:C:464:GLY:N	2.31	0.45
1:D:461:ILE:CD1	1:E:475:MET:SD	2.97	0.45
1:D:467:GLN:O	1:D:470:ALA:HB3	2.17	0.45
1:E:482:LYS:HD2	1:E:488:ASP:HA	1.98	0.45
1:E:545:PRO:HA	1:E:567:PRO:CG	2.46	0.45
1:E:563:LYS:HA	1:E:584:ILE:HG13	1.99	0.45
1:A:478:SER:C	1:A:480:ILE:N	2.68	0.44
1:B:431:GLY:CA	1:B:533:MET:O	2.44	0.44
1:E:420:ILE:HG13	1:E:428:ARG:NE	2.31	0.44
1:F:477:VAL:CG2	1:F:515:ALA:CB	2.94	0.44
1:F:592:ILE:CG2	1:F:593:ASN:N	2.79	0.44
1:A:442:VAL:C	1:A:444:PRO:HD3	2.42	0.44
1:C:477:VAL:C	2:C:629:HOH:O	2.60	0.44
1:D:611:SER:O	1:D:614:LYS:HE2	2.17	0.44
1:E:603:GLY:O	1:E:607:ASN:ND2	2.50	0.44
1:F:418:LEU:HB3	1:F:499:VAL:HG12	1.98	0.44
1:F:523:GLU:HB2	1:F:525:ILE:HD12	2.00	0.44
1:A:435:ILE:O	1:A:436:GLY:C	2.61	0.44
1:E:417:LYS:N	1:E:417:LYS:HD2	2.31	0.44
1:B:539:VAL:C	1:B:541:GLY:N	2.73	0.44
1:D:564:VAL:HG22	1:D:565:ILE:N	2.27	0.44
1:D:583:LYS:HB2	1:D:583:LYS:HE3	1.67	0.44
1:E:601:GLU:HG2	2:E:690:HOH:O	2.16	0.44
1:B:611:SER:HA	1:B:614:LYS:HD3	2.00	0.44
1:C:537:LEU:HG	1:C:538:SER:N	2.33	0.44
1:A:444:PRO:C	1:A:445:ILE:HD13	2.43	0.44
1:B:505:VAL:CG1	1:B:506:GLU:N	2.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:VAL:CG1	1:D:545:PRO:HG2	2.48	0.44
1:D:556:ALA:O	1:D:557:ILE:C	2.60	0.44
1:E:505:VAL:HG12	1:E:506:GLU:N	2.27	0.44
1:F:452:SER:O	1:F:453:MET:HG2	2.17	0.44
1:F:478:SER:HA	1:F:481:ILE:CB	2.34	0.44
1:E:453:MET:HE2	1:E:453:MET:HB2	1.83	0.44
1:A:472:GLU:HG3	2:A:626:HOH:O	2.18	0.44
1:A:482:LYS:C	1:A:484:TYR:N	2.76	0.44
1:D:432:LEU:HD21	1:D:532:ALA:HB1	2.00	0.44
1:F:432:LEU:HD23	1:F:432:LEU:HA	1.67	0.44
1:F:576:LEU:HD23	1:F:576:LEU:HA	1.89	0.44
1:E:520:SER:C	1:E:522:ILE:N	2.75	0.43
1:E:545:PRO:HA	1:E:567:PRO:CB	2.47	0.43
1:E:596:LEU:O	1:E:597:GLU:C	2.61	0.43
1:F:562:LYS:HG2	2:F:626:HOH:O	2.17	0.43
1:A:501:THR:HG22	1:B:547:GLY:H	1.82	0.43
1:B:435:ILE:HG22	1:B:503:GLU:O	2.17	0.43
1:D:565:ILE:HD13	1:D:565:ILE:HG21	1.54	0.43
1:E:509:SER:O	1:E:510:ALA:C	2.61	0.43
1:B:418:LEU:N	1:B:418:LEU:CD2	2.81	0.43
1:D:440:GLY:O	1:D:441:ILE:HG23	2.18	0.43
1:F:474:VAL:O	1:F:477:VAL:HG12	2.18	0.43
1:A:426:VAL:CG1	1:A:524:GLY:HA2	2.48	0.43
1:A:488:ASP:OD2	1:A:490:SER:OG	2.35	0.43
1:B:430:ASN:HB3	1:B:442:VAL:CG1	2.48	0.43
1:C:469:ILE:HG21	1:C:508:ASP:O	2.19	0.43
1:D:476:ASN:ND2	1:D:537:LEU:O	2.44	0.43
1:B:489:ILE:O	1:B:490:SER:C	2.61	0.43
1:C:609:LEU:O	1:C:610:MET:C	2.61	0.43
1:E:550:THR:HB	1:E:551:GLN:OE1	2.19	0.43
1:A:571:ILE:HD11	1:A:588:PRO:HB3	2.01	0.43
