



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:38 AM UTC

PDB ID : 1Z0T / pdb_00001z0t
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:

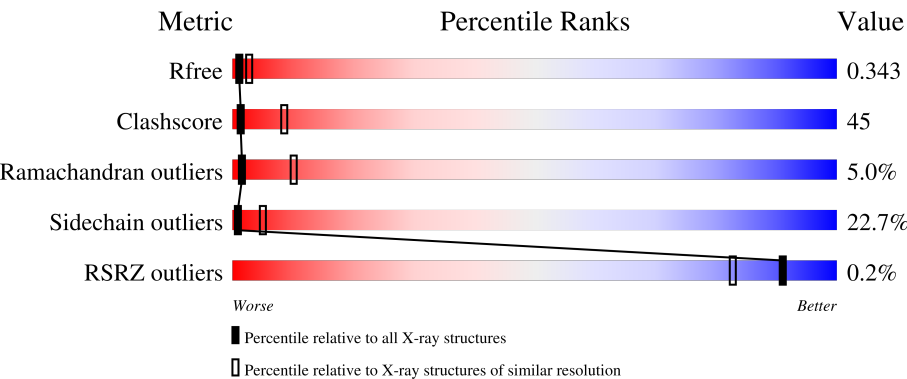
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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	31%36%25%5%
1	B	205	% 19%33%30%14%
1	C	205	34%35%20%7%
1	D	205	29%39%20%8%
1	E	205	18%36%31%11%5%

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Mol	Chain	Length	Quality of chain
1	F	205	27% 39% 20% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9870 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			

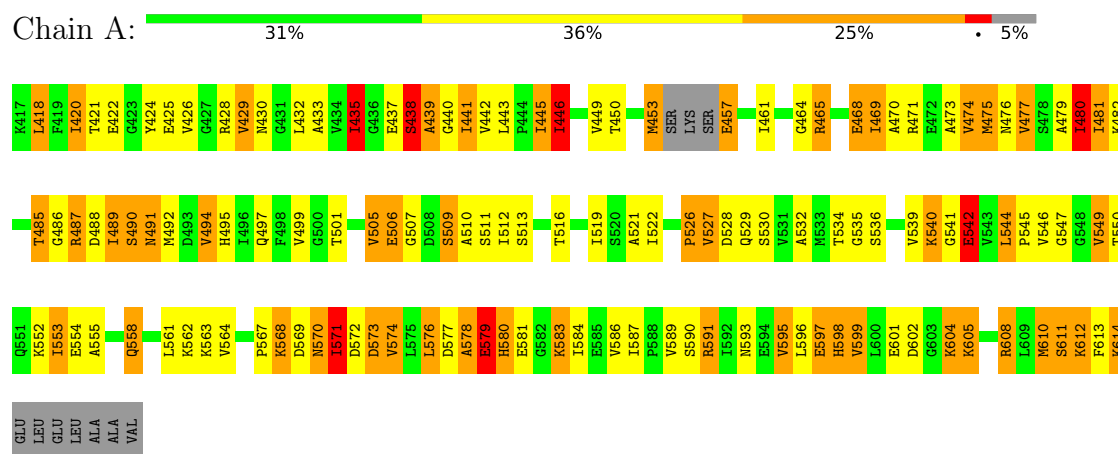
- Molecule 2 is water.

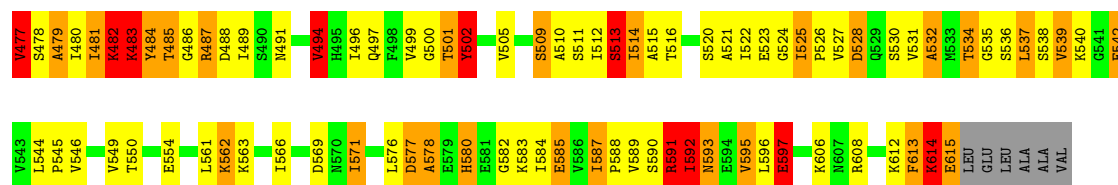
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	159	Total	O	0	0
			159	159		
2	B	164	Total	O	0	0
			164	164		
2	C	208	Total	O	0	0
			208	208		
2	D	190	Total	O	0	0
			190	190		
2	E	145	Total	O	0	0
			145	145		
2	F	226	Total	O	0	0
			226	226		

3 Residue-property plots

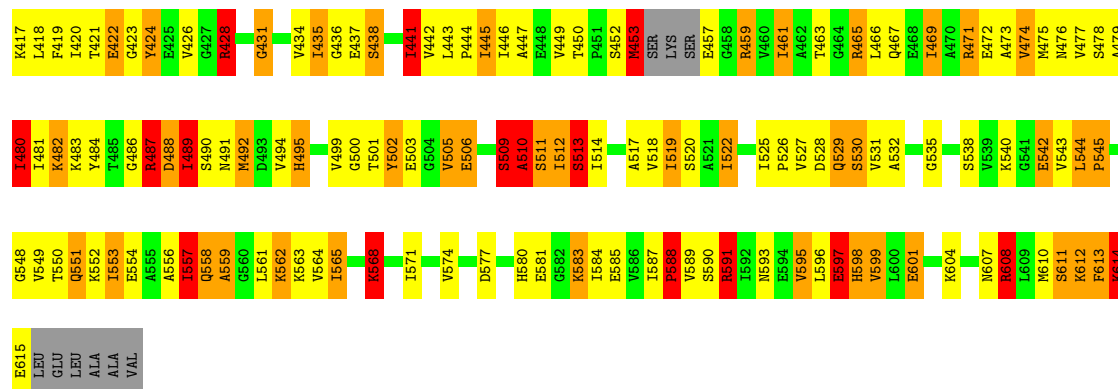
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

