



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:28 AM UTC

PDB ID : 1Z0G / pdb_00001z0g
Title : Crystal Structure of A. fulgidus Lon proteolytic domain
Authors : Botos, I.; Melnikov, E.E.; Cherry, S.; Kozlov, S.; Makhovskaya, O.V.; Tropea, J.E.; Gustchina, A.; Rotanova, T.V.; Wlodawer, A.
Deposited on : 2005-03-01
Resolution : 2.27 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:

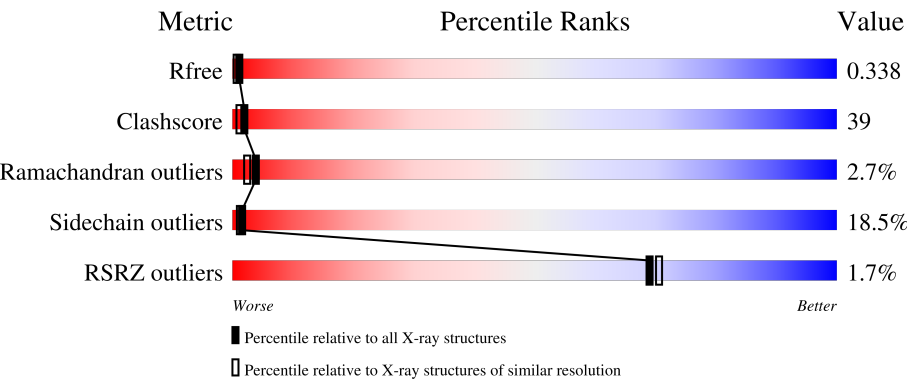
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.27 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	33%40%18%5%
1	B	205	3% 27%40%22%6%
1	C	205	2% 24%40%23%8%
1	D	205	28%42%21%
1	E	205	% 30%38%20%7%5%

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Mol	Chain	Length	Quality of chain
1	F	205	3% 27% 40% 21% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9873 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	196	Total	C	N	O	S	0	0	0
			1466	926	248	287	5			
1	C	196	Total	C	N	O	S	0	0	0
			1466	926	248	287	5			
1	D	196	Total	C	N	O	S	0	0	0
			1466	926	248	287	5			
1	E	195	Total	C	N	O	S	0	0	0
			1457	921	247	284	5			
1	F	196	Total	C	N	O	S	0	0	0
			1466	926	248	287	5			

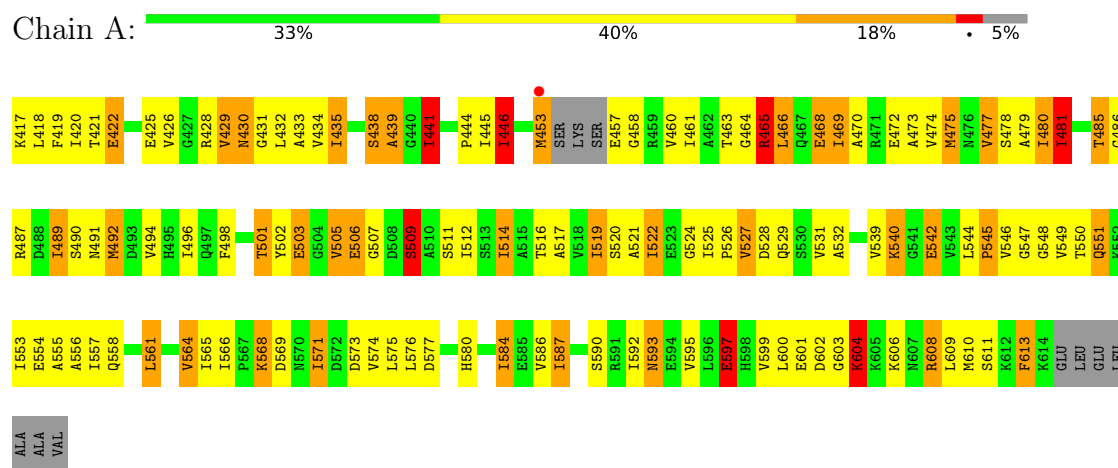
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	163	Total	O	0	0
			163	163		
2	B	165	Total	O	0	0
			165	165		
2	C	198	Total	O	0	0
			198	198		
2	D	197	Total	O	0	0
			197	197		
2	E	147	Total	O	0	0
			147	147		
2	F	225	Total	O	0	0
			225	225		

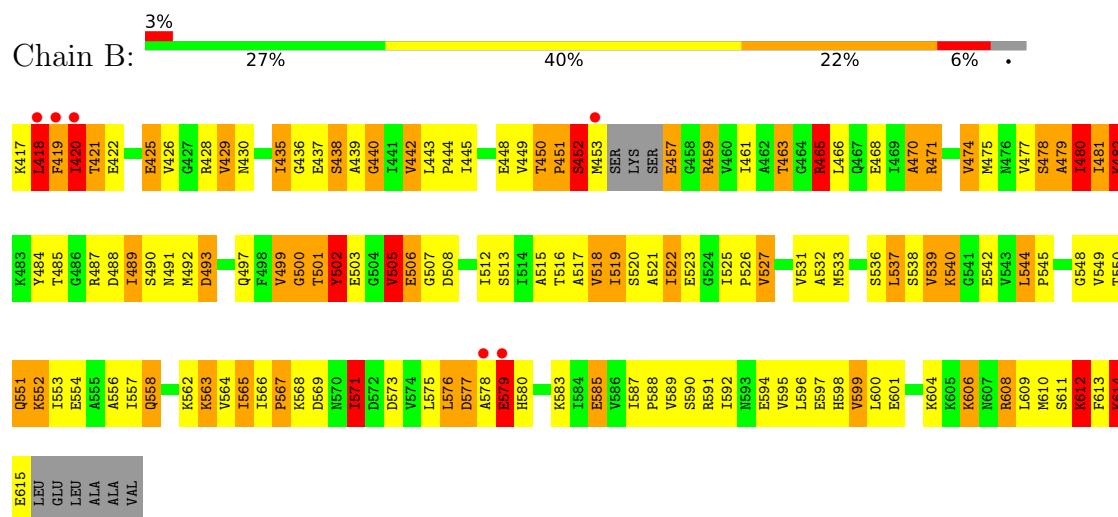
3 Residue-property plots

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.

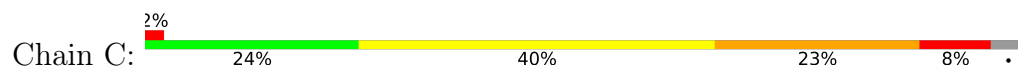
• Molecule 1: Putative protease La homolog type

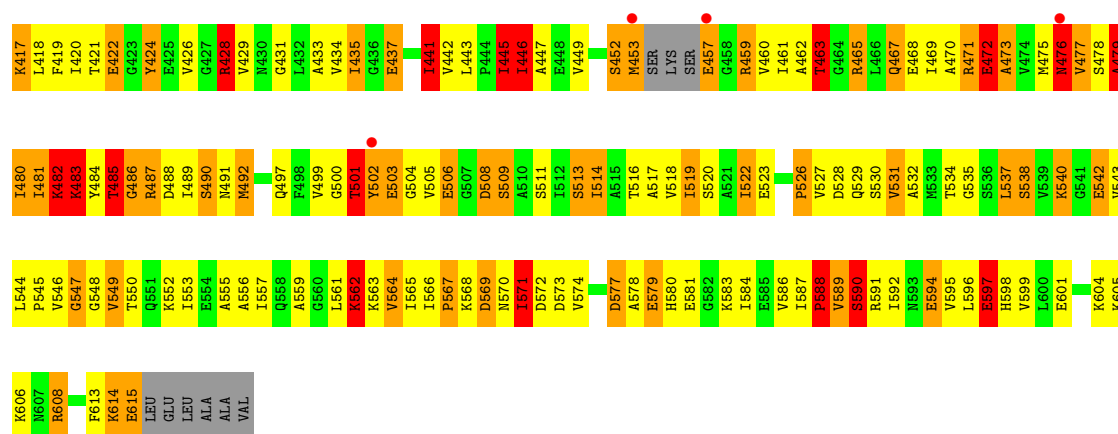


• Molecule 1: Putative protease La homolog type



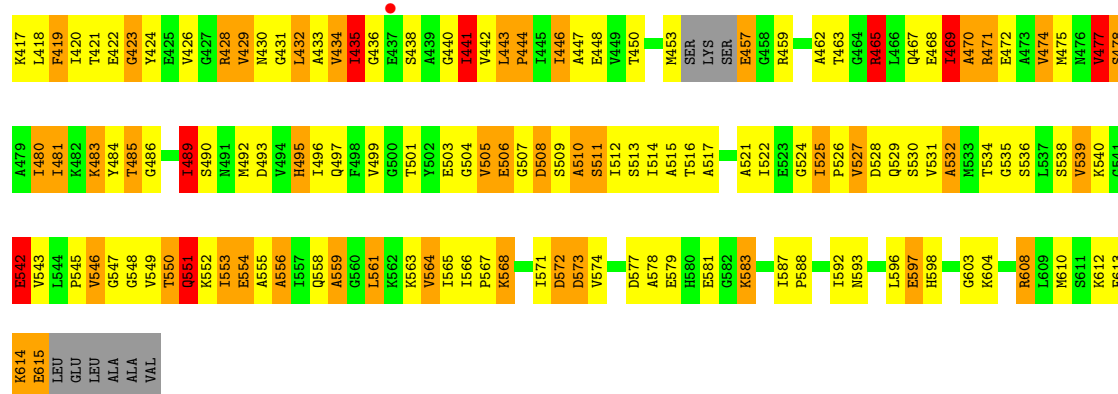
• Molecule 1: Putative protease La homolog type





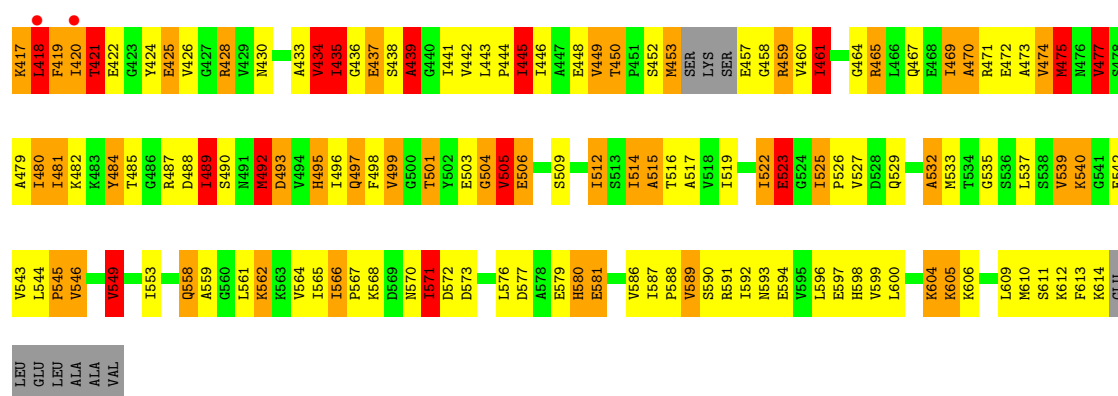
• Molecule 1: Putative protease La homolog type

Chain D: 28% 42% 21% . .



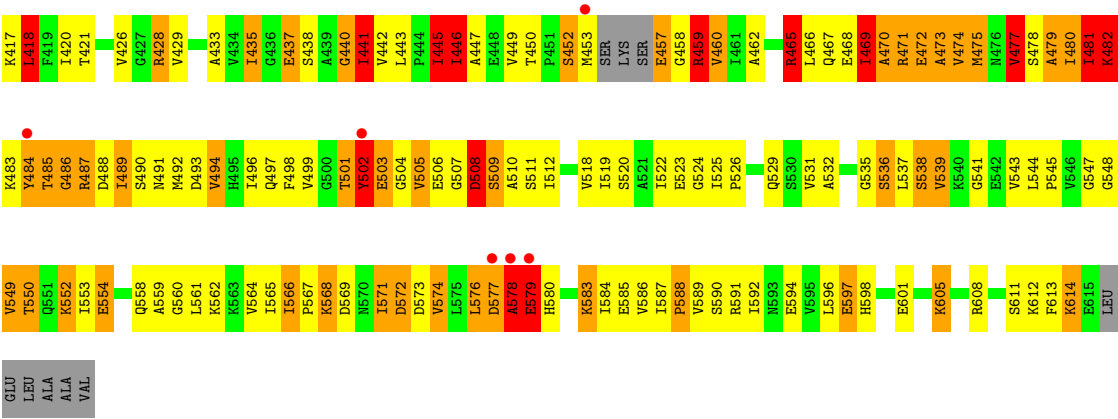
• Molecule 1: Putative protease La homolog type

Chain E: 30% 38% 20% 7% 5%



• Molecule 1: Putative protease La homolog type

Chain F: 3% 27% 40% 21% 7% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.65Å 88.69Å 147.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.27 15.00 – 2.27	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.27) 95.7 (15.00-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.195 , 0.329 0.211 , 0.338	Depositor DCC
R_{free} test set	1038 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.42$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9873	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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 57.46 % 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 2.3605e-05. 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	2.56	82/1470 (5.6%)	1.95	47/1983 (2.4%)
1	B	2.46	75/1479 (5.1%)	1.96	39/1995 (2.0%)
1	C	2.70	99/1479 (6.7%)	2.11	58/1995 (2.9%)
1	D	2.64	103/1479 (7.0%)	2.10	56/1995 (2.8%)
1	E	2.39	73/1470 (5.0%)	1.96	43/1983 (2.2%)
1	F	2.50	79/1479 (5.3%)	2.08	60/1995 (3.0%)
All	All	2.54	511/8856 (5.8%)	2.03	303/11946 (2.5%)

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	B	0	1
1	C	0	2
1	D	1	1
1	E	0	3
1	F	1	3
All	All	2	10