1:F:466:LEU:HA	1:F:466:LEU:HD23	1.61	0.43
1:A:428:ARG:HD2	1:A:446:ILE:HB	2.00	0.43
1:A:512:ILE:HG13	1:A:513:SER:N	2.33	0.43
1:B:426:VAL:CG2	1:B:526:PRO:HA	2.49	0.43
1:B:550:THR:HB	1:B:551:GLN:NE2	2.33	0.43
1:C:463:THR:CG2	1:D:469:ILE:CD1	2.94	0.43
1:C:537:LEU:HD11	1:C:592:ILE:HB	2.01	0.43
1:E:477:VAL:CG1	1:E:478:SER:N	2.82	0.43
1:F:561:LEU:HA	2:F:626:HOH:O	2.17	0.43
1:A:554:GLU:HA	2:A:695:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:LYS:C	1:B:614:LYS:CD	2.91	0.43
1:E:427:GLY:O	1:E:446:ILE:HA	2.19	0.43
1:A:526:PRO:HG2	1:A:601:GLU:OE1	2.18	0.43
1:B:580:HIS:O	1:B:583:LYS:CB	2.67	0.43
1:E:477:VAL:O	1:E:480:ILE:HB	2.19	0.43
1:F:467:GLN:OE1	1:F:471:ARG:NH2	2.41	0.43
1:C:448:GLU:CD	1:D:539:VAL:HG13	2.43	0.42
1:C:596:LEU:O	1:C:597:GLU:C	2.62	0.42
1:D:463:THR:HG22	1:E:468:GLU:HB3	2.00	0.42
1:A:562:LYS:C	1:A:563:LYS:HG3	2.43	0.42
1:A:601:GLU:O	1:A:606:LYS:HD2	2.19	0.42
1:C:477:VAL:O	1:C:477:VAL:CG2	2.67	0.42
1:E:432:LEU:HD21	1:E:556:ALA:HB2	2.01	0.42
1:F:562:LYS:HG3	2:F:626:HOH:O	2.18	0.42
1:B:450:THR:O	1:B:451:PRO:C	2.62	0.42
1:B:494:VAL:HG13	1:B:496:ILE:HD11	1.98	0.42
1:B:426:VAL:HG12	1:B:427:GLY:N	2.34	0.42
1:B:435:ILE:CG1	1:B:441:ILE:HG23	2.50	0.42
1:E:450:THR:HG21	1:F:482:LYS:NZ	2.35	0.42
1:B:420:ILE:HG22	1:B:421:THR:H	1.84	0.42
1:B:426:VAL:HG12	1:B:427:GLY:H	1.84	0.42
1:B:515:ALA:O	1:B:519:ILE:HG13	2.19	0.42
1:B:528:ASP:O	1:B:530:SER:N	2.52	0.42
1:B:565:ILE:HD11	1:B:599:VAL:HG13	2.00	0.42
1:D:510:ALA:O	1:D:511:SER:C	2.61	0.42
1:E:475:MET:HB2	1:E:475:MET:HE2	1.39	0.42
1:E:533:MET:HB3	1:E:565:ILE:HB	2.02	0.42
1:E:551:GLN:HG3	2:E:641:HOH:O	2.19	0.42
1:F:444:PRO:HB2	1:F:499:VAL:HB	1.99	0.42
1:C:462:ALA:HB2	1:C:496:ILE:HB	2.02	0.42
1:C:473:ALA:HA	1:C:476:ASN:HD22	1.85	0.42
1:C:527:VAL:HG12	1:C:528:ASP:N	2.34	0.42
1:F:548:GLY:O	1:F:551:GLN:HB2	2.20	0.42
1:A:432:LEU:HD13	1:A:552:LYS:HB3	2.02	0.42
1:A:483:LYS:NZ	1:A:483:LYS:CD	2.71	0.42
1:A:512:ILE:O	1:A:513:SER:C	2.59	0.42
1:B:429:VAL:HG23	1:B:517:ALA:HA	2.01	0.42
1:B:482:LYS:HA	1:B:487:ARG:O	2.19	0.42
1:B:532:ALA:HB2	1:B:561:LEU:HD13	2.00	0.42
1:C:581:GLU:OE2	1:C:581:GLU:N	2.53	0.42
1:D:489:ILE:C	1:D:491:ASN:N	2.78	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:568:LYS:CE	1:E:569:ASP:OD1	2.67	0.42
1:F:447:ALA:O	1:F:521:ALA:HB2	2.19	0.42
1:F:601:GLU:O	1:F:602:ASP:C	2.63	0.42
1:F:608:ARG:HE	1:F:608:ARG:HB3	1.23	0.42