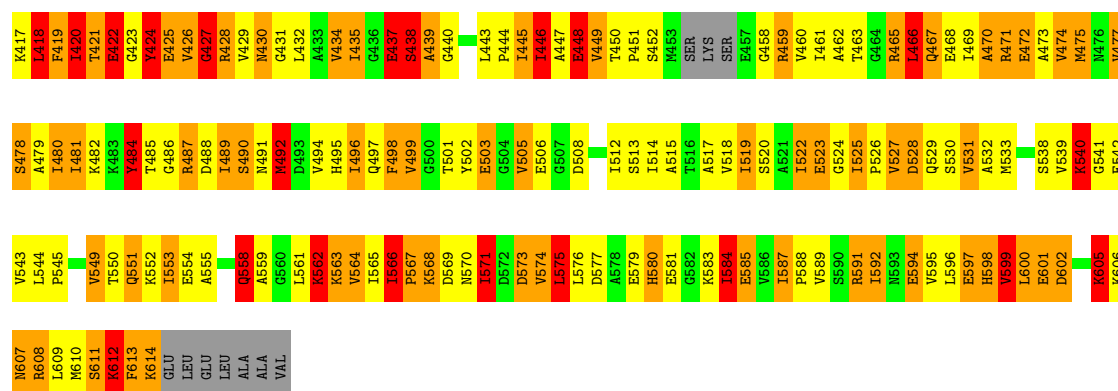




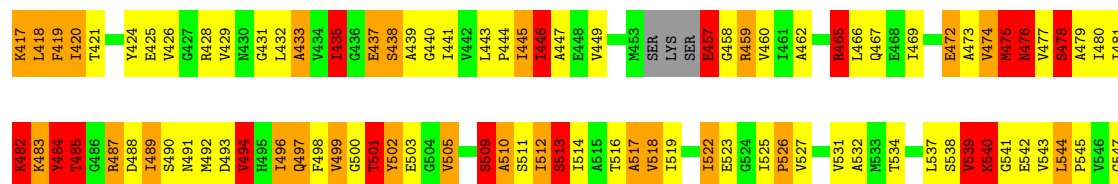
- Molecule 1: Putative protease La homolog type

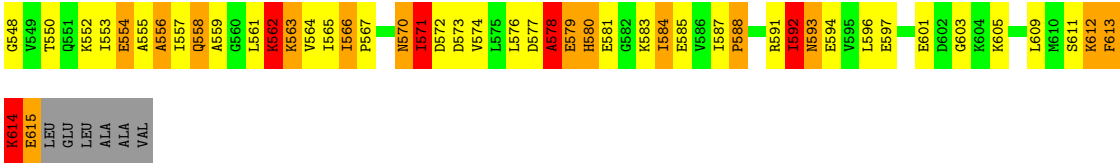


- Molecule 1: Putative protease La homolog type



- Molecule 1: Putative protease La homolog type





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.25Å 90.55Å 147.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 15.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-3.00) 99.0 (15.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.94 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.330 0.211 , 0.343	Depositor DCC
R_{free} test set	1210 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	41.7	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9870	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 54.90 % 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 3.4165e-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	2.28	55/1470 (3.7%)	2.10	56/1983 (2.8%)
1	B	2.43	79/1479 (5.3%)	2.09	51/1995 (2.6%)
1	C	2.33	52/1479 (3.5%)	1.92	47/1995 (2.4%)
1	D	2.25	53/1479 (3.6%)	2.11	47/1995 (2.4%)
1	E	2.38	67/1470 (4.6%)	2.11	57/1983 (2.9%)
1	F	2.23	49/1479 (3.3%)	1.99	49/1995 (2.5%)
All	All	2.32	355/8856 (4.0%)	2.05	307/11946 (2.6%)

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	2
1	C	0	1
1	D	0	2
1	E	0	2
1	F	0	1
All	All	0	8