All (511) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	479	ALA	CA-CB	16.31	1.81	1.53
1	B	579	GLU	CD-OE1	15.63	1.55	1.25
1	C	473	ALA	CA-CB	-14.31	1.31	1.53
1	A	481	ILE	CA-CB	13.96	1.69	1.54
1	E	527	VAL	CA-CB	13.71	1.70	1.54
1	C	527	VAL	CA-CB	13.46	1.72	1.54
1	B	480	ILE	CA-CB	13.35	1.69	1.54
1	F	473	ALA	CA-CB	-13.30	1.32	1.53
1	D	556	ALA	CA-CB	12.75	1.73	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	480	ILE	CA-CB	12.63	1.69	1.54
1	D	480	ILE	CA-CB	12.18	1.71	1.54
1	B	579	GLU	CD-OE2	11.96	1.48	1.25
1	F	578	ALA	C-O	11.72	1.38	1.24
1	F	525	ILE	CA-CB	11.12	1.64	1.54
1	E	515	ALA	CA-CB	10.77	1.70	1.53
1	C	542	GLU	CA-C	-10.52	1.39	1.52
1	D	597	GLU	CD-OE1	10.42	1.45	1.25
1	A	527	VAL	N-CA	10.35	1.58	1.46
1	C	542	GLU	C-O	-10.31	1.11	1.23
1	A	577	ASP	N-CA	10.04	1.59	1.46
1	D	592	ILE	CA-CB	10.03	1.68	1.54
1	E	565	ILE	CA-CB	-10.02	1.42	1.54
1	C	489	ILE	CA-CB	10.02	1.68	1.54
1	A	531	VAL	CA-CB	-10.01	1.41	1.53
1	E	525	ILE	CA-C	9.99	1.59	1.52
1	A	426	VAL	CA-C	9.92	1.64	1.52
1	A	519	ILE	CA-CB	9.84	1.66	1.54
1	C	597	GLU	CG-CD	9.83	1.76	1.52
1	A	429	VAL	C-O	-9.74	1.14	1.24
1	C	595	VAL	N-CA	-9.71	1.35	1.46
1	B	513	SER	C-O	-9.64	1.12	1.24
1	C	587	ILE	CA-CB	9.61	1.66	1.54
1	F	566	ILE	CA-CB	9.58	1.66	1.54
1	C	564	VAL	CA-CB	9.51	1.67	1.54
1	A	597	GLU	CG-CD	9.37	1.75	1.52
1	E	471	ARG	CZ-NH1	9.17	1.45	1.32
1	B	445	ILE	CA-CB	9.03	1.66	1.54
1	F	477	VAL	C-O	-9.01	1.14	1.24
1	F	567	PRO	C-O	8.91	1.34	1.23
1	C	426	VAL	CA-C	8.84	1.63	1.52
1	E	420	ILE	CA-C	8.77	1.63	1.52
1	A	502	TYR	CA-C	-8.70	1.41	1.53
1	D	536	SER	N-CA	-8.55	1.35	1.46
1	B	579	GLU	CG-CD	8.48	1.73	1.52
1	D	448	GLU	CA-C	-8.48	1.42	1.52
1	F	543	VAL	CA-CB	8.47	1.64	1.53
1	A	611	SER	C-O	-8.46	1.13	1.24
1	A	468	GLU	CA-C	8.41	1.63	1.52
1	A	473	ALA	CA-CB	-8.39	1.40	1.53
1	B	587	ILE	CA-CB	8.38	1.61	1.54
1	D	531	VAL	C-O	8.38	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	527	VAL	N-CA	-8.32	1.36	1.46
1	D	443	LEU	C-O	-8.30	1.14	1.24
1	C	614	LYS	CA-C	8.28	1.63	1.52
1	B	527	VAL	CA-CB	8.22	1.64	1.54
1	F	466	LEU	CA-C	-8.22	1.42	1.52
1	D	513	SER	CA-C	-8.22	1.41	1.52
1	F	505	VAL	CA-CB	8.22	1.64	1.54
1	F	564	VAL	CA-CB	8.22	1.65	1.54
1	C	514	ILE	CA-C	-8.21	1.42	1.52
1	D	578	ALA	C-O	8.20	1.33	1.24
1	A	432	LEU	CA-C	-8.19	1.42	1.52
1	C	566	ILE	CA-CB	8.17	1.66	1.54
1	D	587	ILE	CA-CB	-8.17	1.47	1.54
1	B	515	ALA	CA-CB	8.13	1.66	1.53
1	A	521	ALA	CA-CB	8.13	1.66	1.53
1	F	592	ILE	CA-CB	8.11	1.65	1.54
1	C	513	SER	N-CA	8.09	1.56	1.46
1	D	419	PHE	C-O	8.07	1.34	1.23
1	C	483	LYS	N-CA	8.06	1.56	1.46
1	A	592	ILE	CA-CB	8.03	1.66	1.54
1	E	535	GLY	N-CA	7.99	1.54	1.45
1	D	553	ILE	CA-CB	7.99	1.64	1.54
1	D	564	VAL	CA-CB	7.93	1.65	1.54
1	D	442	VAL	CA-C	7.91	1.61	1.52
1	B	518	VAL	N-CA	-7.88	1.37	1.46
1	C	449	VAL	C-O	-7.88	1.16	1.24
1	D	506	GLU	C-O	7.87	1.33	1.24
1	D	472	GLU	CA-C	7.84	1.62	1.52
1	E	543	VAL	CA-C	7.83	1.61	1.52
1	C	565	ILE	CA-CB	7.81	1.64	1.54
1	C	459	ARG	C-O	7.76	1.33	1.23
1	C	587	ILE	CA-C	7.74	1.61	1.52
1	F	481	ILE	CA-CB	7.72	1.62	1.54
1	D	507	GLY	C-O	-7.69	1.16	1.23
1	F	499	VAL	CA-C	7.68	1.61	1.53
1	A	441	ILE	CA-CB	7.68	1.68	1.55
1	C	449	VAL	CA-C	-7.65	1.43	1.52
1	D	471	ARG	N-CA	-7.65	1.37	1.46
1	D	429	VAL	C-O	-7.62	1.16	1.24
1	B	450	THR	CA-C	7.61	1.60	1.52
1	B	479	ALA	CA-CB	7.59	1.65	1.53
1	E	516	THR	C-O	7.58	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	452	SER	CA-C	7.56	1.63	1.52
1	E	545	PRO	C-O	7.55	1.32	1.23
1	D	535	GLY	N-CA	7.51	1.56	1.45
1	C	597	GLU	CD-OE2	7.48	1.39	1.25
1	B	571	ILE	CA-C	7.47	1.62	1.52
1	B	595	VAL	CA-CB	-7.45	1.46	1.54
1	E	514	ILE	CA-CB	7.42	1.63	1.54
1	E	514	ILE	CA-C	7.36	1.61	1.52
1	A	571	ILE	CA-CB	7.34	1.63	1.54
1	C	592	ILE	CA-CB	7.32	1.64	1.54
1	D	426	VAL	CA-CB	7.30	1.62	1.54
1	A	481	ILE	CA-C	7.30	1.61	1.52
1	F	612	LYS	CD-CE	7.27	1.74	1.52
1	F	531	VAL	C-O	7.26	1.32	1.24
1	B	429	VAL	CA-CB	7.26	1.63	1.54
1	E	421	THR	CA-CB	7.25	1.65	1.53
1	B	481	ILE	CA-C	7.25	1.61	1.52
1	B	567	PRO	CA-C	7.24	1.61	1.52
1	C	520	SER	C-O	-7.24	1.15	1.24
1	D	539	VAL	CB-CG1	7.22	1.76	1.52
1	F	583	LYS	N-CA	7.21	1.55	1.46
1	D	447	ALA	CA-CB	-7.21	1.37	1.53
1	D	470	ALA	CA-C	7.19	1.61	1.52
1	F	471	ARG	C-O	-7.19	1.15	1.24
1	B	526	PRO	C-O	7.17	1.32	1.23
1	E	474	VAL	CA-CB	7.17	1.63	1.54
1	B	482	LYS	CG-CD	7.17	1.74	1.52
1	F	474	VAL	CB-CG1	7.16	1.76	1.52
1	C	549	VAL	N-CA	7.16	1.55	1.46
1	D	489	ILE	CA-CB	7.15	1.64	1.54
1	D	551	GLN	CD-OE1	7.11	1.37	1.23
1	B	599	VAL	N-CA	7.09	1.52	1.46
1	B	429	VAL	N-CA	7.09	1.54	1.46
1	C	555	ALA	CA-CB	7.08	1.64	1.53
1	E	479	ALA	C-O	-7.07	1.16	1.24
1	E	505	VAL	CA-CB	7.05	1.64	1.54
1	E	587	ILE	N-CA	7.03	1.52	1.46
1	D	539	VAL	N-CA	7.02	1.55	1.46
1	F	532	ALA	CA-CB	7.02	1.64	1.53
1	D	574	VAL	CA-CB	6.99	1.60	1.53
1	D	531	VAL	CA-C	6.98	1.61	1.52
1	A	472	GLU	CA-C	6.98	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	521	ALA	C-O	-6.97	1.16	1.24
1	A	465	ARG	CA-C	6.94	1.62	1.52
1	D	481	ILE	CA-CB	6.91	1.62	1.54
1	D	471	ARG	CD-NE	6.90	1.55	1.46
1	D	431	GLY	C-O	6.88	1.29	1.23
1	D	514	ILE	CA-CB	6.88	1.63	1.54
1	A	531	VAL	CA-C	6.86	1.61	1.52
1	C	599	VAL	N-CA	6.85	1.52	1.46
1	D	477	VAL	C-O	6.84	1.32	1.24
1	A	606	LYS	N-CA	6.84	1.54	1.46
1	B	448	GLU	C-O	-6.84	1.15	1.23
1	B	461	ILE	CA-C	6.83	1.61	1.52
1	E	480	ILE	CA-CB	6.83	1.61	1.54
1	E	543	VAL	N-CA	-6.80	1.38	1.46
1	A	516	THR	C-O	-6.80	1.16	1.24
1	C	502	TYR	CE1-CZ	6.80	1.54	1.38
1	C	442	VAL	N-CA	6.79	1.54	1.46
1	B	512	ILE	CA-CB	6.79	1.63	1.54
1	B	445	ILE	CA-C	-6.77	1.44	1.52
1	D	555	ALA	C-O	-6.77	1.16	1.24
1	C	477	VAL	CA-C	6.76	1.60	1.52
1	F	442	VAL	CA-CB	6.76	1.62	1.54
1	F	470	ALA	N-CA	6.76	1.54	1.46
1	A	498	PHE	C-O	-6.75	1.15	1.24
1	F	594	GLU	CD-OE1	-6.75	1.12	1.25
1	A	574	VAL	CA-CB	6.74	1.60	1.53
1	F	504	GLY	C-O	-6.74	1.15	1.24
1	A	446	ILE	N-CA	6.72	1.53	1.46
1	D	469	ILE	CA-CB	6.72	1.62	1.54
1	D	497	GLN	C-O	-6.72	1.15	1.23
1	A	522	ILE	N-CA	-6.71	1.38	1.46
1	F	450	THR	C-O	-6.68	1.18	1.24
1	C	567	PRO	CA-C	6.68	1.61	1.52
1	B	442	VAL	CA-C	6.67	1.61	1.52
1	A	517	ALA	CA-CB	6.66	1.63	1.53
1	F	558	GLN	C-O	-6.66	1.16	1.24
1	C	531	VAL	C-O	6.66	1.31	1.24
1	C	462	ALA	CA-CB	-6.65	1.42	1.53
1	E	559	ALA	N-CA	6.65	1.54	1.46
1	C	517	ALA	C-O	-6.63	1.16	1.24
1	C	429	VAL	C-O	-6.62	1.17	1.24
1	D	546	VAL	CA-CB	6.61	1.65	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	547	GLY	C-O	6.61	1.29	1.23
1	D	525	ILE	CA-CB	-6.59	1.49	1.54
1	A	516	THR	CA-CB	6.58	1.63	1.53
1	E	588	PRO	CA-CB	-6.58	1.45	1.53
1	D	506	GLU	CB-CG	-6.58	1.32	1.52
1	F	508	ASP	N-CA	6.57	1.54	1.45
1	E	433	ALA	CA-CB	6.57	1.63	1.54
1	C	598	HIS	C-N	6.56	1.39	1.33
1	E	522	ILE	CB-CG2	6.56	1.74	1.52
1	F	584	ILE	C-O	-6.56	1.17	1.23
1	D	571	ILE	CB-CG2	6.55	1.74	1.52
1	A	586	VAL	C-O	-6.51	1.17	1.24
1	C	428	ARG	CB-CG	6.50	1.72	1.52
1	D	565	ILE	CA-CB	-6.48	1.46	1.54
1	F	460	VAL	CA-CB	-6.48	1.46	1.54
1	E	428	ARG	CA-C	-6.48	1.44	1.52
1	E	434	VAL	CA-CB	6.46	1.63	1.54
1	A	561	LEU	N-CA	6.45	1.54	1.45
1	F	592	ILE	C-O	6.42	1.31	1.24
1	C	522	ILE	CB-CG2	6.41	1.73	1.52
1	F	509	SER	CA-C	-6.41	1.44	1.53
1	E	571	ILE	N-CA	6.40	1.54	1.46
1	A	520	SER	C-O	-6.40	1.16	1.24
1	E	445	ILE	CG1-CD1	6.38	1.76	1.51
1	D	577	ASP	CG-OD2	6.37	1.37	1.25
1	A	584	ILE	CA-CB	6.37	1.64	1.54
1	F	611	SER	CA-C	6.37	1.61	1.52
1	A	514	ILE	CA-C	-6.37	1.45	1.52
1	B	542	GLU	CA-C	-6.35	1.44	1.53
1	A	517	ALA	CA-C	6.35	1.61	1.52
1	D	424	TYR	N-CA	-6.34	1.38	1.46
1	C	503	GLU	CB-CG	6.33	1.71	1.52
1	A	460	VAL	CA-C	-6.33	1.44	1.52
1	A	555	ALA	CA-C	6.31	1.60	1.52
1	C	485	THR	CA-CB	6.29	1.64	1.53
1	E	539	VAL	CA-CB	-6.28	1.45	1.54
1	E	515	ALA	C-O	6.28	1.31	1.24
1	C	562	LYS	C-O	-6.28	1.15	1.24
1	E	519	ILE	N-CA	-6.28	1.39	1.46
1	C	485	THR	CA-C	6.27	1.61	1.52
1	F	586	VAL	CA-CB	6.27	1.61	1.54
1	C	428	ARG	N-CA	-6.26	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	522	ILE	CA-CB	6.24	1.62	1.54
1	D	587	ILE	CB-CG2	6.24	1.73	1.52
1	A	593	ASN	N-CA	-6.24	1.38	1.46
1	F	445	ILE	N-CA	6.22	1.53	1.46
1	F	541	GLY	C-O	-6.22	1.16	1.24
1	A	565	ILE	CA-CB	6.21	1.61	1.54
1	D	426	VAL	CA-C	6.21	1.59	1.52
1	C	472	GLU	CG-CD	6.20	1.67	1.52
1	A	599	VAL	CA-CB	6.19	1.61	1.54
1	A	490	SER	C-O	-6.18	1.16	1.24
1	B	459	ARG	CA-C	6.18	1.60	1.52
1	C	499	VAL	C-O	6.17	1.31	1.23
1	E	461	ILE	CG1-CD1	6.17	1.75	1.51
1	D	440	GLY	C-O	-6.17	1.15	1.23
1	C	538	SER	C-O	6.14	1.32	1.23
1	C	476	ASN	CA-C	6.13	1.60	1.52
1	C	540	LYS	CA-C	-6.12	1.44	1.52
1	B	587	ILE	C-N	6.11	1.40	1.33
1	B	592	ILE	CA-C	6.11	1.61	1.52
1	F	449	VAL	N-CA	-6.11	1.39	1.46
1	A	434	VAL	N-CA	6.10	1.53	1.46
1	A	512	ILE	CA-CB	6.08	1.62	1.54
1	F	429	VAL	N-CA	-6.08	1.39	1.46
1	E	596	LEU	CA-C	-6.08	1.45	1.52
1	D	468	GLU	C-O	-6.07	1.17	1.24
1	F	518	VAL	N-CA	-6.07	1.39	1.46
1	F	520	SER	C-O	-6.07	1.16	1.24
1	C	589	VAL	C-O	6.07	1.29	1.24
1	E	439	ALA	CA-C	6.06	1.60	1.52
1	A	546	VAL	CA-CB	6.06	1.64	1.55
1	C	526	PRO	CA-C	6.06	1.60	1.52
1	E	460	VAL	CA-CB	6.05	1.61	1.54
1	C	465	ARG	N-CA	-6.05	1.38	1.46
1	A	525	ILE	CA-C	6.04	1.58	1.52
1	C	506	GLU	C-O	6.03	1.31	1.24