1:B:512:ILE:HG22	1:B:537:LEU:HB2	2.02	0.42
1:C:463:THR:HG21	1:D:469:ILE:CD1	2.50	0.42
1:C:606:LYS:HG2	1:C:610:MET:HG2	2.01	0.42
1:D:443:LEU:HD21	1:D:466:LEU:HD13	2.01	0.42
1:F:421:THR:HA	1:F:561:LEU:HD21	2.01	0.42
1:A:587:ILE:HA	1:A:588:PRO:HD3	1.91	0.42
1:E:514:ILE:O	1:E:518:VAL:HG23	2.19	0.42
1:E:528:ASP:HB3	1:E:531:VAL:HG23	2.02	0.42
1:C:587:ILE:HA	1:C:588:PRO:HD3	1.76	0.42
1:F:467:GLN:CG	1:F:471:ARG:HH22	2.32	0.42
1:A:535:GLY:HA3	1:A:567:PRO:HG3	2.02	0.41
1:B:512:ILE:CG2	1:B:537:LEU:HB2	2.50	0.41
1:C:483:LYS:HD2	1:C:483:LYS:O	2.19	0.41
1:D:498:PHE:CD2	1:D:498:PHE:N	2.88	0.41
1:E:574:VAL:HG12	1:E:576:LEU:HB2	2.01	0.41
1:F:466:LEU:CB	1:F:498:PHE:CE2	3.02	0.41
1:F:483:LYS:O	1:F:483:LYS:HG3	2.19	0.41
1:F:538:SER:OG	1:F:540:LYS:N	2.53	0.41
1:F:546:VAL:N	1:F:570:ASN:OD1	2.35	0.41
1:C:445:ILE:CG2	1:C:445:ILE:HD13	2.50	0.41
1:A:478:SER:HA	1:A:489:ILE:CD1	2.45	0.41
1:B:448:GLU:HB3	1:C:539:VAL:CG2	2.47	0.41
1:B:477:VAL:CG2	1:B:515:ALA:HB1	2.45	0.41
1:C:433:ALA:HB1	1:C:506:GLU:O	2.20	0.41
1:C:488:ASP:O	1:C:491:ASN:HB2	2.20	0.41
1:E:474:VAL:O	1:E:477:VAL:HG12	2.20	0.41
1:A:469:ILE:HD12	1:A:469:ILE:HA	1.70	0.41
1:A:549:VAL:H	1:A:549:VAL:HG23	1.60	0.41
1:C:445:ILE:HG21	1:C:445:ILE:HD13	2.02	0.41
1:E:463:THR:HG21	1:F:472:GLU:CB	2.50	0.41
1:A:484:TYR:CD1	1:A:613:PHE:HA	2.56	0.41
1:B:606:LYS:O	1:B:607:ASN:C	2.62	0.41
1:E:531:VAL:HG21	1:E:599:VAL:HG12	2.02	0.41
1:C:480:ILE:CG2	2:C:707:HOH:O	2.67	0.41
1:E:417:LYS:HG3	1:E:419:PHE:CE2	2.56	0.41
1:E:446:ILE:HG12	2:F:630:HOH:O	2.20	0.41
1:F:464:GLY:O	1:F:467:GLN:HB3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:ILE:C	1:B:491:ASN:N	2.77	0.41
1:B:553:ILE:C	1:B:556:ALA:HB3	2.45	0.41
1:D:448:GLU:OE2	1:E:540:LYS:NZ	2.53	0.41
1:E:483:LYS:HE3	1:E:484:TYR:CZ	2.55	0.41
1:E:540:LYS:NZ	1:E:540:LYS:HB2	2.36	0.41
1:F:537:LEU:HD11	1:F:541:GLY:HA2	2.03	0.41
1:A:581:GLU:HB3	1:A:582:GLY:H	1.70	0.41
1:B:448:GLU:HG2	1:C:539:VAL:O	2.20	0.41
1:B:466:LEU:H	1:B:466:LEU:HG	1.68	0.41
1:B:531:VAL:HG12	1:B:565:ILE:HG13	2.00	0.41
1:C:608:ARG:CZ	1:C:612:LYS:HE3	2.51	0.41
1:D:542:GLU:OE2	1:D:542:GLU:HA	2.20	0.41
1:A:512:ILE:O	1:A:516:THR:OG1	2.34	0.41
1:B:426:VAL:HG22	1:B:525:ILE:C	2.46	0.41
1:B:442:VAL:HB	2:B:663:HOH:O	2.20	0.41
1:B:609:LEU:HD11	1:B:613:PHE:CE2	2.56	0.41
1:D:463:THR:HB	1:D:464:GLY:H	1.67	0.41
1:D:528:ASP:OD2	1:D:531:VAL:HG23	2.21	0.41
1:D:596:LEU:O	1:D:600:LEU:HG	2.21	0.41