All (355) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	613	PHE	CA-C	17.77	1.63	1.52
1	F	612	LYS	CE-NZ	11.18	1.82	1.49
1	C	483	LYS	N-CA	10.84	1.60	1.46
1	C	473	ALA	CA-CB	-10.67	1.36	1.53
1	E	466	LEU	C-O	10.35	1.37	1.23
1	B	450	THR	CA-C	10.22	1.62	1.52
1	C	420	ILE	CG1-CD1	10.17	1.91	1.51
1	F	485	THR	N-CA	10.14	1.52	1.46
1	A	429	VAL	C-O	10.04	1.33	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	418	LEU	CA-C	9.60	1.65	1.52
1	E	462	ALA	CA-CB	-9.51	1.38	1.53
1	C	614	LYS	CA-C	9.38	1.64	1.52
1	B	505	VAL	CA-C	9.37	1.64	1.52
1	D	506	GLU	C-O	9.37	1.34	1.23
1	C	479	ALA	CA-CB	9.33	1.69	1.53
1	B	420	ILE	CA-C	9.29	1.64	1.52
1	B	518	VAL	CA-CB	9.13	1.65	1.54
1	B	439	ALA	CA-CB	9.12	1.62	1.53
1	C	484	TYR	CA-C	9.04	1.64	1.52
1	B	587	ILE	CA-CB	8.94	1.65	1.54
1	D	543	VAL	N-CA	-8.85	1.34	1.46
1	B	568	LYS	N-CA	8.74	1.56	1.46
1	A	480	ILE	CA-CB	8.68	1.64	1.54
1	A	579	GLU	C-O	8.67	1.34	1.24
1	E	527	VAL	CA-C	8.66	1.62	1.52
1	B	420	ILE	CA-CB	8.62	1.66	1.54
1	A	580	HIS	N-CA	8.50	1.57	1.46
1	A	576	LEU	CA-C	8.37	1.62	1.52
1	B	420	ILE	N-CA	8.25	1.56	1.46
1	F	449	VAL	C-O	8.21	1.32	1.24
1	F	571	ILE	CA-CB	8.18	1.63	1.54
1	A	553	ILE	CA-CB	8.17	1.63	1.54
1	C	460	VAL	CA-C	8.14	1.61	1.52
1	B	505	VAL	CA-CB	8.13	1.65	1.54
1	A	604	LYS	CE-NZ	8.13	1.73	1.49
1	F	485	THR	CA-C	-8.11	1.49	1.53
1	C	426	VAL	CA-CB	-8.10	1.44	1.54
1	D	562	LYS	C-O	-8.07	1.14	1.24
1	F	484	TYR	CA-C	7.97	1.63	1.52
1	A	527	VAL	CA-CB	-7.92	1.44	1.54
1	C	420	ILE	CB-CG2	7.92	1.78	1.52
1	A	546	VAL	CA-CB	7.85	1.66	1.55
1	D	574	VAL	C-O	7.82	1.33	1.24
1	C	589	VAL	N-CA	-7.80	1.37	1.46
1	A	599	VAL	CA-CB	7.78	1.64	1.54
1	E	553	ILE	N-CA	7.77	1.55	1.46
1	C	587	ILE	N-CA	7.76	1.52	1.46
1	C	515	ALA	C-O	7.66	1.33	1.24
1	B	474	VAL	CA-CB	7.65	1.62	1.54
1	E	463	THR	N-CA	7.60	1.56	1.45
1	E	461	ILE	C-O	-7.56	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	605	LYS	CE-NZ	7.53	1.72	1.49
1	D	517	ALA	N-CA	7.53	1.55	1.46
1	A	583	LYS	CE-NZ	7.48	1.71	1.49
1	F	484	TYR	CB-CG	7.35	1.67	1.51
1	A	587	ILE	C-O	7.33	1.33	1.24
1	B	501	THR	N-CA	7.33	1.54	1.46
1	C	435	ILE	CA-C	-7.28	1.45	1.53
1	D	601	GLU	CA-C	7.27	1.61	1.52
1	A	475	MET	SD-CE	7.14	1.97	1.79
1	C	597	GLU	CG-CD	7.11	1.69	1.52
1	F	522	ILE	CG1-CD1	7.10	1.79	1.51
1	B	571	ILE	CA-C	7.08	1.61	1.52
1	B	450	THR	CA-CB	7.06	1.62	1.53
1	E	461	ILE	CA-C	-7.03	1.43	1.52
1	F	476	ASN	CA-C	7.03	1.62	1.52
1	E	519	ILE	CA-CB	-7.01	1.45	1.54
1	E	592	ILE	CA-CB	7.00	1.61	1.54
1	D	612	LYS	CE-NZ	7.00	1.70	1.49