1	D	423	GLY	C-O	-6.03	1.13	1.24
1	F	589	VAL	N-CA	-6.03	1.39	1.46
1	D	509	SER	C-O	-6.03	1.16	1.23
1	E	474	VAL	N-CA	6.03	1.53	1.46
1	B	420	ILE	CA-CB	6.03	1.62	1.54
1	B	471	ARG	CA-C	-6.02	1.44	1.52
1	C	601	GLU	N-CA	-6.02	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	592	ILE	CA-C	6.02	1.60	1.52
1	A	542	GLU	CA-C	6.01	1.60	1.52
1	F	561	LEU	C-O	-6.00	1.16	1.23
1	B	521	ALA	CA-CB	-6.00	1.44	1.53
1	D	597	GLU	CG-CD	5.99	1.67	1.52
1	B	501	THR	CA-CB	5.99	1.63	1.53
1	C	596	LEU	CA-CB	5.99	1.62	1.53
1	B	519	ILE	N-CA	-5.99	1.39	1.46
1	F	589	VAL	C-O	5.98	1.30	1.23
1	C	476	ASN	N-CA	5.96	1.53	1.46
1	F	503	GLU	N-CA	-5.95	1.38	1.46
1	B	465	ARG	N-CA	-5.93	1.38	1.46
1	B	478	SER	N-CA	5.93	1.53	1.46
1	B	507	GLY	N-CA	5.93	1.50	1.44
1	C	441	ILE	C-O	-5.93	1.17	1.23
1	A	566	ILE	CB-CG1	5.92	1.65	1.53
1	C	528	ASP	N-CA	5.92	1.53	1.46
1	D	532	ALA	CA-CB	-5.92	1.44	1.53
1	C	565	ILE	N-CA	-5.92	1.39	1.46
1	A	540	LYS	C-O	-5.90	1.16	1.24
1	C	529	GLN	CD-OE1	5.90	1.34	1.23
1	A	547	GLY	N-CA	-5.89	1.37	1.45
1	F	529	GLN	N-CA	5.88	1.53	1.46
1	C	535	GLY	N-CA	5.87	1.52	1.45
1	E	498	PHE	CA-C	-5.87	1.45	1.52
1	E	445	ILE	CA-CB	5.87	1.61	1.54
1	E	493	ASP	C-O	5.86	1.31	1.24
1	F	594	GLU	CB-CG	5.86	1.70	1.52
1	E	459	ARG	C-O	-5.86	1.16	1.23
1	E	517	ALA	CA-C	5.85	1.60	1.52
1	C	490	SER	CA-C	5.84	1.60	1.52
1	E	512	ILE	CG1-CD1	5.84	1.74	1.51
1	D	581	GLU	C-O	-5.84	1.16	1.24
1	A	566	ILE	CA-C	-5.83	1.47	1.52
1	C	588	PRO	N-CA	-5.83	1.40	1.47
1	A	556	ALA	CA-CB	5.81	1.62	1.53
1	D	559	ALA	CA-CB	5.81	1.63	1.53
1	C	461	ILE	CG1-CD1	-5.80	1.29	1.51
1	B	552	LYS	N-CA	-5.80	1.39	1.46
1	D	573	ASP	C-O	-5.80	1.16	1.24
1	D	588	PRO	C-O	-5.79	1.18	1.23
1	E	477	VAL	CB-CG1	5.78	1.71	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	475	MET	C-O	-5.78	1.17	1.24
1	D	446	ILE	CA-CB	5.78	1.61	1.54
1	E	481	ILE	N-CA	5.78	1.53	1.46
1	B	596	LEU	CA-CB	5.78	1.62	1.53
1	C	518	VAL	N-CA	-5.77	1.39	1.46
1	D	465	ARG	CA-C	5.76	1.60	1.52
1	E	450	THR	CA-CB	5.76	1.62	1.53
1	B	493	ASP	CA-CB	5.75	1.60	1.53
1	B	440	GLY	C-O	-5.75	1.16	1.23
1	B	429	VAL	CB-CG2	-5.74	1.33	1.52
1	C	519	ILE	CA-CB	5.74	1.61	1.54
1	A	434	VAL	CA-CB	5.73	1.61	1.54
1	E	567	PRO	CA-C	5.73	1.59	1.52
1	C	572	ASP	CA-C	5.73	1.60	1.52
1	D	545	PRO	C-O	5.72	1.30	1.23
1	B	477	VAL	C-O	-5.72	1.16	1.24
1	F	421	THR	N-CA	5.71	1.53	1.46
1	A	592	ILE	C-O	-5.70	1.17	1.24
1	F	560	GLY	CA-C	5.70	1.59	1.51
1	D	468	GLU	CD-OE1	5.70	1.36	1.25
1	E	467	GLN	CA-C	5.68	1.60	1.52
1	A	564	VAL	CA-CB	5.68	1.61	1.54
1	E	527	VAL	CA-C	5.68	1.59	1.52
1	C	503	GLU	CG-CD	5.68	1.66	1.52
1	E	527	VAL	CB-CG1	5.67	1.71	1.52
1	F	466	LEU	C-O	-5.67	1.16	1.24
1	C	429	VAL	CA-CB	5.66	1.62	1.54
1	D	529	GLN	CD-OE1	-5.65	1.12	1.23
1	E	445	ILE	CB-CG2	5.65	1.71	1.52
1	C	597	GLU	CB-CG	5.64	1.69	1.52
1	D	421	THR	CA-CB	-5.64	1.44	1.53
1	F	493	ASP	CA-C	5.64	1.59	1.52
1	C	538	SER	N-CA	-5.63	1.38	1.45
1	C	516	THR	C-O	5.62	1.30	1.24
1	A	469	ILE	C-O	5.62	1.30	1.24
1	E	481	ILE	CA-CB	5.61	1.61	1.54
1	D	597	GLU	N-CA	5.61	1.53	1.46
1	A	480	ILE	N-CA	5.60	1.53	1.46
1	E	461	ILE	CA-CB	5.60	1.60	1.53
1	A	430	ASN	N-CA	5.59	1.53	1.46
1	F	502	TYR	CB-CG	5.59	1.64	1.51
1	C	483	LYS	CA-C	5.58	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	429	VAL	C-O	-5.58	1.18	1.24
1	A	496	ILE	CA-CB	5.58	1.62	1.54
1	F	440	GLY	N-CA	5.57	1.50	1.44
1	C	606	LYS	CG-CD	-5.55	1.35	1.52
1	D	543	VAL	CA-C	-5.55	1.45	1.52
1	A	590	SER	CA-C	-5.55	1.45	1.52
1	B	517	ALA	CA-CB	5.55	1.62	1.53
1	E	589	VAL	CA-CB	5.54	1.62	1.54
1	A	461	ILE	CA-CB	5.54	1.60	1.53
1	E	571	ILE	CA-CB	5.54	1.61	1.54
1	D	613	PHE	CA-C	-5.53	1.45	1.52
1	D	565	ILE	C-O	5.53	1.30	1.24
1	B	537	LEU	CA-CB	-5.53	1.45	1.53
1	B	526	PRO	N-CA	5.53	1.53	1.47
1	D	550	THR	C-O	-5.52	1.17	1.24
1	F	522	ILE	CB-CG2	5.52	1.70	1.52
1	D	581	GLU	N-CA	5.51	1.53	1.46
1	A	528	ASP	C-O	5.51	1.30	1.24
1	B	601	GLU	C-O	5.51	1.30	1.23
1	B	565	ILE	CA-CB	-5.50	1.47	1.53
1	D	463	THR	C-O	5.50	1.30	1.24
1	C	470	ALA	CA-CB	-5.50	1.44	1.53
1	D	428	ARG	CB-CG	5.49	1.69	1.52
1	D	477	VAL	CA-C	5.48	1.60	1.52
1	B	497	GLN	CA-C	5.47	1.59	1.52
1	A	496	ILE	C-O	-5.46	1.18	1.24
1	A	593	ASN	C-O	-5.46	1.17	1.24
1	A	603	GLY	CA-C	-5.46	1.46	1.51
1	E	495	HIS	CA-CB	5.46	1.60	1.53
1	F	577	ASP	N-CA	-5.46	1.39	1.46
1	D	516	THR	CA-CB	5.46	1.61	1.53
1	F	457	GLU	CA-C	5.46	1.64	1.52
1	C	574	VAL	N-CA	-5.46	1.40	1.46
1	A	425	GLU	CA-C	-5.45	1.46	1.52
1	B	592	ILE	CA-CB	5.44	1.62	1.54
1	C	601	GLU	C-O	5.44	1.30	1.23
1	B	564	VAL	CB-CG2	5.43	1.70	1.52
1	B	425	GLU	CA-C	-5.43	1.46	1.52
1	D	528	ASP	C-O	5.42	1.30	1.23
1	F	443	LEU	C-O	5.42	1.31	1.24
1	D	561	LEU	N-CA	5.42	1.52	1.45
1	C	543	VAL	CA-CB	5.41	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	506	GLU	CB-CG	-5.41	1.36	1.52
1	B	527	VAL	CA-C	5.41	1.59	1.52
1	D	524	GLY	C-N	5.41	1.37	1.33
1	D	552	LYS	N-CA	5.41	1.52	1.46
1	B	482	LYS	CB-CG	5.41	1.68	1.52
1	D	604	LYS	N-CA	-5.40	1.39	1.46
1	B	527	VAL	CB-CG1	5.39	1.70	1.52
1	C	584	ILE	C-O	-5.39	1.18	1.23
1	D	505	VAL	CA-CB	-5.39	1.47	1.54
1	D	596	LEU	CG-CD2	5.39	1.70	1.52
1	A	492	MET	CA-C	-5.38	1.46	1.52
1	B	612	LYS	CA-C	5.38	1.59	1.52
1	A	542	GLU	CG-CD	5.38	1.65	1.52
1	C	449	VAL	CB-CG1	5.38	1.70	1.52
1	F	597	GLU	CG-CD	5.38	1.65	1.52
1	D	434	VAL	N-CA	5.37	1.52	1.46
1	F	498	PHE	CA-C	-5.37	1.46	1.52
1	D	432	LEU	N-CA	-5.36	1.39	1.45
1	E	549	VAL	CA-CB	-5.36	1.47	1.54
1	E	489	ILE	CA-C	5.36	1.59	1.52
1	F	459	ARG	CZ-NH1	5.36	1.40	1.32
1	A	464	GLY	N-CA	5.34	1.54	1.45
1	C	530	SER	CA-C	-5.34	1.45	1.52
1	F	539	VAL	CA-CB	5.34	1.62	1.54
1	A	542	GLU	CD-OE2	5.33	1.35	1.25
1	D	444	PRO	CA-C	5.33	1.58	1.52
1	D	527	VAL	CB-CG2	-5.33	1.34	1.52
1	F	446	ILE	CA-CB	5.33	1.61	1.54
1	D	517	ALA	CA-CB	5.33	1.61	1.53
1	F	426	VAL	CA-C	5.33	1.58	1.52
1	E	498	PHE	CA-CB	-5.32	1.45	1.53
1	E	499	VAL	CA-CB	5.32	1.60	1.54
1	A	505	VAL	CA-CB	5.32	1.60	1.54
1	B	426	VAL	CA-CB	5.31	1.60	1.54
1	E	506	GLU	CA-C	5.31	1.59	1.52
1	F	597	GLU	CD-OE2	5.31	1.35	1.25
1	B	421	THR	CA-CB	5.30	1.62	1.53
1	C	504	GLY	C-O	-5.30	1.16	1.24
1	E	558	GLN	CG-CD	5.30	1.65	1.52
1	F	535	GLY	C-O	5.30	1.31	1.23
1	B	502	TYR	N-CA	5.30	1.52	1.45
1	F	526	PRO	CA-C	5.30	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	520	SER	CA-C	-5.29	1.46	1.52
1	B	556	ALA	CA-C	5.29	1.59	1.52
1	F	420	ILE	CA-CB	5.28	1.61	1.54
1	D	450	THR	CA-C	5.28	1.57	1.52
1	F	472	GLU	CB-CG	5.28	1.68	1.52
1	E	532	ALA	CA-CB	-5.27	1.45	1.53
1	D	510	ALA	N-CA	5.27	1.54	1.46
1	F	418	LEU	CG-CD1	-5.27	1.35	1.52
1	C	453	MET	CB-CG	5.27	1.68	1.52
1	F	525	ILE	C-O	-5.26	1.18	1.23
1	A	566	ILE	N-CA	5.26	1.51	1.46
1	D	493	ASP	CA-C	-5.26	1.46	1.52
1	F	559	ALA	CA-C	5.25	1.60	1.52
1	D	598	HIS	CA-C	5.25	1.59	1.52
1	B	597	GLU	C-O	-5.25	1.17	1.24
1	A	551	GLN	C-O	-5.25	1.17	1.24
1	B	551	GLN	N-CA	5.25	1.52	1.46
1	E	497	GLN	CA-C	5.25	1.59	1.52
1	D	471	ARG	NE-CZ	5.25	1.38	1.33
1	C	449	VAL	N-CA	5.24	1.52	1.46
1	D	603	GLY	N-CA	5.24	1.50	1.45
1	C	574	VAL	CA-C	5.24	1.58	1.53
1	E	495	HIS	C-O	-5.24	1.17	1.24
1	E	509	SER	CA-C	-5.24	1.46	1.52
1	C	484	TYR	CA-CB	5.24	1.62	1.53
1	B	439	ALA	CA-CB	5.23	1.58	1.53
1	F	462	ALA	N-CA	5.23	1.52	1.45
1	C	578	ALA	CA-CB	5.22	1.61	1.53
1	C	502	TYR	CZ-OH	5.22	1.49	1.38
1	F	511	SER	C-O	5.22	1.30	1.24
1	D	552	LYS	C-O	-5.22	1.18	1.24
1	D	478	SER	N-CA	5.22	1.52	1.46
1	E	542	GLU	N-CA	5.21	1.52	1.45
1	F	474	VAL	CA-C	-5.21	1.46	1.52
1	B	585	GLU	CA-C	5.21	1.59	1.52
1	C	518	VAL	CB-CG2	5.20	1.69	1.52
1	D	430	ASN	N-CA	5.19	1.53	1.46
1	D	470	ALA	N-CA	5.19	1.52	1.46
1	C	606	LYS	N-CA	5.18	1.52	1.46
1	E	445	ILE	N-CA	5.18	1.52	1.46
1	F	597	GLU	CD-OE1	5.18	1.35	1.25
1	B	557	ILE	CA-CB	5.17	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	522	ILE	CG1-CD1	-5.17	1.31	1.51
1	E	464	GLY	C-O	5.17	1.30	1.23
1	B	481	ILE	N-CA	5.16	1.52	1.46
1	C	500	GLY	N-CA	5.16	1.52	1.45
1	B	587	ILE	C-O	5.16	1.28	1.23
1	E	599	VAL	CA-C	-5.15	1.46	1.52
1	F	552	LYS	CA-C	5.14	1.59	1.52
1	A	593	ASN	CB-CG	5.13	1.64	1.52
1	A	494	VAL	CA-CB	-5.13	1.48	1.54
1	D	596	LEU	N-CA	-5.13	1.40	1.46
1	A	509	SER	C-O	-5.12	1.17	1.24
1	F	472	GLU	C-O	-5.12	1.17	1.24
1	B	522	ILE	CG1-CD1	-5.12	1.31	1.51
1	D	499	VAL	CB-CG2	5.12	1.69	1.52
1	F	506	GLU	C-O	5.11	1.30	1.24
1	C	424	TYR	CA-C	-5.10	1.46	1.52
1	A	602	ASP	N-CA	5.10	1.52	1.46
1	A	507	GLY	C-N	-5.09	1.26	1.33
1	E	442	VAL	CA-C	5.09	1.58	1.52
1	F	471	ARG	CZ-NH1	5.09	1.39	1.32
1	D	552	LYS	CE-NZ	5.09	1.64	1.49
1	C	537	LEU	CA-CB	5.08	1.60	1.53
1	B	562	LYS	C-O	-5.07	1.17	1.24
1	C	473	ALA	CA-C	5.07	1.59	1.52
1	D	496	ILE	CA-CB	5.06	1.62	1.54
1	B	445	ILE	CG1-CD1	5.05	1.71	1.51
1	C	446	ILE	C-O	-5.05	1.19	1.24
1	F	568	LYS	CD-CE	5.05	1.67	1.52
1	D	547	GLY	C-N	5.04	1.39	1.33
1	C	472	GLU	CB-CG	5.04	1.67	1.52
1	B	500	GLY	N-CA	-5.02	1.40	1.45
1	D	469	ILE	CA-C	-5.02	1.46	1.52
1	D	536	SER	C-O	5.02	1.30	1.24
1	C	514	ILE	C-O	-5.02	1.18	1.24
1	F	569	ASP	C-O	-5.02	1.17	1.24
1	E	475	MET	N-CA	-5.02	1.40	1.46
1	A	613	PHE	C-O	-5.02	1.17	1.24
1	A	609	LEU	C-O	5.01	1.29	1.24
1	E	581	GLU	C-O	5.01	1.29	1.24
1	F	585	GLU	C-O	-5.00	1.18	1.24