1:E:441:ILE:HD12	1:E:502:TYR:CE1	2.56	0.41
1:E:596:LEU:C	1:E:598:HIS:N	2.77	0.41
1:F:478:SER:CA	1:F:481:ILE:HB	2.35	0.41
1:F:592:ILE:HG23	1:F:593:ASN:N	2.35	0.41
1:B:531:VAL:HG11	1:B:565:ILE:HD11	2.03	0.41
1:C:511:SER:HB3	1:C:514:ILE:HB	2.03	0.41
1:C:563:LYS:HD3	1:C:587:ILE:HD11	2.02	0.41
1:E:545:PRO:HA	1:E:567:PRO:HG2	2.02	0.41
1:F:429:VAL:O	1:F:445:ILE:HG12	2.21	0.41
1:F:581:GLU:C	1:F:583:LYS:H	2.29	0.41
1:B:427:GLY:HA3	1:B:447:ALA:O	2.21	0.40
1:C:465:ARG:HD2	1:C:503:GLU:OE2	2.19	0.40
1:C:467:GLN:HB2	1:C:471:ARG:CZ	2.51	0.40
1:F:477:VAL:HG21	1:F:515:ALA:CB	2.51	0.40
1:A:558:GLN:CB	2:A:693:HOH:O	2.54	0.40
1:C:429:VAL:HG22	1:C:527:VAL:HG11	2.03	0.40
1:D:424:TYR:CD1	1:D:528:ASP:N	2.89	0.40
1:D:555:ALA:O	1:D:558:GLN:HB2	2.21	0.40
1:C:445:ILE:H	1:C:445:ILE:HG12	1.59	0.40
1:E:434:VAL:C	1:E:435:ILE:O	2.64	0.40
1:C:482:LYS:O	1:C:485:THR:N	2.55	0.40
1:D:552:LYS:C	1:D:554:GLU:H	2.28	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:557:ILE:HG12	1:E:584:ILE:HG21	2.02	0.40
1:B:469:ILE:HD13	1:B:508:ASP:O	2.22	0.40
1:B:609:LEU:CD1	1:B:613:PHE:HE2	2.35	0.40
1:D:549:VAL:H	1:D:549:VAL:HG23	1.48	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:486:GLY:O	1:F:578:ALA:CB[1_455]	1.65	0.55

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	191/205 (93%)	164 (86%)	16 (8%)	11 (6%)	1	8
1	B	191/205 (93%)	140 (73%)	35 (18%)	16 (8%)	0	3
1	C	190/205 (93%)	162 (85%)	18 (10%)	10 (5%)	1	9
1	D	191/205 (93%)	169 (88%)	16 (8%)	6 (3%)	3	19
1	E	191/205 (93%)	151 (79%)	35 (18%)	5 (3%)	4	23
1	F	191/205 (93%)	155 (81%)	25 (13%)	11 (6%)	1	8
All	All	1145/1230 (93%)	941 (82%)	145 (13%)	59 (5%)	1	9

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	486	GLY
1	A	549	VAL
1	A	578	ALA
1	A	581	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	582	GLY
1	B	559	ALA
1	B	569	ASP
1	B	586	VAL
1	C	439	ALA
1	C	465	ARG
1	C	549	VAL
1	C	578	ALA
1	C	579	GLU
1	F	476	ASN
1	F	477	VAL
1	F	486	GLY
1	F	579	GLU
1	A	436	GLY
1	A	483	LYS
1	A	613	PHE
1	B	427	GLY
1	B	436	GLY
1	B	484	TYR
1	B	529	GLN
1	C	436	GLY
1	C	483	LYS
1	C	572	ASP
1	C	607	ASN
1	D	579	GLU
1	E	435	ILE
1	E	524	GLY
1	F	436	GLY
1	F	437	GLU
1	F	510	ALA
1	F	549	VAL
1	B	418	LEU
1	C	490	SER
1	D	490	SER
1	D	509	SER
1	E	439	ALA
1	E	510	ALA
1	A	509	SER
1	A	510	ALA
1	B	421	THR
1	B	490	SER
1	D	553	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	451	PRO
1	B	435	ILE
1	B	437	GLU
1	B	451	PRO
1	D	499	VAL
1	E	513	SER