1	F	443	LEU	N-CA	-6.95	1.39	1.46
1	B	569	ASP	N-CA	6.93	1.56	1.46
1	B	458	GLY	N-CA	6.87	1.53	1.45
1	B	445	ILE	CA-CB	6.85	1.62	1.54
1	D	480	ILE	CA-CB	6.84	1.62	1.54
1	D	461	ILE	CA-CB	6.84	1.61	1.53
1	B	519	ILE	CA-CB	-6.83	1.46	1.54
1	E	594	GLU	N-CA	6.83	1.54	1.46
1	B	594	GLU	N-CA	6.80	1.54	1.46
1	B	470	ALA	CA-CB	-6.80	1.42	1.53
1	E	602	ASP	N-CA	6.79	1.53	1.45
1	D	447	ALA	C-O	6.76	1.32	1.24
1	E	525	ILE	C-O	6.74	1.32	1.24
1	F	522	ILE	CA-C	6.73	1.61	1.52
1	B	463	THR	CB-CG2	6.72	1.74	1.52
1	E	474	VAL	CA-CB	6.68	1.63	1.54
1	F	559	ALA	CA-CB	6.67	1.65	1.53
1	D	550	THR	C-O	6.66	1.31	1.24
1	E	599	VAL	N-CA	6.66	1.54	1.46
1	C	488	ASP	N-CA	6.63	1.54	1.46
1	F	558	GLN	C-O	-6.63	1.16	1.24
1	F	612	LYS	CD-CE	6.62	1.72	1.52
1	B	463	THR	C-O	6.62	1.31	1.23
1	D	596	LEU	CA-C	6.61	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	513	SER	N-CA	6.61	1.54	1.46
1	E	591	ARG	CG-CD	6.60	1.72	1.52
1	A	471	ARG	CA-CB	6.56	1.64	1.53
1	C	426	VAL	CA-C	-6.56	1.44	1.52
1	B	614	LYS	CA-C	6.55	1.61	1.52
1	A	430	ASN	CA-C	-6.54	1.44	1.52
1	D	608	ARG	CB-CG	6.54	1.72	1.52
1	B	609	LEU	C-O	-6.51	1.16	1.24
1	D	562	LYS	N-CA	6.50	1.54	1.46
1	F	483	LYS	N-CA	6.50	1.54	1.46
1	E	542	GLU	N-CA	6.47	1.54	1.45
1	D	568	LYS	CD-CE	6.46	1.71	1.52
1	A	453	MET	CG-SD	6.46	1.97	1.80
1	D	591	ARG	CG-CD	6.45	1.71	1.52
1	B	611	SER	N-CA	6.44	1.54	1.46
1	C	472	GLU	CB-CG	6.44	1.71	1.52
1	F	497	GLN	C-O	6.43	1.32	1.23
1	A	540	LYS	CD-CE	6.42	1.71	1.52
1	A	526	PRO	C-O	6.41	1.31	1.23
1	B	418	LEU	CA-C	6.39	1.62	1.52
1	A	509	SER	C-O	6.38	1.31	1.23
1	C	484	TYR	CA-CB	6.37	1.63	1.53
1	C	435	ILE	CG1-CD1	6.36	1.76	1.51
1	F	426	VAL	C-O	6.36	1.31	1.24
1	C	591	ARG	C-O	6.35	1.31	1.23
1	C	578	ALA	N-CA	6.35	1.54	1.46
1	B	532	ALA	CA-C	-6.33	1.44	1.52
1	C	481	ILE	C-O	6.33	1.31	1.24
1	A	597	GLU	CG-CD	6.33	1.67	1.52
1	A	587	ILE	CA-C	6.32	1.58	1.53
1	E	445	ILE	C-O	6.32	1.32	1.23
1	B	470	ALA	N-CA	-6.28	1.39	1.46
1	E	558	GLN	CG-CD	6.26	1.67	1.52
1	E	564	VAL	CA-CB	6.24	1.61	1.54
1	B	419	PHE	CA-C	6.23	1.60	1.52
1	C	452	SER	N-CA	6.23	1.54	1.46
1	C	421	THR	CA-C	6.22	1.61	1.52
1	B	472	GLU	N-CA	6.21	1.54	1.46
1	E	555	ALA	N-CA	6.20	1.53	1.46
1	A	445	ILE	CA-CB	-6.18	1.45	1.54
1	B	608	ARG	N-CA	6.17	1.53	1.46
1	C	595	VAL	N-CA	-6.17	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	481	ILE	CA-CB	6.16	1.61	1.54
1	E	594	GLU	C-O	-6.15	1.17	1.24
1	B	441	ILE	N-CA	-6.14	1.39	1.46
1	D	489	ILE	CA-CB	6.14	1.62	1.54
1	A	420	ILE	N-CA	6.12	1.53	1.46