All (303) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	523	GLU	N-CA-C	-10.93	99.51	113.72
1	B	479	ALA	N-CA-C	-10.66	99.35	110.97
1	F	509	SER	N-CA-C	-10.47	95.03	110.52
1	D	506	GLU	CA-C-N	-10.38	111.99	122.27
1	D	506	GLU	C-N-CA	-10.38	111.99	122.27
1	B	474	VAL	N-CA-C	9.90	120.52	110.23
1	E	479	ALA	N-CA-C	-9.67	100.70	111.14
1	B	506	GLU	CA-C-N	-9.30	114.15	122.43
1	B	506	GLU	C-N-CA	-9.30	114.15	122.43
1	B	565	ILE	CB-CA-C	-9.24	98.95	111.33
1	F	498	PHE	N-CA-C	-9.06	94.47	109.24
1	A	479	ALA	N-CA-C	-8.92	101.00	112.23
1	C	509	SER	N-CA-C	-8.87	98.00	110.50
1	A	446	ILE	CB-CA-C	-8.84	97.44	110.62
1	E	544	LEU	CA-C-N	8.82	128.86	119.78
1	E	544	LEU	C-N-CA	8.82	128.86	119.78
1	D	573	ASP	N-CA-C	-8.75	102.61	113.38
1	B	480	ILE	N-CA-CB	8.74	120.15	110.62
1	D	598	HIS	N-CA-C	8.60	120.73	111.36
1	C	569	ASP	N-CA-C	8.36	122.90	112.87
1	E	544	LEU	N-CA-C	-8.28	97.63	110.14
1	C	446	ILE	N-CA-C	-8.17	96.72	108.48
1	D	507	GLY	O-C-N	-8.11	115.18	122.88
1	D	443	LEU	CA-C-N	8.04	128.34	119.90
1	D	443	LEU	C-N-CA	8.04	128.34	119.90
1	A	520	SER	N-CA-C	7.99	120.70	111.11
1	B	445	ILE	CB-CA-C	-7.96	99.75	110.98
1	D	470	ALA	N-CA-C	7.89	119.67	111.14
1	F	465	ARG	N-CA-C	7.72	121.80	112.38
1	F	482	LYS	N-CA-C	7.65	120.70	111.82
1	E	445	ILE	CB-CA-C	-7.64	99.44	110.83
1	F	574	VAL	N-CA-C	-7.62	95.30	106.88
1	F	502	TYR	N-CA-C	7.60	124.89	107.48
1	D	468	GLU	N-CA-C	-7.57	102.97	111.07
1	A	446	ILE	CA-CB-CG2	7.56	123.35	110.50
1	F	549	VAL	N-CA-C	7.54	118.31	110.62
1	E	470	ALA	N-CA-C	-7.49	103.12	111.28
1	B	516	THR	N-CA-C	-7.46	103.64	112.89
1	B	525	ILE	CA-C-N	7.46	127.50	119.89
1	B	525	ILE	C-N-CA	7.46	127.50	119.89
1	C	472	GLU	CB-CG-CD	7.40	125.18	112.60
1	C	467	GLN	N-CA-C	7.40	121.22	111.75
1	C	546	VAL	CA-C-N	-7.40	114.94	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	546	VAL	C-N-CA	-7.40	114.94	122.27
1	C	597	GLU	CB-CG-CD	7.40	125.17	112.60
1	B	599	VAL	CB-CA-C	-7.38	103.69	110.63
1	C	596	LEU	N-CA-C	7.38	119.32	111.28
1	D	448	GLU	CA-CB-CG	-7.34	99.42	114.10
1	A	489	ILE	N-CA-C	7.33	121.28	111.17
1	F	519	ILE	N-CA-C	-7.32	103.65	110.53
1	D	450	THR	CA-C-N	-7.29	112.25	119.76
1	D	450	THR	C-N-CA	-7.29	112.25	119.76
1	C	446	ILE	CB-CG1-CD1	-7.25	98.58	113.80
1	F	479	ALA	CA-C-N	7.25	130.26	120.77
1	F	479	ALA	C-N-CA	7.25	130.26	120.77
1	B	614	LYS	N-CA-C	-7.21	95.44	110.80
1	C	463	THR	CA-CB-CG2	7.21	122.76	110.50
1	E	446	ILE	N-CA-C	-7.15	98.18	108.48
1	A	505	VAL	N-CA-C	7.04	118.03	108.17
1	F	569	ASP	N-CA-C	6.99	121.40	113.01
1	E	471	ARG	NE-CZ-NH2	-6.97	112.92	119.20
1	B	539	VAL	N-CA-C	6.94	119.72	111.05
1	A	604	LYS	N-CA-C	6.93	118.84	111.28
1	B	480	ILE	CA-CB-CG2	6.93	122.28	110.50
1	A	466	LEU	N-CA-C	6.92	121.74	113.16
1	C	483	LYS	N-CA-C	6.91	125.51	110.80
1	A	480	ILE	N-CA-CB	6.90	119.41	110.57
1	E	566	ILE	CA-C-N	-6.89	112.39	119.83
1	E	566	ILE	C-N-CA	-6.89	112.39	119.83
1	F	509	SER	CA-C-O	-6.89	113.59	121.72
1	F	443	LEU	CA-C-N	-6.89	112.55	119.99
1	F	443	LEU	C-N-CA	-6.89	112.55	119.99
1	F	550	THR	N-CA-C	-6.87	103.24	111.69
1	E	445	ILE	CB-CG1-CD1	6.83	128.15	113.80
1	C	508	ASP	N-CA-CB	6.82	120.06	109.48
1	C	502	TYR	CA-CB-CG	-6.80	101.65	113.90
1	C	445	ILE	CB-CA-C	-6.77	100.40	110.82
1	C	577	ASP	N-CA-C	6.77	119.06	110.33
1	A	465	ARG	CB-CG-CD	6.75	126.84	111.30
1	C	441	ILE	CB-CA-C	-6.67	98.78	110.71
1	C	481	ILE	N-CA-C	6.66	117.16	110.23
1	C	478	SER	CA-C-N	6.66	134.26	121.54
1	C	478	SER	C-N-CA	6.66	134.26	121.54
1	A	556	ALA	N-CA-C	-6.62	104.15	111.36
1	E	469	ILE	N-CA-C	6.61	119.36	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	500	GLY	N-CA-C	6.61	118.23	111.95
1	F	479	ALA	O-C-N	6.61	128.90	122.03
1	A	580	HIS	N-CA-C	6.59	119.47	111.82
1	E	596	LEU	N-CA-C	-6.56	103.39	111.40
1	E	516	THR	N-CA-C	-6.56	104.21	111.36
1	B	470	ALA	N-CA-C	-6.54	103.26	111.11
1	F	446	ILE	CA-CB-CG2	6.50	121.55	110.50
1	A	549	VAL	N-CA-C	6.50	117.28	110.72
1	C	614	LYS	N-CA-C	6.48	119.16	110.35
1	D	552	LYS	N-CA-C	6.47	117.99	111.07
1	C	540	LYS	N-CA-C	6.45	121.30	113.17
1	D	597	GLU	CG-CD-OE2	-6.43	103.62	118.40
1	B	522	ILE	N-CA-C	-6.43	104.23	110.72
1	A	446	ILE	N-CA-C	-6.42	99.23	108.48
1	A	461	ILE	N-CA-C	6.41	116.86	107.37
1	E	436	GLY	N-CA-C	-6.40	98.00	113.18
1	C	564	VAL	CB-CA-C	6.38	117.69	110.41
1	F	549	VAL	CG1-CB-CG2	-6.34	96.84	110.80
1	D	542	GLU	N-CA-C	6.33	119.43	110.50
1	D	568	LYS	CB-CG-CD	6.32	125.84	111.30
1	A	544	LEU	CA-C-N	-6.31	113.04	120.11
1	A	544	LEU	C-N-CA	-6.31	113.04	120.11
1	A	481	ILE	CA-CB-CG2	6.31	121.23	110.50
1	B	571	ILE	N-CA-CB	-6.30	101.97	110.54
1	C	463	THR	N-CA-CB	-6.30	101.27	111.22
1	E	492	MET	N-CA-C	6.26	119.40	109.50
1	D	428	ARG	CG-CD-NE	6.24	125.73	112.00
1	D	429	VAL	CB-CA-C	6.23	119.43	110.33
1	B	606	LYS	N-CA-C	-6.23	104.57	111.36
1	F	475	MET	N-CA-C	6.22	118.58	111.11
1	C	446	ILE	CA-CB-CG2	6.21	121.06	110.50
1	A	603	GLY	O-C-N	6.21	129.80	123.78
1	C	452	SER	N-CA-C	6.20	119.95	112.38
1	D	615	GLU	N-CA-C	6.20	128.34	111.00
1	D	530	SER	CA-C-N	6.19	131.17	123.12
1	D	530	SER	C-N-CA	6.19	131.17	123.12
1	C	509	SER	CA-C-O	-6.19	114.81	121.56
1	C	446	ILE	CB-CA-C	-6.18	101.40	110.62
1	A	524	GLY	CA-C-N	-6.18	117.35	123.04
1	A	524	GLY	C-N-CA	-6.18	117.35	123.04
1	B	565	ILE	CB-CG1-CD1	6.18	126.78	113.80
1	D	441	ILE	CB-CG1-CD1	-6.16	100.86	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	608	ARG	N-CA-C	-6.14	104.59	111.28
1	D	495	HIS	N-CA-C	-6.13	98.29	108.34
1	D	480	ILE	N-CA-CB	6.10	120.74	110.56
1	C	471	ARG	CA-C-N	6.09	128.68	120.65
1	C	471	ARG	C-N-CA	6.09	128.68	120.65
1	A	600	LEU	CB-CG-CD1	-6.06	92.51	110.70
1	C	594	GLU	N-CA-CB	-6.04	101.26	110.01
1	C	590	SER	CA-CB-OG	-6.03	99.03	111.10
1	C	596	LEU	CA-C-N	6.03	128.65	120.38
1	C	596	LEU	C-N-CA	6.03	128.65	120.38
1	D	474	VAL	CB-CA-C	-6.03	103.90	112.22
1	C	471	ARG	CG-CD-NE	-6.03	98.74	112.00
1	B	573	ASP	N-CA-C	-6.02	105.23	113.30
1	E	573	ASP	N-CA-C	-6.02	104.58	113.61
1	D	504	GLY	N-CA-C	-5.96	107.09	115.32
1	E	435	ILE	N-CA-C	-5.96	106.69	112.29
1	F	462	ALA	CA-C-O	-5.96	114.32	120.99
1	B	452	SER	CA-CB-OG	-5.95	99.21	111.10
1	D	434	VAL	CB-CA-C	-5.95	101.76	110.62
1	E	512	ILE	N-CA-C	5.91	118.44	111.05
1	A	509	SER	CA-CB-OG	-5.91	99.28	111.10
1	B	544	LEU	N-CA-C	-5.91	102.14	110.29
1	F	547	GLY	N-CA-C	-5.90	103.56	112.89
1	B	442	VAL	N-CA-CB	5.89	117.83	110.05
1	A	431	GLY	CA-C-N	-5.86	112.29	122.37
1	A	431	GLY	C-N-CA	-5.86	112.29	122.37
1	E	540	LYS	N-CA-C	-5.86	105.79	113.17
1	C	431	GLY	N-CA-C	-5.84	103.20	112.66
1	D	505	VAL	N-CA-C	5.83	116.50	107.99
1	D	441	ILE	CB-CA-C	-5.83	100.27	110.71
1	B	610	MET	N-CA-C	5.82	117.62	111.28
1	F	471	ARG	NE-CZ-NH2	-5.81	113.97	119.20
1	F	447	ALA	CA-C-N	5.80	132.13	122.73
1	F	447	ALA	C-N-CA	5.80	132.13	122.73
1	D	495	HIS	CA-C-N	-5.79	114.89	122.94
1	D	495	HIS	C-N-CA	-5.79	114.89	122.94
1	A	545	PRO	N-CA-C	5.78	119.60	111.33
1	F	421	THR	N-CA-C	5.78	120.45	113.17
1	A	609	LEU	N-CA-C	5.78	118.05	111.11
1	F	496	ILE	N-CA-C	5.77	116.24	108.17
1	F	494	VAL	CB-CA-C	5.76	119.37	111.31
1	A	481	ILE	CB-CA-C	5.75	119.06	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	512	ILE	N-CA-C	5.75	118.24	111.05
1	D	499	VAL	CA-C-N	5.74	131.06	122.05
1	D	499	VAL	C-N-CA	5.74	131.06	122.05
1	D	555	ALA	N-CA-C	-5.72	105.04	111.28
1	E	604	LYS	N-CA-C	5.72	117.97	111.11
1	D	538	SER	O-C-N	-5.71	116.51	122.96
1	D	547	GLY	N-CA-C	5.71	121.90	112.66
1	B	499	VAL	N-CA-C	5.70	116.95	108.23
1	D	435	ILE	CB-CA-C	-5.69	102.70	110.90
1	F	512	ILE	CB-CG1-CD1	-5.69	101.84	113.80
1	F	596	LEU	CA-C-N	5.68	128.16	120.38
1	F	596	LEU	C-N-CA	5.68	128.16	120.38
1	B	492	MET	N-CA-C	5.67	118.13	108.90
1	F	612	LYS	CD-CE-NZ	5.67	130.03	111.90
1	C	579	GLU	CA-C-N	5.65	127.85	120.28
1	C	579	GLU	C-N-CA	5.65	127.85	120.28
1	E	426	VAL	CA-C-N	-5.64	111.92	121.85
1	E	426	VAL	C-N-CA	-5.64	111.92	121.85
1	E	434	VAL	N-CA-CB	5.63	120.60	111.36
1	F	572	ASP	N-CA-C	5.63	120.00	113.18
1	C	487	ARG	CG-CD-NE	-5.63	99.62	112.00
1	C	447	ALA	CA-C-N	5.62	131.83	121.94
1	C	447	ALA	C-N-CA	5.62	131.83	121.94
1	F	594	GLU	OE1-CD-OE2	-5.62	109.41	122.90
1	D	554	GLU	N-CA-C	5.62	117.85	111.11
1	E	471	ARG	N-CA-C	5.59	117.06	111.07
1	C	421	THR	N-CA-C	5.59	120.22	113.17
1	A	480	ILE	CA-CB-CG2	5.58	119.98	110.50
1	D	540	LYS	N-CA-C	-5.58	106.48	113.28
1	C	605	LYS	N-CA-C	5.57	117.03	111.07
1	F	466	LEU	N-CA-C	-5.55	105.20	112.41
1	A	426	VAL	CA-C-N	5.54	131.51	120.77
1	A	426	VAL	C-N-CA	5.54	131.51	120.77
1	C	571	ILE	N-CA-C	-5.53	104.98	110.62
1	F	585	GLU	N-CA-C	-5.53	100.23	109.24
1	F	469	ILE	N-CA-C	5.53	120.83	109.34
1	E	523	GLU	N-CA-C	-5.52	105.76	112.88
1	B	608	ARG	N-CA-CB	5.51	118.77	109.78
1	C	478	SER	N-CA-C	-5.51	105.82	112.54
1	F	592	ILE	N-CA-C	5.51	120.80	109.34
1	B	598	HIS	CA-C-N	-5.49	113.84	121.53
1	B	598	HIS	C-N-CA	-5.49	113.84	121.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	428	ARG	NE-CZ-NH2	5.48	124.13	119.20
1	F	468	GLU	N-CA-CB	5.47	117.91	109.98
1	A	521	ALA	N-CA-C	-5.47	105.23	111.14
1	F	558	GLN	CB-CA-C	-5.47	102.30	110.88
1	D	431	GLY	CA-C-N	-5.46	112.19	121.85
1	D	431	GLY	C-N-CA	-5.46	112.19	121.85
1	A	603	GLY	CA-C-N	5.45	127.59	120.28
1	A	603	GLY	C-N-CA	5.45	127.59	120.28
1	E	480	ILE	N-CA-CB	5.44	116.55	110.51
1	C	513	SER	N-CA-C	5.44	117.21	111.28
1	D	597	GLU	N-CA-CB	5.44	118.11	110.12
1	D	604	LYS	N-CA-C	5.44	117.64	111.11
1	E	421	THR	CA-C-N	5.44	131.10	122.94
1	E	421	THR	C-N-CA	5.44	131.10	122.94
1	D	556	ALA	N-CA-C	-5.43	105.27	111.14
1	C	471	ARG	N-CA-C	5.42	117.19	111.28
1	A	465	ARG	CA-CB-CG	5.42	124.94	114.10
1	A	481	ILE	N-CA-CB	5.41	116.30	110.62
1	A	603	GLY	CA-C-O	-5.38	116.34	121.83
1	A	531	VAL	N-CA-CB	-5.38	104.90	111.67
1	D	506	GLU	CB-CG-CD	-5.37	103.48	112.60
1	D	510	ALA	CA-C-O	5.35	127.65	121.28
1	D	563	LYS	CA-C-N	-5.34	113.79	122.33
1	D	563	LYS	C-N-CA	-5.34	113.79	122.33
1	F	441	ILE	CB-CG1-CD1	-5.33	102.60	113.80
1	B	506	GLU	O-C-N	-5.33	116.47	123.02
1	F	544	LEU	CA-C-N	5.32	125.22	119.85
1	F	544	LEU	C-N-CA	5.32	125.22	119.85
1	B	451	PRO	CB-CA-C	-5.31	104.43	111.23
1	F	524	GLY	CA-C-N	-5.31	115.79	123.28
1	F	524	GLY	C-N-CA	-5.31	115.79	123.28
1	F	550	THR	CA-C-N	5.31	127.34	120.44
1	F	550	THR	C-N-CA	5.31	127.34	120.44
1	F	577	ASP	CB-CA-C	5.31	120.98	110.42
1	E	527	VAL	CA-CB-CG1	5.30	119.41	110.40
1	A	548	GLY	N-CA-C	5.30	121.21	113.48
1	A	558	GLN	CB-CG-CD	-5.30	103.60	112.60
1	F	509	SER	O-C-N	5.29	128.86	122.94
1	B	481	ILE	CB-CG1-CD1	-5.26	102.75	113.80
1	A	587	ILE	CB-CG1-CD1	-5.26	102.76	113.80
1	C	486	GLY	N-CA-C	5.25	125.63	113.18
1	A	613	PHE	CB-CA-C	-5.25	99.97	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	601	GLU	N-CA-C	5.25	117.96	110.24
1	A	568	LYS	N-CA-C	5.25	117.41	111.11
1	F	543	VAL	N-CA-C	5.23	115.31	107.51
1	C	483	LYS	CA-C-N	-5.23	112.46	121.66
1	C	483	LYS	C-N-CA	-5.23	112.46	121.66
1	C	476	ASN	N-CA-C	5.22	121.93	110.80
1	F	512	ILE	N-CA-C	5.22	116.58	110.62
1	A	580	HIS	CA-C-N	5.20	127.25	120.28
1	A	580	HIS	C-N-CA	5.20	127.25	120.28
1	D	471	ARG	CA-C-O	-5.20	115.34	120.90
1	D	572	ASP	N-CA-C	5.19	119.37	113.19
1	F	486	GLY	N-CA-C	-5.18	100.90	113.18
1	E	592	ILE	N-CA-C	5.18	115.39	110.42
1	D	508	ASP	N-CA-CB	-5.17	102.21	110.63
1	D	583	LYS	CD-CE-NZ	5.16	128.43	111.90
1	E	469	ILE	CB-CG1-CD1	-5.16	102.96	113.80
1	E	480	ILE	CA-C-N	5.16	127.75	120.42
1	E	480	ILE	C-N-CA	5.16	127.75	120.42
1	B	418	LEU	CA-CB-CG	5.14	134.30	116.30
1	D	566	ILE	CB-CA-C	-5.14	104.34	109.89
1	C	518	VAL	N-CA-C	-5.13	105.41	111.00
1	D	462	ALA	N-CA-C	-5.12	100.95	108.79
1	B	442	VAL	CG1-CB-CG2	-5.12	99.53	110.80
1	E	539	VAL	CB-CA-C	-5.12	104.23	112.16
1	C	522	ILE	N-CA-C	5.12	119.20	112.04
1	E	566	ILE	N-CA-CB	-5.11	104.05	111.21
1	E	572	ASP	N-CA-C	5.11	120.42	113.37
1	C	501	THR	N-CA-C	5.11	117.81	109.59
1	B	549	VAL	N-CA-C	5.10	115.82	110.62
1	E	505	VAL	N-CA-C	5.09	119.93	109.34
1	F	507	GLY	N-CA-C	-5.09	105.25	112.37
1	F	561	LEU	N-CA-C	5.08	117.67	110.50
1	B	550	THR	N-CA-C	-5.07	105.66	111.14
1	D	467	GLN	N-CA-C	5.07	117.69	111.82
1	F	440	GLY	CA-C-N	-5.06	115.88	122.51
1	F	440	GLY	C-N-CA	-5.06	115.88	122.51
1	C	557	ILE	N-CA-CB	5.06	116.47	110.55
1	E	480	ILE	N-CA-C	5.06	115.67	110.36
1	F	446	ILE	CB-CA-C	-5.05	103.13	110.81
1	C	476	ASN	O-C-N	-5.05	115.87	122.59
1	E	525	ILE	N-CA-C	5.05	113.62	107.61
1	E	517	ALA	CA-C-N	5.04	127.10	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	517	ALA	C-N-CA	5.04	127.10	120.60
1	B	482	LYS	CG-CD-CE	5.04	122.89	111.30
1	E	586	VAL	CB-CA-C	5.04	117.16	110.91
1	B	550	THR	CB-CA-C	5.01	118.82	110.90
1	C	502	TYR	N-CA-C	5.01	116.46	110.44
1	F	564	VAL	CB-CA-C	5.01	116.94	110.12
1	A	498	PHE	CA-C-N	-5.00	114.90	122.01
1	A	498	PHE	C-N-CA	-5.00	114.90	122.01