1	F	597	GLU
1	B	540	LYS
1	D	510	ALA
1	B	599	VAL
1	F	458	GLY
1	F	499	VAL
1	B	571	ILE

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	160/168 (95%)	110 (69%)	50 (31%)	0	1
1	B	160/168 (95%)	115 (72%)	45 (28%)	0	2
1	C	159/168 (95%)	120 (76%)	39 (24%)	1	4
1	D	160/168 (95%)	127 (79%)	33 (21%)	1	7
1	E	160/168 (95%)	114 (71%)	46 (29%)	0	2
1	F	160/168 (95%)	126 (79%)	34 (21%)	1	6
All	All	959/1008 (95%)	712 (74%)	247 (26%)	0	3

All (247) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	GLU
1	A	424	TYR
1	A	426	VAL
1	A	429	VAL
1	A	435	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	446	ILE
1	A	453	MET
1	A	457	GLU
1	A	459	ARG
1	A	467	GLN
1	A	468	GLU
1	A	469	ILE
1	A	471	ARG
1	A	475	MET
1	A	478	SER
1	A	480	ILE
1	A	482	LYS
1	A	483	LYS
1	A	485	THR
1	A	487	ARG
1	A	488	ASP
1	A	492	MET
1	A	493	ASP
1	A	496	ILE
1	A	501	THR
1	A	503	GLU
1	A	508	ASP
1	A	509	SER
1	A	516	THR
1	A	529	GLN
1	A	533	MET
1	A	539	VAL
1	A	540	LYS
1	A	542	GLU
1	A	546	VAL
1	A	562	LYS
1	A	563	LYS
1	A	568	LYS
1	A	569	ASP
1	A	571	ILE
1	A	579	GLU
1	A	585	GLU
1	A	590	SER
1	A	592	ILE
1	A	594	GLU
1	A	598	HIS
1	A	599	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	602	ASP
1	A	608	ARG
1	A	612	LYS
1	B	417	LYS
1	B	418	LEU
1	B	420	ILE
1	B	421	THR
1	B	425	GLU
1	B	434	VAL
1	B	435	ILE
1	B	443	LEU
1	B	449	VAL
1	B	451	PRO
1	B	463	THR
1	B	466	LEU
1	B	469	ILE
1	B	478	SER
1	B	480	ILE
1	B	482	LYS
1	B	483	LYS
1	B	487	ARG
1	B	492	MET
1	B	496	ILE
1	B	502	TYR
1	B	503	GLU
1	B	518	VAL
1	B	522	ILE
1	B	531	VAL
1	B	534	THR
1	B	542	GLU
1	B	546	VAL
1	B	549	VAL
1	B	550	THR
1	B	562	LYS
1	B	564	VAL
1	B	568	LYS
1	B	570	ASN
1	B	571	ILE
1	B	573	ASP
1	B	575	LEU
1	B	579	GLU
1	B	580	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	583	LYS
1	B	584	ILE
1	B	605	LYS
1	B	608	ARG
1	B	609	LEU
1	B	614	LYS
1	C	420	ILE
1	C	422	GLU
1	C	425	GLU
1	C	435	ILE
1	C	437	GLU
1	C	438	SER
1	C	441	ILE
1	C	445	ILE
1	C	446	ILE
1	C	463	THR
1	C	465	ARG
1	C	468	GLU
1	C	472	GLU
1	C	476	ASN
1	C	477	VAL
1	C	480	ILE
1	C	482	LYS
1	C	483	LYS
1	C	485	THR
1	C	488	ASP
1	C	489	ILE
1	C	501	THR
1	C	506	GLU
1	C	508	ASP
1	C	509	SER
1	C	514	ILE
1	C	519	ILE
1	C	549	VAL
1	C	558	GLN
1	C	564	VAL
1	C	568	LYS
1	C	570	ASN
1	C	571	ILE
1	C	572	ASP
1	C	577	ASP
1	C	580	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	581	GLU
1	C	597	GLU
1	C	614	LYS
1	D	417	LYS
1	D	418	LEU
1	D	420	ILE
1	D	435	ILE
1	D	437	GLU
1	D	442	VAL