1	D	511	SER	CB-OG	6.11	1.54	1.42
1	F	562	LYS	CG-CD	6.09	1.70	1.52
1	E	427	GLY	N-CA	6.09	1.54	1.45
1	D	559	ALA	CA-CB	-6.08	1.42	1.53
1	C	534	THR	N-CA	-6.07	1.38	1.45
1	D	557	ILE	CA-CB	6.06	1.62	1.54
1	E	523	GLU	CA-CB	6.06	1.63	1.53
1	B	442	VAL	N-CA	6.06	1.53	1.46
1	E	419	PHE	N-CA	6.06	1.54	1.46
1	E	529	GLN	C-O	6.06	1.32	1.24
1	C	477	VAL	CB-CG2	6.05	1.72	1.52
1	B	595	VAL	CA-CB	-6.04	1.46	1.54
1	B	551	GLN	N-CA	6.04	1.53	1.46
1	D	608	ARG	CG-CD	6.02	1.70	1.52
1	E	421	THR	CA-C	6.02	1.60	1.52
1	A	442	VAL	C-O	6.01	1.31	1.24
1	B	563	LYS	CA-C	6.00	1.59	1.52
1	E	563	LYS	CA-C	-5.99	1.45	1.52
1	B	469	ILE	N-CA	5.99	1.53	1.46
1	C	597	GLU	CD-OE2	5.99	1.36	1.25
1	A	595	VAL	N-CA	-5.98	1.39	1.46
1	E	419	PHE	C-O	5.97	1.31	1.23
1	E	484	TYR	CA-C	5.97	1.60	1.52
1	F	614	LYS	CA-C	5.95	1.60	1.52
1	E	445	ILE	CA-C	5.95	1.59	1.52
1	D	557	ILE	N-CA	5.94	1.53	1.46
1	E	559	ALA	N-CA	5.93	1.53	1.46
1	E	420	ILE	CA-C	5.92	1.62	1.53
1	A	430	ASN	C-O	-5.91	1.16	1.23
1	C	536	SER	CA-C	-5.89	1.45	1.52
1	E	437	GLU	C-O	5.89	1.31	1.24
1	F	475	MET	SD-CE	5.88	1.94	1.79
1	B	450	THR	N-CA	5.86	1.51	1.45
1	A	440	GLY	C-O	5.86	1.32	1.23
1	C	535	GLY	C-O	5.86	1.28	1.23
1	C	525	ILE	N-CA	-5.86	1.41	1.46
1	D	613	PHE	CA-C	-5.86	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479	ALA	CA-C	-5.85	1.45	1.52
1	B	441	ILE	CA-CB	5.84	1.61	1.54
1	B	565	ILE	C-O	5.84	1.31	1.24
1	E	428	ARG	CZ-NH1	5.84	1.41	1.32
1	E	477	VAL	CA-CB	5.83	1.61	1.54
1	F	525	ILE	CA-CB	5.83	1.59	1.54
1	F	502	TYR	C-O	5.83	1.32	1.23
1	B	432	LEU	CA-C	5.83	1.59	1.52
1	F	554	GLU	N-CA	-5.82	1.39	1.46
1	B	608	ARG	CB-CG	5.80	1.69	1.52
1	E	489	ILE	CA-CB	5.80	1.62	1.54
1	F	578	ALA	C-O	5.80	1.31	1.24
1	B	506	GLU	CA-C	5.80	1.60	1.53
1	A	577	ASP	CG-OD1	5.80	1.36	1.25
1	C	465	ARG	CA-C	5.79	1.60	1.52
1	B	593	ASN	CA-CB	5.77	1.63	1.53
1	C	591	ARG	CA-C	5.75	1.59	1.52
1	D	510	ALA	C-O	5.74	1.31	1.24
1	F	447	ALA	CA-CB	-5.74	1.43	1.53
1	B	443	LEU	C-N	5.73	1.41	1.33
1	D	422	GLU	CG-CD	5.72	1.66	1.52
1	F	438	SER	CB-OG	5.72	1.53	1.42
1	B	462	ALA	CA-C	5.72	1.59	1.52
1	B	555	ALA	N-CA	5.71	1.53	1.46
1	E	515	ALA	CA-C	-5.71	1.45	1.52
1	E	458	GLY	N-CA	5.68	1.50	1.44
1	A	437	GLU	N-CA	5.68	1.52	1.46
1	B	544	LEU	C-O	5.66	1.31	1.23
1	F	517	ALA	CA-CB	-5.65	1.44	1.53
1	A	599	VAL	C-O	-5.64	1.18	1.24
1	B	497	GLN	C-O	5.64	1.30	1.24
1	B	613	PHE	CA-C	-5.63	1.47	1.53
1	F	505	VAL	N-CA	5.63	1.52	1.46
1	C	542	GLU	CB-CG	5.62	1.69	1.52
1	B	495	HIS	N-CA	-5.61	1.39	1.46
1	A	521	ALA	CA-CB	-5.61	1.44	1.53