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	615	GLU	CA
1	F	502	TYR	CA

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	435	ILE	Peptide
1	C	562	LYS	Mainchain
1	C	613	PHE	Peptide
1	D	614	LYS	Peptide
1	E	435	ILE	Peptide
1	E	438	SER	Peptide
1	E	504	GLY	Peptide
1	F	484	TYR	Peptide
1	F	576	LEU	Peptide
1	F	578	ALA	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	89	0
1	B	1466	0	1529	140	0
1	C	1466	0	1529	161	0
1	D	1466	0	1529	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1457	0	1523	119	0
1	F	1466	0	1529	139	0
2	A	163	0	0	21	0
2	B	165	0	0	42	0
2	C	198	0	0	71	2
2	D	197	0	0	34	2
2	E	147	0	0	37	0
2	F	225	0	0	50	0
All	All	9873	0	9162	693	2

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 39.

All (693) 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:E:461:ILE:CD1	1:E:461:ILE:CG1	1.75	1.60
1:E:445:ILE:CG1	1:E:445:ILE:CD1	1.76	1.60
1:E:512:ILE:CD1	1:E:512:ILE:CG1	1.74	1.59
1:C:479:ALA:CB	1:C:479:ALA:CA	1.81	1.59
1:F:474:VAL:CG1	1:F:474:VAL:CB	1.76	1.55
1:C:597:GLU:CD	1:C:597:GLU:CG	1.76	1.55
1:D:539:VAL:CB	1:D:539:VAL:CG1	1.76	1.54
1:A:597:GLU:CD	1:A:597:GLU:CG	1.75	1.53
1:D:428:ARG:HG2	2:D:818:HOH:O	1.25	1.29
1:C:420:ILE:HG13	2:C:768:HOH:O	1.38	1.24
1:E:497:GLN:HG2	2:E:727:HOH:O	1.35	1.22
1:F:445:ILE:HD11	2:F:811:HOH:O	1.37	1.19
1:C:614:LYS:HA	1:C:615:GLU:C	1.69	1.16
1:D:608:ARG:HE	1:D:612:LYS:HE3	1.11	1.15
1:E:419:PHE:HB2	2:E:763:HOH:O	1.49	1.13
1:B:418:LEU:HD11	2:C:800:HOH:O	1.48	1.12
1:F:554:GLU:HG2	2:F:837:HOH:O	1.46	1.12
1:C:465:ARG:HB2	1:C:503:GLU:OE1	1.49	1.10
1:E:425:GLU:HG2	2:F:828:HOH:O	1.50	1.08
1:F:477:VAL:HG22	1:F:481:ILE:HD12	1.10	1.08
1:A:492:MET:HE1	1:A:522:ILE:HD13	1.34	1.08
1:C:550:THR:HG23	2:C:807:HOH:O	1.54	1.06
1:B:576:LEU:HD22	1:B:580:HIS:HB3	1.28	1.06
1:F:472:GLU:OE1	1:F:509:SER:HA	1.58	1.02
1:B:420:ILE:HG21	2:B:701:HOH:O	1.60	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:MET:HE1	1:F:459:ARG:HH22	1.26	1.00
1:D:428:ARG:NE	2:D:818:HOH:O	1.93	1.00
1:F:578:ALA:HB1	2:F:803:HOH:O	1.61	1.00
1:D:608:ARG:HH11	1:D:608:ARG:HG2	1.25	1.00
1:D:428:ARG:CD	2:D:818:HOH:O	2.05	0.99
1:B:419:PHE:HA	1:B:428:ARG:HH22	1.24	0.99
1:A:466:LEU:HB3	2:A:781:HOH:O	1.62	0.98
1:D:542:GLU:HG3	2:D:650:HOH:O	1.62	0.98
1:A:475:MET:HE1	1:F:459:ARG:NH2	1.79	0.97
1:C:446:ILE:HD11	1:C:497:GLN:HB2	1.43	0.97
1:B:482:LYS:HG2	2:B:753:HOH:O	1.62	0.97
1:F:614:LYS:HA	2:F:835:HOH:O	1.65	0.97
1:F:472:GLU:HG3	2:F:665:HOH:O	1.61	0.97
1:B:419:PHE:HA	1:B:428:ARG:NH2	1.79	0.96
1:C:428:ARG:HD2	2:C:666:HOH:O	1.65	0.96
2:A:758:HOH:O	1:B:540:LYS:HE2	1.64	0.96
1:C:577:ASP:OD1	1:C:579:GLU:HB2	1.66	0.95
1:C:482:LYS:HG2	1:C:483:LYS:H	1.32	0.95
1:F:502:TYR:HB2	2:F:734:HOH:O	1.64	0.95
1:F:477:VAL:CG2	1:F:481:ILE:HD12	1.95	0.94
1:D:583:LYS:HG3	2:D:790:HOH:O	1.67	0.94
1:A:492:MET:HE1	1:A:522:ILE:CD1	1.98	0.94
1:C:463:THR:HG23	2:C:771:HOH:O	1.68	0.94
2:E:746:HOH:O	1:F:539:VAL:HG11	1.67	0.93
1:C:445:ILE:HD11	2:C:782:HOH:O	1.69	0.92
1:B:444:PRO:HB2	1:B:499:VAL:HB	1.52	0.92
1:B:614:LYS:HD2	2:B:710:HOH:O	1.70	0.91
1:B:489:ILE:O	1:B:489:ILE:HG22	1.68	0.91
1:B:478:SER:O	1:B:482:LYS:HD3	1.69	0.91
1:C:506:GLU:HG3	2:C:798:HOH:O	1.69	0.90
1:A:445:ILE:HD11	2:A:767:HOH:O	1.70	0.90
1:B:482:LYS:HB3	2:B:753:HOH:O	1.72	0.89
1:C:465:ARG:CB	1:C:503:GLU:OE1	2.20	0.89
1:D:539:VAL:CG1	1:D:539:VAL:CG2	2.50	0.89
1:A:446:ILE:CD1	1:B:544:LEU:HD13	2.02	0.89
1:F:477:VAL:HB	2:F:658:HOH:O	1.71	0.89
1:C:571:ILE:HG12	2:C:711:HOH:O	1.72	0.89
1:B:419:PHE:HB3	2:B:771:HOH:O	1.71	0.89
1:C:550:THR:HA	2:C:807:HOH:O	1.73	0.89
1:F:469:ILE:O	1:F:472:GLU:HG2	1.73	0.88
1:D:612:LYS:NZ	2:D:744:HOH:O	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:502:TYR:CE1	2:C:626:HOH:O	2.28	0.87
1:B:487:ARG:HD3	2:B:762:HOH:O	1.75	0.86
1:E:418:LEU:HD21	2:F:810:HOH:O	1.75	0.86
1:E:492:MET:HE1	1:E:522:ILE:HG12	1.57	0.86
1:C:482:LYS:HG2	1:C:483:LYS:N	1.88	0.86
1:D:465:ARG:HE	1:D:503:GLU:HB2	1.39	0.85
1:A:463:THR:HG22	1:B:468:GLU:HG3	1.57	0.85
1:D:489:ILE:HA	1:D:492:MET:HE3	1.59	0.84
1:C:502:TYR:CD2	1:C:505:VAL:HG21	2.12	0.84
1:D:417:LYS:HD2	2:D:777:HOH:O	1.76	0.84
1:F:435:ILE:HG12	1:F:441:ILE:HG23	1.57	0.84
1:C:608:ARG:CB	2:C:713:HOH:O	2.25	0.84
1:D:608:ARG:NE	1:D:612:LYS:HE3	1.92	0.84
1:F:428:ARG:NH2	2:F:686:HOH:O	2.10	0.84
1:F:477:VAL:HG22	1:F:481:ILE:CD1	2.04	0.83
1:B:501:THR:HB	2:B:660:HOH:O	1.78	0.83
1:E:613:PHE:HB3	2:E:747:HOH:O	1.78	0.83
1:F:605:LYS:HE3	2:F:705:HOH:O	1.76	0.83
1:E:418:LEU:CD2	2:F:810:HOH:O	2.26	0.83
1:C:441:ILE:HG21	1:C:502:TYR:OH	1.79	0.83
1:C:446:ILE:CD1	1:C:497:GLN:HB2	2.08	0.82
1:F:502:TYR:CE1	2:F:709:HOH:O	2.31	0.82
1:B:465:ARG:HG2	2:B:746:HOH:O	1.80	0.82
1:C:476:ASN:HB2	2:C:681:HOH:O	1.79	0.82
1:A:477:VAL:HG22	1:A:519:ILE:HD11	1.59	0.82
1:E:424:TYR:HE2	2:E:668:HOH:O	1.62	0.82
1:E:465:ARG:HD3	2:E:745:HOH:O	1.79	0.82
1:B:609:LEU:O	1:B:612:LYS:HB2	1.80	0.82
2:E:746:HOH:O	1:F:539:VAL:HG21	1.79	0.81
1:C:457:GLU:HA	2:C:715:HOH:O	1.78	0.81
1:C:502:TYR:HD1	2:C:699:HOH:O	1.63	0.81
1:B:437:GLU:HB3	2:B:763:HOH:O	1.81	0.81
1:A:481:ILE:CD1	1:A:485:THR:HG21	2.10	0.81
1:D:435:ILE:HG23	1:D:505:VAL:HG22	1.62	0.81
1:D:469:ILE:HD12	2:D:788:HOH:O	1.81	0.81
1:F:502:TYR:HB3	1:F:505:VAL:HG21	1.64	0.80
1:C:608:ARG:HG2	2:C:713:HOH:O	1.81	0.80
1:F:578:ALA:C	1:F:580:HIS:H	1.90	0.80
1:A:429:VAL:HG22	1:A:527:VAL:HG11	1.64	0.80
1:A:419:PHE:HB3	1:A:444:PRO:HG3	1.64	0.79
2:A:758:HOH:O	1:B:540:LYS:CE	2.27	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:LYS:HD2	2:B:785:HOH:O	1.80	0.79
1:C:502:TYR:CD1	2:C:699:HOH:O	2.36	0.79
1:D:615:GLU:HB3	2:D:811:HOH:O	1.81	0.79
1:C:614:LYS:N	2:C:710:HOH:O	2.14	0.79
1:C:459:ARG:HD2	2:C:814:HOH:O	1.82	0.79
1:E:512:ILE:CD1	1:E:512:ILE:CB	2.61	0.79
1:F:577:ASP:O	1:F:578:ALA:O	2.00	0.79
1:A:540:LYS:HG2	1:A:540:LYS:O	1.82	0.78
1:C:437:GLU:OE2	1:C:437:GLU:N	2.14	0.78
1:A:481:ILE:HD11	1:A:485:THR:HG21	1.63	0.78
1:F:579:GLU:N	2:F:803:HOH:O	2.15	0.78
1:D:597:GLU:HG2	1:D:610:MET:HE2	1.65	0.78
1:F:597:GLU:HG2	2:F:815:HOH:O	1.84	0.78
1:C:459:ARG:HB3	2:C:814:HOH:O	1.83	0.78
1:C:614:LYS:CA	1:C:615:GLU:C	2.54	0.77
1:D:433:ALA:HA	2:D:808:HOH:O	1.83	0.77
1:F:445:ILE:CG2	2:F:701:HOH:O	2.33	0.77
1:B:482:LYS:CB	2:B:753:HOH:O	2.31	0.77
1:E:435:ILE:HD11	1:E:441:ILE:CG2	2.15	0.77
1:B:548:GLY:HA2	1:B:551:GLN:NE2	2.00	0.77
1:A:446:ILE:HD11	1:B:544:LEU:HD13	1.67	0.77
1:E:609:LEU:O	1:E:612:LYS:HB2	1.85	0.76
1:F:479:ALA:HB3	2:F:805:HOH:O	1.84	0.76
1:C:492:MET:HE1	1:C:522:ILE:HD11	1.67	0.76
1:F:508:ASP:O	2:F:839:HOH:O	2.03	0.76
1:E:437:GLU:HB2	2:E:736:HOH:O	1.84	0.76
1:F:472:GLU:CA	2:F:697:HOH:O	2.33	0.76
1:D:428:ARG:CG	2:D:818:HOH:O	1.90	0.76
1:C:457:GLU:N	2:C:817:HOH:O	2.18	0.75
1:C:545:PRO:HG3	1:C:569:ASP:HB2	1.69	0.75
1:E:419:PHE:HD2	2:E:733:HOH:O	1.70	0.75
1:A:466:LEU:HD22	2:A:781:HOH:O	1.87	0.74
1:E:485:THR:HG22	1:E:487:ARG:H	1.53	0.74
1:A:446:ILE:CD1	1:B:544:LEU:CD1	2.65	0.74
1:C:594:GLU:CD	2:C:785:HOH:O	2.30	0.74
1:E:568:LYS:HE2	2:E:744:HOH:O	1.85	0.74
1:B:482:LYS:CG	2:B:753:HOH:O	2.26	0.74
1:F:441:ILE:HG21	2:F:715:HOH:O	1.86	0.74
1:F:472:GLU:CB	2:F:697:HOH:O	2.34	0.74
1:C:480:ILE:HD13	1:C:537:LEU:HD21	1.68	0.74
1:B:508:ASP:OD2	2:B:769:HOH:O	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:LEU:CD2	1:B:580:HIS:HB3	2.12	0.73
1:A:481:ILE:HD12	1:A:485:THR:HB	1.70	0.73
1:B:480:ILE:HG13	1:B:481:ILE:N	2.00	0.73
1:D:429:VAL:HG22	1:D:527:VAL:HG11	1.69	0.73
1:C:422:GLU:HG2	2:C:818:HOH:O	1.87	0.73
1:D:579:GLU:OE1	2:D:784:HOH:O	2.07	0.73
1:C:475:MET:HG3	2:C:788:HOH:O	1.87	0.73
1:E:576:LEU:HD22	1:E:580:HIS:HB3	1.71	0.72
1:C:608:ARG:CG	2:C:713:HOH:O	2.35	0.72
1:D:608:ARG:HH11	1:D:608:ARG:CG	2.02	0.72
1:E:497:GLN:HE22	1:F:538:SER:HA	1.53	0.72
1:B:505:VAL:HG23	1:B:505:VAL:O	1.89	0.72
1:D:489:ILE:HA	1:D:492:MET:CE	2.20	0.72
1:F:473:ALA:O	1:F:477:VAL:HG12	1.90	0.72
1:A:608:ARG:HG2	2:A:687:HOH:O	1.89	0.71
1:C:435:ILE:HG22	2:C:813:HOH:O	1.90	0.71
1:E:613:PHE:CB	2:E:747:HOH:O	2.34	0.71
1:C:465:ARG:CG	1:C:503:GLU:OE1	2.38	0.71
1:A:463:THR:CG2	1:B:468:GLU:HG3	2.20	0.71
1:A:478:SER:HB2	2:A:707:HOH:O	1.90	0.71
1:E:492:MET:CE	1:E:522:ILE:HG12	2.21	0.71
1:B:465:ARG:CG	2:B:746:HOH:O	2.35	0.70
1:E:448:GLU:HG3	2:E:732:HOH:O	1.90	0.70
1:C:547:GLY:O	1:C:552:LYS:NZ	2.17	0.70
1:B:608:ARG:HG3	2:B:639:HOH:O	1.91	0.70
1:D:597:GLU:CG	1:D:610:MET:HE2	2.22	0.70
1:E:489:ILE:O	1:E:492:MET:HG2	1.91	0.70
1:B:482:LYS:CD	2:B:785:HOH:O	2.39	0.69
1:F:435:ILE:HG12	1:F:441:ILE:CG2	2.22	0.69
1:F:502:TYR:HD2	1:F:503:GLU:N	1.89	0.69
1:B:505:VAL:HG22	2:B:745:HOH:O	1.92	0.69
1:F:549:VAL:O	1:F:553:ILE:HG13	1.93	0.69
1:F:435:ILE:CG1	1:F:441:ILE:HG23	2.23	0.69
1:B:553:ILE:HG21	1:B:576:LEU:HD11	1.76	0.69
1:F:485:THR:HG23	1:F:523:GLU:OE2	1.93	0.69
1:B:418:LEU:HA	1:C:545:PRO:HG2	1.74	0.68
1:A:435:ILE:CG2	1:A:505:VAL:HG22	2.22	0.68
1:C:435:ILE:HB	2:C:813:HOH:O	1.93	0.68
1:A:475:MET:HG3	2:A:754:HOH:O	1.91	0.68
1:C:548:GLY:O	1:C:552:LYS:HG3	1.94	0.68
1:F:578:ALA:C	1:F:580:HIS:N	2.52	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ILE:HG12	1:A:441:ILE:HG23	1.75	0.68
1:A:509:SER:HB3	1:F:497:GLN:OE1	1.93	0.68
1:C:476:ASN:HD22	1:C:476:ASN:C	2.01	0.68
1:C:550:THR:CG2	2:C:807:HOH:O	2.24	0.68
1:C:463:THR:CG2	2:C:771:HOH:O	2.31	0.68
1:C:597:GLU:HG2	2:C:769:HOH:O	1.92	0.68
1:D:428:ARG:CZ	2:D:818:HOH:O	2.36	0.68
1:A:597:GLU:CD	1:A:597:GLU:CB	2.65	0.67
1:F:613:PHE:HB3	2:F:802:HOH:O	1.94	0.67
1:C:472:GLU:HB2	2:C:757:HOH:O	1.94	0.67
1:A:481:ILE:HD11	1:A:485:THR:CG2	2.24	0.67
1:E:439:ALA:HB2	2:E:736:HOH:O	1.93	0.67
1:C:434:VAL:HB	2:C:806:HOH:O	1.95	0.67
1:C:435:ILE:CB	2:C:813:HOH:O	2.42	0.67
1:C:550:THR:CA	2:C:807:HOH:O	2.33	0.67
1:F:472:GLU:CG	1:F:473:ALA:N	2.58	0.67
1:A:481:ILE:CD1	1:A:485:THR:CG2	2.73	0.66
1:D:422:GLU:HG2	1:D:423:GLY:H	1.61	0.66
1:A:453:MET:HG2	2:A:711:HOH:O	1.94	0.66
1:E:453:MET:HE3	1:E:453:MET:HA	1.77	0.66
1:E:504:GLY:N	1:E:505:VAL:HG22	2.10	0.66
1:F:474:VAL:CG1	1:F:474:VAL:CA	2.70	0.66
1:E:501:THR:HG23	1:E:501:THR:O	1.95	0.66
1:C:550:THR:CB	2:C:807:HOH:O	2.42	0.66
1:F:502:TYR:CA	2:F:829:HOH:O	2.43	0.66
1:C:522:ILE:HG22	1:C:522:ILE:O	1.96	0.66
1:D:612:LYS:HE2	2:D:812:HOH:O	1.94	0.66
1:F:502:TYR:HE1	2:F:709:HOH:O	1.73	0.66
1:D:484:TYR:HB2	2:D:780:HOH:O	1.94	0.65
1:F:445:ILE:HG22	2:F:701:HOH:O	1.95	0.65