1	D	443	LEU
1	D	453	MET
1	D	457	GLU
1	D	459	ARG
1	D	465	ARG
1	D	468	GLU
1	D	469	ILE
1	D	480	ILE
1	D	487	ARG
1	D	506	GLU
1	D	533	MET
1	D	539	VAL
1	D	540	LYS
1	D	551	GLN
1	D	557	ILE
1	D	562	LYS
1	D	564	VAL
1	D	575	LEU
1	D	576	LEU
1	D	579	GLU
1	D	583	LYS
1	D	592	ILE
1	D	597	GLU
1	D	604	LYS
1	D	610	MET
1	D	612	LYS
1	D	614	LYS
1	E	418	LEU
1	E	419	PHE
1	E	420	ILE
1	E	421	THR
1	E	422	GLU
1	E	425	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	434	VAL
1	E	435	ILE
1	E	443	LEU
1	E	446	ILE
1	E	450	THR
1	E	453	MET
1	E	457	GLU
1	E	459	ARG
1	E	461	ILE
1	E	463	THR
1	E	475	MET
1	E	477	VAL
1	E	482	LYS
1	E	485	THR
1	E	487	ARG
1	E	488	ASP
1	E	489	ILE
1	E	491	ASN
1	E	492	MET
1	E	496	ILE
1	E	502	TYR
1	E	503	GLU
1	E	505	VAL
1	E	508	ASP
1	E	518	VAL
1	E	531	VAL
1	E	536	SER
1	E	539	VAL
1	E	540	LYS
1	E	544	LEU
1	E	551	GLN
1	E	558	GLN
1	E	562	LYS
1	E	563	LYS
1	E	579	GLU
1	E	599	VAL
1	E	605	LYS
1	E	608	ARG
1	E	609	LEU
1	E	614	LYS
1	F	417	LYS
1	F	418	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	420	ILE
1	F	425	GLU
1	F	437	GLU
1	F	445	ILE
1	F	446	ILE
1	F	467	GLN
1	F	469	ILE
1	F	472	GLU
1	F	480	ILE
1	F	482	LYS
1	F	489	ILE
1	F	495	HIS
1	F	501	THR
1	F	519	ILE
1	F	527	VAL
1	F	540	LYS
1	F	546	VAL
1	F	549	VAL
1	F	550	THR
1	F	558	GLN
1	F	562	LYS
1	F	564	VAL
1	F	565	ILE
1	F	566	ILE
1	F	572	ASP
1	F	575	LEU
1	F	581	GLU
1	F	593	ASN
1	F	595	VAL
1	F	605	LYS
1	F	608	ARG
1	F	614	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	491	ASN
1	A	593	ASN
1	B	430	ASN
1	B	529	GLN
1	B	551	GLN
1	B	580	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	476	ASN
1	D	598	HIS
1	E	558	GLN
1	E	580	HIS
1	E	607	ASN
1	F	491	ASN

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	531:VAL	C	532:ALA	N	1.67

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	532:ALA	C	533:MET	N	1.66

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	195/205 (95%)	-0.31	2 (1%) 79 59	5, 17, 35, 47	0
1	B	195/205 (95%)	-0.08	1 (0%) 87 72	11, 25, 43, 61	0
1	C	194/205 (94%)	-0.63	0 100 100	2, 10, 27, 35	0
1	D	195/205 (95%)	-0.61	0 100 100	2, 8, 24, 34	0
1	E	195/205 (95%)	-0.31	0 100 100	5, 17, 42, 57	0
1	F	195/205 (95%)	-0.46	0 100 100	2, 17, 36, 50	0
All	All	1169/1230 (95%)	-0.40	3 (0%) 90 79	2, 16, 37, 61	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	420	ILE	2.9
1	A	489	ILE	2.5
1	B	501	THR	2.4

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.