1	D	428	ARG	CA-C	5.60	1.59	1.52
1	C	466	LEU	N-CA	-5.59	1.40	1.46
1	B	472	GLU	CA-C	5.58	1.60	1.52
1	D	495	HIS	CA-C	-5.57	1.46	1.52
1	D	492	MET	N-CA	5.57	1.52	1.45
1	A	506	GLU	C-O	5.56	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	483	LYS	CA-CB	5.55	1.62	1.53
1	D	591	ARG	CD-NE	5.55	1.54	1.46
1	E	505	VAL	CA-C	5.55	1.59	1.52
1	A	473	ALA	CA-CB	-5.55	1.44	1.53
1	E	470	ALA	N-CA	-5.55	1.39	1.46
1	B	427	GLY	N-CA	5.54	1.53	1.45
1	A	469	ILE	N-CA	-5.54	1.40	1.46
1	A	513	SER	C-O	5.54	1.31	1.24
1	C	539	VAL	CA-CB	5.54	1.61	1.54
1	B	549	VAL	CA-CB	5.54	1.60	1.54
1	A	552	LYS	CA-C	5.53	1.59	1.52
1	F	478	SER	CA-C	5.53	1.60	1.52
1	D	511	SER	N-CA	-5.53	1.38	1.46
1	F	419	PHE	CA-C	5.53	1.59	1.52
1	F	614	LYS	C-O	5.53	1.30	1.24
1	B	474	VAL	CA-C	5.52	1.59	1.52
1	E	443	LEU	N-CA	5.52	1.52	1.46
1	F	420	ILE	CG1-CD1	5.52	1.73	1.51
1	C	532	ALA	CA-CB	-5.50	1.44	1.53
1	E	461	ILE	C-N	-5.50	1.26	1.33
1	A	597	GLU	CB-CG	5.50	1.69	1.52
1	A	541	GLY	C-O	5.50	1.31	1.24
1	B	599	VAL	CA-CB	-5.49	1.48	1.54
1	D	527	VAL	N-CA	5.49	1.52	1.46
1	F	588	PRO	CA-C	-5.48	1.44	1.52
1	B	475	MET	SD-CE	5.48	1.93	1.79
1	D	422	GLU	CD-OE2	5.48	1.35	1.25
1	F	518	VAL	N-CA	-5.48	1.39	1.46
1	E	512	ILE	N-CA	5.48	1.53	1.46
1	C	592	ILE	CB-CG1	-5.47	1.42	1.53
1	E	424	TYR	C-O	5.45	1.30	1.23
1	D	489	ILE	CB-CG2	5.45	1.70	1.52
1	C	422	GLU	N-CA	5.43	1.53	1.46
1	C	483	LYS	C-O	5.42	1.30	1.24
1	B	608	ARG	CG-CD	5.42	1.68	1.52
1	D	450	THR	CA-C	5.42	1.59	1.52
1	E	487	ARG	CA-C	5.42	1.59	1.52
1	E	540	LYS	CB-CG	5.42	1.68	1.52
1	F	544	LEU	CG-CD2	5.42	1.70	1.52
1	B	522	ILE	CG1-CD1	5.41	1.72	1.51
1	F	494	VAL	CA-CB	5.41	1.60	1.53
1	E	552	LYS	CA-C	5.41	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	585	GLU	C-O	5.39	1.30	1.24
1	E	494	VAL	C-O	5.38	1.29	1.24
1	B	429	VAL	CA-CB	5.38	1.61	1.54
1	C	521	ALA	N-CA	5.38	1.52	1.46
1	D	608	ARG	CD-NE	5.37	1.53	1.46
1	E	465	ARG	CA-C	5.36	1.60	1.52
1	C	449	VAL	CA-C	-5.35	1.46	1.52
1	C	537	LEU	CA-C	-5.35	1.46	1.52
1	B	516	THR	CA-C	5.35	1.60	1.52
1	D	438	SER	C-O	5.33	1.30	1.24
1	E	421	THR	N-CA	5.32	1.52	1.46
1	D	479	ALA	CA-C	-5.31	1.46	1.52
1	E	498	PHE	C-O	5.31	1.30	1.23
1	D	530	SER	N-CA	5.30	1.53	1.46
1	E	528	ASP	CA-C	5.30	1.60	1.52
1	F	485	THR	CA-CB	5.30	1.61	1.53
1	B	566	ILE	CA-CB	5.29	1.60	1.55
1	E	496	ILE	CB-CG2	5.29	1.70	1.52
1	B	532	ALA	CA-CB	-5.29	1.46	1.53
1	D	564	VAL	CA-CB	5.29	1.61	1.54
1	A	597	GLU	CD-OE2	5.28	1.35	1.25
1	A	433	ALA	CA-CB	-5.28	1.46	1.53
1	C	471	ARG	C-O	5.28	1.30	1.24