1:A:604:LYS:HD2	2:A:779:HOH:O	1.97	0.65
1:C:452:SER:O	1:C:453:MET:HG2	1.96	0.65
1:D:501:THR:HB	2:E:753:HOH:O	1.96	0.65
1:F:477:VAL:CG2	1:F:477:VAL:O	2.44	0.65
1:C:501:THR:HG21	2:D:678:HOH:O	1.95	0.65
1:A:470:ALA:O	1:A:474:VAL:HG23	1.96	0.65
1:B:489:ILE:O	1:B:489:ILE:CG2	2.38	0.65
1:C:522:ILE:O	1:C:522:ILE:CG2	2.44	0.65
1:B:450:THR:HG21	1:C:483:LYS:HB2	1.79	0.65
1:B:471:ARG:NE	2:B:760:HOH:O	2.29	0.65
1:E:417:LYS:HD2	1:E:419:PHE:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:PHE:CA	1:B:428:ARG:NH2	2.60	0.64
1:B:465:ARG:HD2	2:B:673:HOH:O	1.96	0.64
1:C:445:ILE:CG2	2:C:645:HOH:O	2.44	0.64
1:C:497:GLN:HB2	2:C:815:HOH:O	1.96	0.64
1:E:419:PHE:CD2	2:E:733:HOH:O	2.47	0.64
1:F:485:THR:HB	1:F:487:ARG:H	1.61	0.64
1:A:422:GLU:HG3	2:A:752:HOH:O	1.97	0.64
1:F:441:ILE:CG2	2:F:715:HOH:O	2.43	0.64
1:A:428:ARG:NH2	2:A:776:HOH:O	2.13	0.64
1:C:479:ALA:CB	1:C:479:ALA:N	2.56	0.64
1:A:438:SER:O	1:A:439:ALA:O	2.15	0.64
1:B:575:LEU:O	1:B:576:LEU:HB2	1.98	0.64
1:C:476:ASN:C	1:C:476:ASN:ND2	2.54	0.64
1:D:422:GLU:HG2	1:D:423:GLY:N	2.12	0.64
1:D:608:ARG:HG2	1:D:608:ARG:NH1	2.05	0.64
1:D:532:ALA:HB2	1:D:561:LEU:HD13	1.79	0.63
1:F:588:PRO:HG2	1:F:588:PRO:O	1.98	0.63
1:E:590:SER:N	1:E:594:GLU:OE1	2.29	0.63
1:F:509:SER:HB3	2:F:717:HOH:O	1.99	0.63
1:A:435:ILE:HG23	1:A:505:VAL:HG22	1.80	0.63
1:D:539:VAL:CG1	1:D:539:VAL:CA	2.71	0.63
1:C:446:ILE:HD11	2:C:815:HOH:O	1.99	0.63
1:F:474:VAL:CG1	1:F:474:VAL:HB	2.15	0.62
1:A:481:ILE:HD11	1:A:487:ARG:HB2	1.82	0.62
1:C:502:TYR:CD1	2:C:626:HOH:O	2.50	0.62
1:E:497:GLN:C	2:E:727:HOH:O	2.41	0.62
1:D:435:ILE:CG2	1:D:505:VAL:HG22	2.28	0.62
1:F:472:GLU:HB3	2:F:697:HOH:O	1.96	0.62
2:A:775:HOH:O	1:F:417:LYS:HE2	1.98	0.62
1:C:441:ILE:CG2	1:C:502:TYR:OH	2.47	0.62
1:E:435:ILE:HD11	1:E:441:ILE:HG21	1.81	0.62
1:F:435:ILE:HG23	1:F:505:VAL:HG22	1.81	0.62
1:A:503:GLU:HG3	1:B:506:GLU:OE1	2.00	0.61
1:C:497:GLN:CB	2:C:815:HOH:O	2.47	0.61
1:C:615:GLU:HB3	2:C:809:HOH:O	1.98	0.61
1:C:501:THR:HB	2:D:775:HOH:O	1.99	0.61
1:C:445:ILE:CD1	1:C:513:SER:HB2	2.30	0.61
1:C:540:LYS:HD3	2:C:764:HOH:O	2.00	0.61
1:E:564:VAL:HG13	1:E:564:VAL:O	2.01	0.61
1:C:477:VAL:O	1:C:477:VAL:HG22	1.99	0.60
1:F:502:TYR:HB3	1:F:505:VAL:CG2	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:VAL:HG22	1:B:563:LYS:HB2	1.82	0.60
1:C:492:MET:HE1	1:C:522:ILE:CD1	2.31	0.60
1:F:472:GLU:HG3	1:F:473:ALA:N	2.16	0.60
1:B:438:SER:HA	1:B:551:GLN:HG2	1.84	0.60
1:E:418:LEU:HD12	2:E:677:HOH:O	2.01	0.60
1:E:549:VAL:O	1:E:553:ILE:HG13	2.02	0.60
1:F:598:HIS:HE1	2:F:664:HOH:O	1.82	0.60
1:B:501:THR:HG22	2:C:794:HOH:O	2.01	0.60
1:C:511:SER:HB3	1:C:514:ILE:HD12	1.81	0.60
1:F:488:ASP:HB3	1:F:491:ASN:ND2	2.17	0.60
1:F:502:TYR:CD2	1:F:503:GLU:O	2.55	0.59
1:E:492:MET:HE2	1:E:522:ILE:HD11	1.84	0.59
1:C:428:ARG:NH2	2:C:714:HOH:O	2.25	0.59
1:C:435:ILE:CG2	2:C:813:HOH:O	2.48	0.59
1:E:484:TYR:HB3	1:E:613:PHE:HD1	1.68	0.58
1:D:438:SER:O	1:D:551:GLN:HG2	2.02	0.58
1:A:501:THR:HG21	2:B:663:HOH:O	2.04	0.58
1:B:480:ILE:HD12	1:B:484:TYR:HD2	1.67	0.58
1:F:477:VAL:CB	2:F:658:HOH:O	2.39	0.58
1:A:428:ARG:CD	1:A:446:ILE:HG23	2.34	0.58
1:C:445:ILE:CG1	2:C:782:HOH:O	2.50	0.58
1:B:501:THR:CA	2:B:660:HOH:O	2.50	0.58
1:D:608:ARG:HE	1:D:612:LYS:CE	2.01	0.58
1:B:480:ILE:HD12	1:B:484:TYR:CD2	2.38	0.58
1:C:597:GLU:HB3	2:C:769:HOH:O	2.04	0.58
1:F:435:ILE:HG21	1:F:502:TYR:CE1	2.39	0.58
1:C:477:VAL:O	1:C:477:VAL:CG2	2.52	0.58
1:D:428:ARG:HD2	2:D:772:HOH:O	2.04	0.58
1:A:428:ARG:HD3	1:A:446:ILE:HG23	1.84	0.57
1:D:478:SER:HB2	1:D:489:ILE:HB	1.85	0.57
1:E:477:VAL:CG2	1:E:515:ALA:HB1	2.34	0.57
1:B:501:THR:CG2	2:C:794:HOH:O	2.51	0.57
1:E:561:LEU:HA	2:E:759:HOH:O	2.04	0.57
1:B:588:PRO:HG3	2:B:696:HOH:O	2.03	0.57
1:B:576:LEU:HD22	1:B:580:HIS:CB	2.20	0.57
1:E:453:MET:C	2:E:700:HOH:O	2.48	0.57
1:C:545:PRO:HG3	1:C:569:ASP:CB	2.35	0.57
1:C:452:SER:O	1:C:453:MET:CG	2.53	0.57
1:C:472:GLU:HG2	2:C:635:HOH:O	2.05	0.57
1:A:477:VAL:CG2	1:A:519:ILE:HD11	2.31	0.56
1:C:433:ALA:HB3	1:C:441:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:470:ALA:O	1:E:474:VAL:HG23	2.05	0.56
1:F:554:GLU:OE1	1:F:580:HIS:CD2	2.58	0.56
1:C:418:LEU:N	1:C:418:LEU:HD12	2.20	0.56
1:C:418:LEU:N	1:C:418:LEU:CD1	2.69	0.56
1:A:481:ILE:HD12	1:A:485:THR:CB	2.36	0.56
1:B:579:GLU:OE1	1:B:579:GLU:HA	2.04	0.56
1:C:476:ASN:HD22	1:C:477:VAL:N	2.04	0.56
1:E:497:GLN:HE22	1:F:539:VAL:H	1.52	0.56
1:F:428:ARG:HD2	1:F:446:ILE:HG23	1.88	0.55
1:F:482:LYS:O	1:F:486:GLY:HA2	2.06	0.55
1:C:446:ILE:CD1	2:C:815:HOH:O	2.52	0.55
1:E:470:ALA:HA	1:E:514:ILE:HD13	1.88	0.55
1:B:449:VAL:HG21	1:B:522:ILE:HD13	1.88	0.55
1:B:578:ALA:C	1:B:580:HIS:H	2.14	0.55
1:B:502:TYR:HB2	1:B:505:VAL:HG12	1.87	0.55
1:B:523:GLU:HG3	1:B:609:LEU:HD22	1.89	0.55
1:C:483:LYS:HG3	1:C:483:LYS:O	2.06	0.55
1:E:549:VAL:HB	2:E:735:HOH:O	2.06	0.55
1:F:502:TYR:N	2:F:829:HOH:O	2.38	0.55
1:A:435:ILE:HG22	1:A:505:VAL:HG22	1.88	0.55
1:B:548:GLY:HA2	1:B:551:GLN:HE21	1.70	0.55
1:C:445:ILE:HD11	1:C:513:SER:HB2	1.88	0.55
1:F:477:VAL:HG22	1:F:477:VAL:O	2.06	0.55
1:C:457:GLU:CA	2:C:715:HOH:O	2.45	0.54
1:C:502:TYR:HE1	2:C:626:HOH:O	1.81	0.54
1:E:484:TYR:CB	1:E:613:PHE:HD1	2.20	0.54
1:A:604:LYS:O	1:A:608:ARG:HB3	2.07	0.54
1:C:614:LYS:CA	2:C:710:HOH:O	2.55	0.54
1:C:597:GLU:CG	2:C:769:HOH:O	2.52	0.54
1:F:485:THR:HG21	1:F:487:ARG:HD2	1.88	0.54
1:C:465:ARG:HG2	1:C:503:GLU:OE1	2.07	0.54
1:C:480:ILE:HD13	1:C:537:LEU:CD2	2.37	0.54
1:F:485:THR:CG2	1:F:487:ARG:HD2	2.38	0.54
1:B:457:GLU:HG2	2:B:689:HOH:O	2.08	0.54
1:A:553:ILE:CG2	1:A:576:LEU:HD21	2.37	0.54
1:F:484:TYR:HB3	1:F:613:PHE:CE2	2.43	0.54
1:C:480:ILE:HD11	1:C:519:ILE:HD11	1.88	0.54
1:E:506:GLU:OE2	1:E:506:GLU:HA	2.08	0.54
1:A:446:ILE:HD11	1:B:544:LEU:CD1	2.34	0.53
1:B:503:GLU:HB2	2:B:783:HOH:O	2.07	0.53
1:B:590:SER:N	1:B:594:GLU:OE1	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:472:GLU:CG	1:F:473:ALA:H	2.21	0.53
1:B:451:PRO:C	1:B:453:MET:H	2.16	0.53
1:B:482:LYS:HG3	1:B:488:ASP:HA	1.91	0.53
1:D:550:THR:O	1:D:554:GLU:HG3	2.09	0.53
1:E:418:LEU:HG	2:F:671:HOH:O	2.08	0.53
1:C:445:ILE:HG22	2:C:645:HOH:O	2.04	0.53
1:C:615:GLU:CB	2:C:809:HOH:O	2.54	0.53
1:D:477:VAL:CG2	1:D:515:ALA:HB1	2.38	0.53
1:E:449:VAL:HB	1:E:492:MET:HE3	1.90	0.53
1:E:497:GLN:NE2	1:F:539:VAL:H	2.06	0.53
1:F:554:GLU:OE1	1:F:580:HIS:HD2	1.92	0.53
1:B:478:SER:HB3	1:B:482:LYS:HE3	1.91	0.53
1:E:613:PHE:O	1:E:614:LYS:O	2.27	0.53
1:A:492:MET:CE	1:A:522:ILE:HD13	2.24	0.53
1:F:479:ALA:O	2:F:831:HOH:O	2.19	0.53
2:E:746:HOH:O	1:F:539:VAL:CG1	2.39	0.52
1:C:503:GLU:CB	2:C:754:HOH:O	2.57	0.52
1:F:457:GLU:HG3	1:F:490:SER:O	2.08	0.52
1:B:553:ILE:CG2	1:B:576:LEU:HD11	2.38	0.52
1:D:432:LEU:HD21	1:D:556:ALA:HB2	1.90	0.52
1:E:434:VAL:O	1:E:505:VAL:HA	2.09	0.52
1:F:590:SER:HB2	2:F:781:HOH:O	2.09	0.52
1:C:424:TYR:HB3	1:C:526:PRO:HB2	1.90	0.52
1:E:448:GLU:CG	2:E:732:HOH:O	2.51	0.52
1:D:483:LYS:HB2	2:D:804:HOH:O	2.08	0.52
1:F:548:GLY:O	1:F:552:LYS:HG3	2.09	0.52
1:C:531:VAL:HG22	1:C:563:LYS:HB2	1.91	0.52
1:E:484:TYR:HB3	1:E:613:PHE:CD1	2.44	0.52
1:F:502:TYR:HD2	1:F:503:GLU:H	1.54	0.52
1:F:502:TYR:CB	2:F:829:HOH:O	2.57	0.52
1:F:597:GLU:HG2	2:F:795:HOH:O	2.08	0.52
1:C:433:ALA:HB3	1:C:441:ILE:CD1	2.40	0.52
1:C:482:LYS:CG	1:C:483:LYS:N	2.67	0.52
1:D:489:ILE:HG12	1:D:492:MET:CE	2.40	0.52
1:E:461:ILE:CG2	1:F:475:MET:HG2	2.39	0.52
1:E:609:LEU:HA	1:E:612:LYS:HG2	1.93	0.51
1:F:445:ILE:HG21	2:F:701:HOH:O	2.01	0.51
1:E:539:VAL:O	1:E:539:VAL:CG1	2.56	0.51
1:A:526:PRO:HG2	1:A:601:GLU:OE1	2.10	0.51
1:F:480:ILE:HD12	1:F:537:LEU:HD21	1.92	0.51
1:C:485:THR:OG1	1:C:486:GLY:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:534:THR:O	1:C:567:PRO:HD3	2.10	0.51
1:B:505:VAL:O	1:B:505:VAL:CG2	2.59	0.51
1:F:588:PRO:O	1:F:588:PRO:CG	2.58	0.51
1:E:477:VAL:HG21	1:E:515:ALA:HB1	1.91	0.51
1:F:536:SER:OG	2:F:846:HOH:O	2.05	0.51
1:A:475:MET:O	2:A:707:HOH:O	2.18	0.51
1:A:568:LYS:HE2	2:A:766:HOH:O	2.10	0.51
1:E:470:ALA:HA	1:E:514:ILE:HG21	1.93	0.51
1:A:568:LYS:HG3	2:A:730:HOH:O	2.10	0.50
1:A:608:ARG:HG3	1:A:608:ARG:HH11	1.75	0.50
1:B:437:GLU:HG3	2:B:674:HOH:O	2.11	0.50
1:B:480:ILE:HD11	1:B:613:PHE:CE2	2.45	0.50
1:A:435:ILE:HG23	1:A:441:ILE:HD12	1.94	0.50
1:B:585:GLU:HB3	2:B:653:HOH:O	2.12	0.50
1:D:435:ILE:O	1:D:436:GLY:C	2.53	0.50
1:A:573:ASP:OD2	1:F:417:LYS:N	2.45	0.50
1:C:428:ARG:CD	2:C:666:HOH:O	2.39	0.50
1:F:435:ILE:HG23	1:F:505:VAL:CG2	2.42	0.50
1:B:453:MET:HG2	1:C:482:LYS:NZ	2.27	0.50
1:B:577:ASP:OD1	1:B:580:HIS:ND1	2.36	0.50
1:C:428:ARG:HH11	1:C:428:ARG:HG3	1.76	0.50
1:D:608:ARG:CG	1:D:608:ARG:NH1	2.66	0.50
1:A:487:ARG:NH1	1:A:487:ARG:HG2	2.27	0.50
1:B:417:LYS:HB2	1:B:419:PHE:CE1	2.46	0.50
1:C:420:ILE:CD1	2:D:722:HOH:O	2.60	0.50
1:C:502:TYR:CE2	1:C:505:VAL:HG21	2.47	0.50
1:D:419:PHE:CE1	1:D:559:ALA:HB1	2.47	0.50
1:D:471:ARG:NH2	2:D:710:HOH:O	2.45	0.50
1:F:577:ASP:C	1:F:578:ALA:O	2.55	0.49
1:B:457:GLU:HG3	1:B:490:SER:O	2.12	0.49
1:B:479:ALA:HB2	2:B:770:HOH:O	2.12	0.49
1:C:475:MET:HE1	2:C:705:HOH:O	2.11	0.49
1:D:534:THR:O	1:D:567:PRO:HD3	2.12	0.49
1:E:593:ASN:O	1:E:610:MET:HE1	2.12	0.49
1:D:459:ARG:HB3	2:D:724:HOH:O	2.12	0.49
1:C:417:LYS:N	1:D:573:ASP:OD2	2.45	0.49
1:E:430:ASN:O	1:E:532:ALA:HA	2.13	0.49
1:F:485:THR:HG21	1:F:487:ARG:CD	2.43	0.49
1:A:475:MET:CG	2:A:754:HOH:O	2.56	0.49
1:E:598:HIS:HE1	2:E:720:HOH:O	1.94	0.49
1:E:501:THR:O	1:E:501:THR:CG2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:562:LYS:N	2:E:759:HOH:O	2.46	0.49
1:F:502:TYR:CE2	1:F:503:GLU:O	2.65	0.49
1:D:477:VAL:HG13	1:D:481:ILE:HD12	1.94	0.49
1:F:470:ALA:O	1:F:474:VAL:HG23	2.12	0.49
1:C:488:ASP:O	1:C:491:ASN:HB2	2.13	0.49
1:A:557:ILE:HG12	1:A:584:ILE:HB	1.95	0.48
1:C:468:GLU:O	1:C:472:GLU:HB3	2.13	0.48
1:F:472:GLU:HG2	1:F:473:ALA:H	1.78	0.48
1:C:586:VAL:HB	2:C:793:HOH:O	2.13	0.48
1:C:469:ILE:HD11	2:C:772:HOH:O	2.12	0.48
1:D:492:MET:HG2	2:D:647:HOH:O	2.13	0.48
1:E:492:MET:HE2	1:E:522:ILE:CD1	2.44	0.48
1:E:577:ASP:O	1:E:581:GLU:HG2	2.12	0.48
1:F:417:LYS:HB3	2:F:780:HOH:O	2.12	0.48
1:B:548:GLY:O	1:B:552:LYS:HG3	2.14	0.48
2:B:774:HOH:O	1:C:545:PRO:HG2	2.12	0.48
1:F:576:LEU:N	2:F:719:HOH:O	2.36	0.48
1:D:548:GLY:HA2	1:D:551:GLN:HE22	1.78	0.48
1:B:450:THR:HG21	1:C:483:LYS:CB	2.43	0.48
1:C:608:ARG:HB3	2:C:713:HOH:O	2.01	0.48
1:D:485:THR:OG1	1:D:486:GLY:N	2.41	0.48
1:B:420:ILE:HD12	1:B:425:GLU:OE2	2.13	0.48