1	E	459	ARG	CA-C	5.27	1.59	1.52
1	E	430	ASN	CA-CB	-5.26	1.45	1.52
1	F	565	ILE	C-O	-5.25	1.17	1.24
1	F	484	TYR	C-N	5.25	1.37	1.33
1	A	552	LYS	CA-CB	5.24	1.61	1.53
1	B	448	GLU	N-CA	5.24	1.52	1.46
1	A	540	LYS	N-CA	-5.24	1.39	1.46
1	B	594	GLU	C-O	5.24	1.30	1.24
1	C	420	ILE	CA-C	5.23	1.59	1.52
1	B	451	PRO	N-CA	5.23	1.52	1.46
1	D	499	VAL	CA-C	-5.22	1.47	1.52
1	D	590	SER	C-O	-5.22	1.17	1.24
1	B	489	ILE	N-CA	-5.21	1.39	1.46
1	D	598	HIS	CA-CB	5.21	1.61	1.53
1	B	461	ILE	C-O	5.21	1.30	1.24
1	E	591	ARG	CA-C	5.19	1.58	1.52
1	F	435	ILE	CG1-CD1	5.19	1.72	1.51
1	F	462	ALA	CA-CB	-5.19	1.44	1.53
1	A	534	THR	C-O	-5.19	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	445	ILE	N-CA	-5.19	1.40	1.46
1	A	425	GLU	C-O	5.18	1.30	1.23
1	A	418	LEU	CA-C	5.18	1.59	1.52
1	B	501	THR	CA-C	5.18	1.58	1.52
1	B	596	LEU	C-O	5.17	1.30	1.24
1	D	589	VAL	CA-CB	5.17	1.60	1.55
1	A	453	MET	SD-CE	5.16	1.92	1.79
1	D	453	MET	SD-CE	5.16	1.92	1.79
1	F	613	PHE	CA-C	5.16	1.59	1.52
1	A	486	GLY	N-CA	5.16	1.52	1.45
1	A	453	MET	N-CA	5.16	1.56	1.46
1	B	533	MET	N-CA	-5.15	1.39	1.46
1	E	591	ARG	CD-NE	5.15	1.53	1.46
1	E	599	VAL	C-O	5.15	1.30	1.24
1	E	499	VAL	CA-C	-5.14	1.46	1.52
1	A	579	GLU	CG-CD	5.14	1.64	1.52
1	C	562	LYS	N-CA	5.14	1.52	1.46
1	F	425	GLU	N-CA	-5.13	1.39	1.46
1	C	462	ALA	CA-C	-5.12	1.46	1.52
1	D	437	GLU	CG-CD	5.11	1.64	1.52
1	F	484	TYR	CA-CB	5.11	1.62	1.54
1	C	528	ASP	N-CA	5.11	1.52	1.46
1	D	428	ARG	CD-NE	5.11	1.53	1.46
1	B	525	ILE	CA-C	5.10	1.57	1.52
1	B	609	LEU	CG-CD2	5.10	1.69	1.52
1	D	520	SER	CA-C	5.09	1.59	1.52
1	B	459	ARG	N-CA	5.09	1.52	1.46
1	E	571	ILE	N-CA	5.09	1.52	1.46
1	B	440	GLY	N-CA	5.09	1.52	1.45
1	D	434	VAL	CA-CB	5.09	1.60	1.54
1	A	435	ILE	C-O	-5.09	1.18	1.24
1	F	493	ASP	C-O	-5.09	1.17	1.24
1	E	459	ARG	CB-CG	5.08	1.67	1.52
1	A	546	VAL	C-O	-5.07	1.18	1.23
1	C	514	ILE	CA-CB	-5.07	1.48	1.54
1	F	446	ILE	CG1-CD1	5.06	1.71	1.51
1	E	506	GLU	CA-C	5.06	1.59	1.52
1	F	540	LYS	CA-C	-5.06	1.45	1.52
1	B	478	SER	CB-OG	5.05	1.52	1.42
1	E	505	VAL	N-CA	5.05	1.52	1.46
1	B	495	HIS	CA-C	-5.05	1.46	1.52
1	C	443	LEU	CA-CB	-5.04	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	571	ILE	CG1-CD1	5.04	1.71	1.51
1	A	578	ALA	N-CA	5.03	1.52	1.46
1	D	584	ILE	CA-CB	-5.03	1.47	1.55
1	D	488	ASP	N-CA	-5.03	1.39	1.46
1	E	471	ARG	CZ-NH1	5.02	1.39	1.32
1	E	544	LEU	C-O	5.02	1.30	1.24
1	D	509	SER	CB-OG	5.02	1.52	1.42
1	C	612	LYS	C-O	5.01	1.30	1.24
1	D	482	LYS	CE-NZ	5.01	1.64	1.49
1	F	603	GLY	N-CA	5.00	1.49	1.45