1:C:503:GLU:HB3	2:C:754:HOH:O	2.12	0.48
1:E:418:LEU:HD23	1:F:545:PRO:HG2	1.95	0.48
1:E:600:LEU:HB2	1:E:606:LYS:HE3	1.95	0.48
1:E:539:VAL:O	1:E:539:VAL:HG12	2.10	0.47
1:E:546:VAL:HG23	2:E:735:HOH:O	2.14	0.47
1:D:483:LYS:NZ	2:D:766:HOH:O	2.47	0.47
1:B:591:ARG:O	1:B:594:GLU:HB2	2.14	0.47
1:E:496:ILE:O	2:E:626:HOH:O	2.20	0.47
1:E:523:GLU:OE2	1:E:609:LEU:HD13	2.14	0.47
1:E:606:LYS:O	1:E:610:MET:HG2	2.15	0.47
1:B:418:LEU:HB3	2:B:771:HOH:O	2.15	0.47
1:B:429:VAL:HG22	1:B:527:VAL:HG11	1.97	0.47
1:B:612:LYS:O	1:B:615:GLU:HG3	2.13	0.47
2:B:773:HOH:O	1:C:482:LYS:HE2	2.13	0.47
1:F:571:ILE:HD13	1:F:571:ILE:HA	1.64	0.47
1:A:481:ILE:HD12	1:A:485:THR:CG2	2.45	0.47
1:B:545:PRO:HA	1:B:567:PRO:HG2	1.96	0.47
1:C:437:GLU:N	1:C:437:GLU:CD	2.73	0.47
1:C:497:GLN:C	2:C:815:HOH:O	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:484:TYR:HB3	1:F:613:PHE:CZ	2.49	0.47
1:A:468:GLU:CD	1:F:467:GLN:HE22	2.21	0.47
1:B:502:TYR:HB2	1:B:505:VAL:CG1	2.45	0.47
2:E:746:HOH:O	1:F:539:VAL:CG2	2.49	0.47
1:D:508:ASP:HB2	2:D:753:HOH:O	2.15	0.47
1:F:474:VAL:CG1	1:F:474:VAL:C	2.88	0.47
1:A:568:LYS:O	1:A:571:ILE:HD12	2.15	0.47
1:D:489:ILE:HG12	1:D:492:MET:HE1	1.96	0.47
1:A:573:ASP:C	1:A:575:LEU:HD22	2.40	0.46
1:A:470:ALA:HA	1:A:514:ILE:HD13	1.96	0.46
1:A:593:ASN:O	1:A:610:MET:HE1	2.16	0.46
1:F:472:GLU:N	2:F:697:HOH:O	2.46	0.46
1:D:418:LEU:HD23	1:E:545:PRO:HB2	1.96	0.46
1:E:449:VAL:HA	1:E:493:ASP:O	2.16	0.46
1:E:503:GLU:C	1:E:505:VAL:HG22	2.40	0.46
1:B:481:ILE:HG21	1:B:481:ILE:HD13	1.46	0.46
1:D:443:LEU:HD23	2:D:679:HOH:O	2.15	0.46
1:F:467:GLN:OE1	1:F:471:ARG:NH2	2.38	0.46
1:C:532:ALA:HB2	1:C:561:LEU:HD13	1.97	0.46
1:F:550:THR:O	1:F:554:GLU:HB2	2.15	0.46
1:C:460:VAL:HG11	1:C:471:ARG:HA	1.97	0.46
1:D:457:GLU:HG3	1:D:490:SER:HB3	1.96	0.46
1:D:612:LYS:CE	2:D:812:HOH:O	2.59	0.46
1:E:613:PHE:HB2	2:E:747:HOH:O	2.09	0.46
1:B:537:LEU:HG	1:B:538:SER:O	2.16	0.46
1:F:566:ILE:O	1:F:588:PRO:HA	2.16	0.46
1:A:446:ILE:HD13	1:B:544:LEU:HD13	1.93	0.46
1:A:604:LYS:CD	2:A:779:HOH:O	2.60	0.46
1:E:480:ILE:HG23	1:E:484:TYR:HD2	1.79	0.46
1:F:472:GLU:O	1:F:473:ALA:C	2.59	0.46
1:A:608:ARG:HG3	1:A:608:ARG:NH1	2.31	0.45
1:B:470:ALA:O	1:B:474:VAL:HG23	2.16	0.45
1:D:593:ASN:O	1:D:597:GLU:HG3	2.16	0.45
1:E:533:MET:HB3	1:E:533:MET:HE2	1.50	0.45
1:F:478:SER:HA	1:F:481:ILE:HB	1.97	0.45
1:B:453:MET:HG2	1:C:482:LYS:HZ2	1.80	0.45
1:E:591:ARG:O	1:E:594:GLU:HB2	2.17	0.45
1:A:466:LEU:O	1:A:469:ILE:HB	2.16	0.45
1:B:588:PRO:CG	2:B:696:HOH:O	2.63	0.45
1:B:418:LEU:CD1	2:C:800:HOH:O	2.30	0.45
1:C:467:GLN:HB2	1:C:471:ARG:NH2	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:558:GLN:NE2	2:D:795:HOH:O	2.48	0.45
1:B:417:LYS:HE3	2:B:779:HOH:O	2.16	0.45
1:B:554:GLU:O	1:B:558:GLN:HB2	2.16	0.45
1:B:599:VAL:HG23	1:B:600:LEU:HD23	1.97	0.45
1:F:472:GLU:CG	2:F:665:HOH:O	2.38	0.45
1:A:485:THR:HG22	1:A:487:ARG:H	1.82	0.45
1:B:451:PRO:O	1:B:453:MET:N	2.47	0.45
1:B:500:GLY:HA2	2:B:659:HOH:O	2.17	0.45
1:B:548:GLY:HA2	1:B:551:GLN:HE22	1.76	0.45
1:C:419:PHE:CE1	1:C:559:ALA:HB1	2.51	0.45
1:E:472:GLU:O	1:E:473:ALA:C	2.58	0.45
1:E:568:LYS:CE	2:E:744:HOH:O	2.54	0.45
1:B:453:MET:CE	2:C:819:HOH:O	2.65	0.45
2:C:779:HOH:O	1:D:475:MET:CG	2.64	0.45
1:F:489:ILE:HD12	1:F:489:ILE:HA	1.48	0.45
1:C:501:THR:HG22	2:D:652:HOH:O	2.17	0.44
1:E:497:GLN:CG	2:E:727:HOH:O	2.18	0.44
1:B:463:THR:HG21	1:C:472:GLU:CG	2.47	0.44
1:B:478:SER:HB3	1:B:482:LYS:CE	2.47	0.44
1:D:548:GLY:HA2	1:D:551:GLN:NE2	2.32	0.44
1:D:553:ILE:HG12	1:D:564:VAL:HG11	1.98	0.44
1:D:419:PHE:HB3	1:D:444:PRO:HG3	1.99	0.44
1:E:480:ILE:HG23	1:E:484:TYR:CD2	2.52	0.44
1:E:484:TYR:CB	1:E:613:PHE:CD1	3.01	0.44
1:E:480:ILE:CD1	1:E:537:LEU:HD21	2.47	0.44
1:F:465:ARG:HH21	1:F:503:GLU:CD	2.25	0.44
1:F:597:GLU:CG	2:F:815:HOH:O	2.54	0.44
1:A:568:LYS:HE3	1:A:568:LYS:HB3	1.77	0.44
1:B:418:LEU:HD13	1:C:545:PRO:HD2	1.99	0.44
1:B:420:ILE:HD12	2:B:701:HOH:O	2.17	0.44
1:C:553:ILE:HG23	1:C:564:VAL:HG11	2.00	0.44
1:E:461:ILE:HG22	1:F:475:MET:HG2	1.99	0.44
1:F:477:VAL:CG2	1:F:481:ILE:CD1	2.82	0.44
1:C:597:GLU:CB	2:C:769:HOH:O	2.62	0.44
1:E:481:ILE:HD13	1:E:481:ILE:HG21	1.68	0.44
1:D:465:ARG:NE	1:D:503:GLU:HB2	2.19	0.44
1:F:597:GLU:HB3	2:F:815:HOH:O	2.17	0.44
1:C:420:ILE:HD12	1:C:420:ILE:HG23	1.61	0.44
1:A:487:ARG:HG2	1:A:487:ARG:HH11	1.82	0.44
1:C:556:ALA:HA	1:C:561:LEU:HD12	1.99	0.44
1:A:433:ALA:HB2	2:A:756:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:465:ARG:HE	1:D:503:GLU:CB	2.20	0.43
1:E:475:MET:SD	2:E:697:HOH:O	2.62	0.43
1:C:475:MET:CE	2:C:705:HOH:O	2.64	0.43
1:E:418:LEU:HA	1:F:545:PRO:HG2	2.00	0.43
1:A:553:ILE:HG21	1:A:576:LEU:HD21	2.00	0.43
1:B:430:ASN:O	1:B:532:ALA:HA	2.18	0.43
1:B:481:ILE:O	1:B:482:LYS:C	2.58	0.43
1:A:430:ASN:ND2	1:A:529:GLN:O	2.51	0.43
1:A:550:THR:O	1:A:554:GLU:HG3	2.19	0.43
1:C:446:ILE:CG1	2:C:815:HOH:O	2.66	0.43
1:C:571:ILE:HD11	1:C:588:PRO:HG3	2.01	0.43
1:A:465:ARG:HD3	1:A:503:GLU:HG2	1.99	0.43
1:B:579:GLU:HB2	2:B:647:HOH:O	2.18	0.43
1:C:502:TYR:CD2	1:C:505:VAL:CG2	2.96	0.43
1:D:441:ILE:HG21	1:D:441:ILE:HD13	1.66	0.43
1:D:470:ALA:O	1:D:474:VAL:HG23	2.18	0.43
1:E:421:THR:HG23	1:E:561:LEU:HD23	2.01	0.43
1:E:540:LYS:HB2	1:E:540:LYS:HE2	1.86	0.43
1:B:449:VAL:HG21	1:B:522:ILE:CD1	2.47	0.43
1:B:568:LYS:O	1:B:571:ILE:HB	2.19	0.43
1:E:526:PRO:HG2	2:E:730:HOH:O	2.18	0.43
1:F:446:ILE:HD12	1:F:497:GLN:H	1.83	0.43
1:F:479:ALA:HB3	2:F:628:HOH:O	2.17	0.43
1:B:417:LYS:HD2	1:B:419:PHE:CE1	2.53	0.43
1:C:457:GLU:OE2	1:C:490:SER:HB2	2.19	0.43
1:E:444:PRO:HG2	1:E:499:VAL:HB	2.01	0.43
1:E:532:ALA:HB2	1:E:561:LEU:HD12	2.00	0.43
1:A:421:THR:HG22	1:A:561:LEU:CD2	2.49	0.43
1:B:450:THR:HG22	1:C:483:LYS:NZ	2.33	0.43
1:B:487:ARG:NH2	2:B:709:HOH:O	2.50	0.43
1:D:446:ILE:HB	2:D:818:HOH:O	2.18	0.43
1:E:419:PHE:HA	1:E:428:ARG:HH22	1.83	0.43
1:E:581:GLU:OE2	1:E:581:GLU:HA	2.18	0.43
1:C:501:THR:CG2	2:D:678:HOH:O	2.59	0.43
2:A:626:HOH:O	1:F:501:THR:HG22	2.17	0.42
1:B:518:VAL:O	1:B:519:ILE:C	2.57	0.42
1:B:551:GLN:CD	1:B:551:GLN:H	2.27	0.42
1:D:495:HIS:HE1	1:E:475:MET:HE2	1.83	0.42
1:D:532:ALA:HB2	1:D:561:LEU:CD1	2.49	0.42
1:D:583:LYS:HE2	2:D:717:HOH:O	2.18	0.42
1:E:452:SER:HA	2:E:754:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:495:HIS:HB3	1:F:539:VAL:HG11	2.01	0.42
1:A:446:ILE:HD12	1:B:544:LEU:HD11	2.02	0.42
1:A:457:GLU:HG2	1:A:458:GLY:H	1.84	0.42
1:C:568:LYS:HA	1:C:588:PRO:HB2	2.00	0.42
1:C:577:ASP:O	1:C:581:GLU:HG3	2.18	0.42
1:C:590:SER:C	1:C:591:ARG:HG3	2.44	0.42
1:D:510:ALA:O	1:D:511:SER:C	2.62	0.42
1:E:480:ILE:HD13	1:E:537:LEU:HD21	2.02	0.42
1:F:549:VAL:HG11	1:F:573:ASP:HB2	2.02	0.42
1:B:485:THR:HG22	1:B:612:LYS:HB3	2.01	0.42
1:B:531:VAL:HG11	1:B:599:VAL:HG12	2.00	0.42
1:C:435:ILE:HG23	1:C:505:VAL:HG22	2.02	0.42
1:C:480:ILE:HG12	1:C:481:ILE:N	2.34	0.42
1:F:477:VAL:HB	1:F:537:LEU:HD23	2.01	0.42
1:F:568:LYS:HA	1:F:588:PRO:HB2	2.01	0.42
1:D:597:GLU:HG3	1:D:610:MET:HE2	2.00	0.42
1:F:502:TYR:CD2	1:F:503:GLU:N	2.79	0.42
1:F:483:LYS:HB2	2:F:804:HOH:O	2.20	0.42
1:B:614:LYS:N	2:B:698:HOH:O	2.52	0.42
1:E:604:LYS:HD3	2:E:645:HOH:O	2.20	0.42
1:B:518:VAL:O	1:B:522:ILE:HG12	2.20	0.42
1:C:446:ILE:HG13	2:C:815:HOH:O	2.20	0.42
1:D:525:ILE:HA	1:D:526:PRO:HD3	1.76	0.42
1:E:417:LYS:HE2	2:E:738:HOH:O	2.18	0.42
1:A:545:PRO:HB2	1:F:418:LEU:HD12	2.01	0.42
1:B:533:MET:HA	1:B:565:ILE:O	2.20	0.42
1:B:576:LEU:HA	1:B:576:LEU:HD23	1.56	0.42
1:E:576:LEU:CD2	1:E:580:HIS:HB3	2.45	0.42
1:A:421:THR:HG22	1:A:561:LEU:HD23	2.02	0.42
1:A:553:ILE:HG22	1:A:576:LEU:HD21	2.00	0.42
1:B:418:LEU:HD22	1:C:545:PRO:O	2.20	0.42
1:C:580:HIS:HA	1:C:583:LYS:HD2	2.01	0.42
1:B:487:ARG:NH1	2:B:762:HOH:O	2.50	0.41
1:E:562:LYS:HD2	1:E:562:LYS:HA	1.73	0.41
1:F:510:ALA:O	1:F:537:LEU:N	2.51	0.41
1:B:418:LEU:CD2	1:C:545:PRO:O	2.68	0.41
1:B:452:SER:O	1:B:453:MET:HB2	2.21	0.41
1:E:605:LYS:HG3	2:E:696:HOH:O	2.19	0.41
1:E:613:PHE:O	1:E:614:LYS:C	2.63	0.41
1:C:417:LYS:C	1:C:418:LEU:HD12	2.45	0.41
1:D:434:VAL:O	1:D:434:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:525:ILE:HA	1:E:526:PRO:HD3	1.88	0.41
1:B:567:PRO:O	1:B:568:LYS:C	2.63	0.41
1:D:572:ASP:HB3	2:D:696:HOH:O	2.20	0.41
1:E:579:GLU:O	1:E:580:HIS:ND1	2.53	0.41
1:A:441:ILE:HD13	1:A:441:ILE:H	1.86	0.41
1:B:503:GLU:C	2:B:783:HOH:O	2.64	0.41
1:E:430:ASN:ND2	1:E:529:GLN:O	2.53	0.41
1:E:457:GLU:HB3	1:E:458:GLY:H	1.77	0.41
1:F:428:ARG:HH11	1:F:428:ARG:HD3	1.73	0.41
1:A:446:ILE:HD12	1:B:544:LEU:CD1	2.48	0.41
1:B:536:SER:HB2	1:B:544:LEU:HB2	2.02	0.41
1:B:614:LYS:O	1:B:615:GLU:HB2	2.21	0.41
1:C:544:LEU:HB3	1:C:545:PRO:HD2	2.02	0.41
1:E:492:MET:CE	1:E:522:ILE:CD1	2.99	0.41
1:F:437:GLU:N	1:F:437:GLU:OE2	2.53	0.41
1:A:453:MET:HB3	2:A:718:HOH:O	2.19	0.41
1:B:566:ILE:O	1:B:589:VAL:HG22	2.21	0.41
1:B:612:LYS:O	1:B:615:GLU:CG	2.68	0.41
1:B:614:LYS:HA	2:B:698:HOH:O	2.21	0.41
1:C:570:ASN:HA	1:C:573:ASP:OD2	2.21	0.41
1:D:435:ILE:HG23	1:D:505:VAL:CG2	2.44	0.41
1:E:564:VAL:O	1:E:564:VAL:CG1	2.69	0.41
1:E:589:VAL:O	1:E:589:VAL:HG23	2.21	0.41
1:F:433:ALA:O	1:F:440:GLY:HA2	2.21	0.41
1:F:460:VAL:HG21	2:F:706:HOH:O	2.21	0.41
1:F:490:SER:HB2	2:F:773:HOH:O	2.20	0.41
1:F:509:SER:CB	2:F:796:HOH:O	2.69	0.41
1:B:449:VAL:HA	1:B:493:ASP:O	2.21	0.41
1:B:600:LEU:HB2	1:B:606:LYS:HE3	2.02	0.41
1:C:443:LEU:HD12	1:C:443:LEU:HA	1.87	0.41
1:E:514:ILE:HD13	1:E:514:ILE:HG21	1.68	0.41
1:A:532:ALA:HB2	1:A:561:LEU:HD13	2.03	0.40
1:B:437:GLU:CB	2:B:763:HOH:O	2.56	0.40
1:B:614:LYS:CA	2:B:698:HOH:O	2.69	0.40
1:D:428:ARG:NE	2:D:772:HOH:O	2.53	0.40
1:D:534:THR:OG1	1:D:546:VAL:HG21	2.21	0.40
1:E:417:LYS:HG2	2:E:659:HOH:O	2.21	0.40
1:F:452:SER:HB3	1:F:458:GLY:HA2	2.03	0.40
1:A:417:LYS:N	1:B:569:ASP:O	2.54	0.40
1:A:569:ASP:O	1:F:417:LYS:N	2.55	0.40
1:B:463:THR:HG21	1:C:472:GLU:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:445:ILE:HD12	1:C:513:SER:HB2	2.03	0.40
1:C:473:ALA:HB2	2:C:716:HOH:O	2.21	0.40
1:D:481:ILE:HD13	1:D:522:ILE:HD12	2.03	0.40
1:E:469:ILE:HD13	1:E:469:ILE:HG21	1.80	0.40
1:E:570:ASN:O	1:E:571:ILE:C	2.65	0.40
1:F:502:TYR:CB	1:F:505:VAL:HG21	2.41	0.40
1:F:565:ILE:HA	1:F:587:ILE:O	2.20	0.40
1:A:587:ILE:HD13	1:A:587:ILE:HG21	1.41	0.40
1:B:576:LEU:CD2	1:B:580:HIS:CB	2.93	0.40
1:C:481:ILE:HD13	1:C:481:ILE:HG21	1.90	0.40
1:C:571:ILE:HD13	1:C:571:ILE:HG21	1.77	0.40
1:F:509:SER:HB3	2:F:796:HOH:O	2.20	0.40

All (2) 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)
2:C:625:HOH:O	2:D:802:HOH:O[4_465]	1.89	0.31
2:C:803:HOH:O	2:D:716:HOH:O[4_465]	2.10	0.10

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	191/205 (93%)	176 (92%)	10 (5%)	5 (3%)	4 2
1	B	192/205 (94%)	166 (86%)	15 (8%)	11 (6%)	1 0
1	C	192/205 (94%)	181 (94%)	8 (4%)	3 (2%)	7 6
1	D	192/205 (94%)	177 (92%)	14 (7%)	1 (0%)	24 29
1	E	191/205 (93%)	167 (87%)	16 (8%)	8 (4%)	2 1
1	F	192/205 (94%)	175 (91%)	14 (7%)	3 (2%)	7 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1150/1230 (94%)	1042 (91%)	77 (7%)	31 (3%)	4 2

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	438	SER
1	A	439	ALA
1	B	438	SER
1	B	505	VAL
1	B	577	ASP
1	B	614	LYS
1	D	614	LYS
1	E	439	ALA
1	E	484	TYR
1	F	578	ALA
1	F	579	GLU
1	B	440	GLY
1	B	612	LYS
1	E	418	LEU
1	E	419	PHE
1	E	421	THR
1	E	505	VAL
1	E	580	HIS
1	A	613	PHE
1	C	479	ALA
1	E	437	GLU
1	F	469	ILE
1	B	452	SER
1	B	482	LYS
1	B	576	LEU
1	C	482	LYS
1	C	483	LYS
1	A	595	VAL
1	A	486	GLY
1	B	436	GLY
1	B	489	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%)	134 (84%)	26 (16%)	2	2
1	B	161/168 (96%)	131 (81%)	30 (19%)	1	1
1	C	161/168 (96%)	128 (80%)	33 (20%)	1	1
1	D	161/168 (96%)	142 (88%)	19 (12%)	5	5
1	E	160/168 (95%)	127 (79%)	33 (21%)	1	1
1	F	161/168 (96%)	124 (77%)	37 (23%)	1	0
All	All	964/1008 (96%)	786 (82%)	178 (18%)	1	1

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	418	LEU
1	A	420	ILE
1	A	422	GLU
1	A	435	ILE
1	A	441	ILE
1	A	446	ILE
1	A	453	MET
1	A	465	ARG
1	A	477	VAL
1	A	480	ILE
1	A	481	ILE
1	A	485	THR
1	A	489	ILE
1	A	491	ASN
1	A	501	THR
1	A	503	GLU
1	A	506	GLU
1	A	509	SER
1	A	511	SER
1	A	539	VAL
1	A	542	GLU
1	A	551	GLN
1	A	564	VAL
1	A	597	GLU
1	A	604	LYS
1	A	608	ARG
1	B	418	LEU

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Mol	Chain	Res	Type
1	B	419	PHE
1	B	420	ILE
1	B	421	THR
1	B	422	GLU
1	B	435	ILE
1	B	442	VAL
1	B	443	LEU
1	B	452	SER
1	B	457	GLU
1	B	459	ARG
1	B	463	THR
1	B	465	ARG
1	B	466	LEU
1	B	475	MET
1	B	480	ILE
1	B	482	LYS
1	B	491	ASN
1	B	502	TYR
1	B	505	VAL
1	B	539	VAL
1	B	540	LYS
1	B	558	GLN
1	B	563	LYS
1	B	571	ILE
1	B	579	GLU
1	B	583	LYS
1	B	604	LYS
1	B	611	SER
1	B	614	LYS
1	C	417	LYS
1	C	422	GLU
1	C	428	ARG
1	C	435	ILE
1	C	437	GLU
1	C	441	ILE
1	C	445	ILE
1	C	446	ILE
1	C	457	GLU
1	C	463	THR
1	C	472	GLU
1	C	476	ASN
1	C	480	ILE

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Mol	Chain	Res	Type
1	C	482	LYS
1	C	483	LYS
1	C	485	THR
1	C	487	ARG
1	C	492	MET
1	C	501	THR
1	C	508	ASP
1	C	509	SER
1	C	538	SER
1	C	542	GLU
1	C	549	VAL
1	C	562	LYS
1	C	571	ILE
1	C	588	PRO
1	C	589	VAL
1	C	590	SER
1	C	597	GLU
1	C	604	LYS
1	C	608	ARG
1	C	615	GLU
1	D	420	ILE
1	D	435	ILE
1	D	441	ILE
1	D	453	MET
1	D	457	GLU
1	D	465	ARG
1	D	469	ILE
1	D	477	VAL
1	D	480	ILE
1	D	483	LYS
1	D	485	THR
1	D	489	ILE
1	D	506	GLU
1	D	511	SER
1	D	542	GLU
1	D	549	VAL
1	D	551	GLN
1	D	568	LYS
1	D	608	ARG
1	E	417	LYS
1	E	418	LEU
1	E	420	ILE

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Mol	Chain	Res	Type
1	E	422	GLU
1	E	425	GLU
1	E	434	VAL
1	E	443	LEU
1	E	445	ILE
1	E	449	VAL
1	E	450	THR
1	E	453	MET
1	E	459	ARG
1	E	461	ILE
1	E	465	ARG
1	E	475	MET
1	E	477	VAL
1	E	482	LYS
1	E	488	ASP
1	E	489	ILE
1	E	490	SER
1	E	492	MET
1	E	501	THR
1	E	505	VAL
1	E	523	GLU
1	E	546	VAL
1	E	549	VAL
1	E	558	GLN
1	E	562	LYS
1	E	566	ILE
1	E	571	ILE
1	E	597	GLU
1	E	605	LYS
1	E	611	SER
1	F	418	LEU
1	F	435	ILE
1	F	437	GLU
1	F	438	SER
1	F	441	ILE
1	F	445	ILE
1	F	446	ILE
1	F	452	SER
1	F	453	MET
1	F	459	ARG
1	F	465	ARG
1	F	469	ILE

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Mol	Chain	Res	Type
1	F	477	VAL
1	F	480	ILE
1	F	481	ILE
1	F	482	LYS
1	F	485	THR
1	F	487	ARG
1	F	489	ILE
1	F	492	MET
1	F	494	VAL
1	F	501	THR
1	F	502	TYR
1	F	508	ASP
1	F	536	SER
1	F	538	SER
1	F	554	GLU
1	F	562	LYS
1	F	571	ILE
1	F	572	ASP
1	F	574	VAL
1	F	579	GLU
1	F	583	LYS
1	F	588	PRO
1	F	591	ARG
1	F	605	LYS
1	F	614	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	551	GLN
1	B	551	GLN
1	B	558	GLN
1	C	476	ASN
1	D	491	ASN
1	D	558	GLN
1	E	497	GLN
1	E	598	HIS
1	F	476	ASN
1	F	580	HIS
1	F	598	HIS

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	195/205 (95%)	-0.36	1 (0%) 87 88	2, 7, 27, 38	0
1	B	196/205 (95%)	0.16	6 (3%) 51 53	3, 13, 35, 54	0
1	C	196/205 (95%)	-0.26	4 (2%) 65 66	2, 6, 27, 41	0
1	D	196/205 (95%)	-0.35	1 (0%) 87 88	2, 7, 25, 40	0
1	E	195/205 (95%)	0.12	2 (1%) 79 81	3, 14, 34, 49	0
1	F	196/205 (95%)	-0.26	6 (3%) 51 53	2, 7, 30, 52	0
All	All	1174/1230 (95%)	-0.16	20 (1%) 69 70	2, 10, 32, 54	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	418	LEU	3.7
1	F	484	TYR	3.3
1	B	578	ALA	3.1
1	F	577	ASP	3.0
1	B	420	ILE	3.0
1	E	418	LEU	2.9
1	C	502	TYR	2.8
1	B	453	MET	2.8
1	B	579	GLU	2.7
1	F	502	TYR	2.6
1	C	453	MET	2.5
1	B	419	PHE	2.5
1	F	453	MET	2.3
1	C	457	GLU	2.3
1	E	420	ILE	2.2
1	D	437	GLU	2.2
1	F	579	GLU	2.2
1	A	453	MET	2.2
1	C	476	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	578	ALA	2.2

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.