All (307) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	587	ILE	CA-C-N	-20.55	94.15	119.84
1	D	587	ILE	C-N-CA	-20.55	94.15	119.84
1	B	587	ILE	CA-C-N	14.03	134.21	119.76
1	B	587	ILE	C-N-CA	14.03	134.21	119.76
1	E	443	LEU	CA-C-N	-12.03	107.39	120.14
1	E	443	LEU	C-N-CA	-12.03	107.39	120.14
1	E	438	SER	N-CA-C	-11.79	89.89	109.46
1	C	502	TYR	N-CA-C	11.78	127.82	111.56
1	F	485	THR	CB-CA-C	-11.63	100.32	117.07
1	D	513	SER	N-CA-C	-11.62	98.61	111.28
1	A	580	HIS	N-CA-C	10.96	124.53	111.82
1	E	460	VAL	N-CA-C	-10.93	91.84	109.12
1	F	502	TYR	N-CA-C	10.44	129.71	107.67
1	F	485	THR	N-CA-C	-10.44	100.22	108.78
1	A	450	THR	CA-C-N	-10.25	110.01	120.98
1	A	450	THR	C-N-CA	-10.25	110.01	120.98
1	D	544	LEU	CA-C-N	10.24	130.17	120.03
1	D	544	LEU	C-N-CA	10.24	130.17	120.03
1	B	598	HIS	N-CA-C	10.19	122.39	111.28
1	C	465	ARG	N-CA-C	10.14	122.42	111.36
1	E	466	LEU	N-CA-C	10.01	125.47	112.26
1	C	484	TYR	CB-CA-C	9.53	125.96	110.90
1	E	527	VAL	N-CA-C	9.52	121.50	108.17
1	E	573	ASP	N-CA-C	-9.35	101.56	113.72
1	B	519	ILE	N-CA-C	-9.21	101.23	110.62
1	F	446	ILE	CB-CA-C	-8.99	98.30	110.98
1	B	462	ALA	N-CA-C	8.70	123.60	109.85
1	A	597	GLU	CB-CG-CD	-8.65	97.89	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	539	VAL	N-CA-C	8.65	121.86	111.05
1	E	575	LEU	N-CA-C	-8.64	92.39	110.80
1	E	555	ALA	N-CA-C	8.55	120.68	111.36
1	C	446	ILE	CB-CA-C	-8.37	97.06	110.28
1	A	490	SER	N-CA-C	-8.21	102.28	111.07
1	C	463	THR	N-CA-C	8.19	121.86	109.41
1	A	552	LYS	N-CA-C	-8.16	102.33	111.14
1	F	437	GLU	N-CA-C	-8.12	102.61	114.39
1	F	563	LYS	CD-CE-NZ	-8.11	85.94	111.90
1	B	434	VAL	N-CA-C	-8.09	95.67	108.86
1	E	525	ILE	CA-C-N	-8.08	112.45	120.21
1	E	525	ILE	C-N-CA	-8.08	112.45	120.21
1	A	505	VAL	CB-CA-C	-8.07	99.86	110.84
1	D	558	GLN	N-CA-C	8.02	121.12	111.82
1	B	555	ALA	N-CA-C	-7.96	102.20	112.23
1	D	491	ASN	N-CA-C	7.91	122.60	113.19
1	E	449	VAL	N-CA-C	7.82	119.06	108.11
1	D	512	ILE	CB-CA-C	-7.80	99.41	110.95
1	E	515	ALA	N-CA-C	-7.79	102.75	111.71
1	E	598	HIS	CB-CA-C	-7.79	98.09	110.94
1	E	471	ARG	NE-CZ-NH2	-7.78	112.20	119.20
1	F	500	GLY	N-CA-C	-7.73	99.99	110.97
1	F	592	ILE	N-CA-C	-7.65	101.19	111.44
1	C	452	SER	N-CA-C	7.63	122.79	113.17
1	E	469	ILE	N-CA-C	7.56	117.63	110.53
1	F	491	ASN	N-CA-C	-7.55	102.28	113.61
1	B	506	GLU	CA-C-N	-7.52	113.35	122.15
1	B	506	GLU	C-N-CA	-7.52	113.35	122.15
1	B	588	PRO	CB-CA-C	-7.50	101.78	111.46
1	E	499	VAL	CB-CA-C	-7.49	99.47	110.62
1	C	502	TYR	CA-CB-CG	-7.44	100.51	113.90
1	A	573	ASP	N-CA-C	-7.42	104.38	113.50
1	D	597	GLU	N-CA-C	-7.42	103.22	111.82
1	F	457	GLU	CA-C-N	7.35	128.22	120.43
1	F	457	GLU	C-N-CA	7.35	128.22	120.43
1	C	441	ILE	CB-CA-C	-7.31	98.02	111.18
1	E	571	ILE	CB-CA-C	-7.29	102.56	111.88
1	D	474	VAL	N-CA-C	-7.18	103.17	111.00
1	D	482	LYS	N-CA-C	-7.17	102.88	111.69
1	C	448	GLU	CA-C-N	-7.14	113.21	123.06
1	C	448	GLU	C-N-CA	-7.14	113.21	123.06
1	D	583	LYS	N-CA-C	7.11	120.44	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	598	HIS	CA-C-N	-7.07	113.85	121.84
1	A	598	HIS	C-N-CA	-7.07	113.85	121.84
1	C	450	THR	CA-C-N	7.07	128.02	120.11
1	C	450	THR	C-N-CA	7.07	128.02	120.11
1	F	580	HIS	N-CA-C	7.06	118.97	111.28
1	A	480	ILE	CB-CA-C	7.05	121.00	111.97
1	F	557	ILE	N-CA-C	-7.05	103.91	110.53
1	B	428	ARG	CG-CD-NE	-7.04	96.51	112.00
1	B	523	GLU	N-CA-C	-7.01	104.84	113.19
1	F	571	ILE	N-CA-CB	6.93	118.21	110.51
1	E	490	SER	N-CA-C	-6.87	104.09	113.30
1	E	599	VAL	CB-CA-C	-6.85	100.05	111.29
1	D	554	GLU	N-CA-C	6.84	119.33	111.11
1	A	468	GLU	N-CA-C	-6.84	103.75	111.07
1	A	512	ILE	CA-C-N	-6.82	110.45	120.28
1	A	512	ILE	C-N-CA	-6.82	110.45	120.28
1	D	587	ILE	C-N-CD	6.81	152.92	125.00
1	F	485	THR	N-CA-CB	6.79	121.97	110.49
1	A	563	LYS	CA-C-N	-6.78	113.56	122.99
1	A	563	LYS	C-N-CA	-6.78	113.56	122.99
1	B	602	ASP	N-CA-C	6.78	119.05	110.24
1	A	465	ARG	CB-CG-CD	6.77	126.88	111.30
1	B	566	ILE	CA-C-N	-6.70	112.86	119.76
1	B	566	ILE	C-N-CA	-6.70	112.86	119.76
1	C	597	GLU	N-CA-C	-6.68	104.00	111.28
1	A	446	ILE	CB-CA-C	-6.66	101.58	110.98
1	A	549	VAL	N-CA-C	6.66	116.76	110.30
1	B	490	SER	N-CA-C	-6.65	105.13	113.18
1	C	483	LYS	CA-C-N	-6.65	111.40	120.44
1	C	483	LYS	C-N-CA	-6.65	111.40	120.44
1	D	441	ILE	N-CA-C	-6.62	98.96	108.42
1	A	544	LEU	CA-C-N	6.61	127.51	120.11
1	A	544	LEU	C-N-CA	6.61	127.51	120.11
1	D	597	GLU	CA-CB-CG	-6.60	100.90	114.10
1	C	613	PHE	CB-CA-C	6.58	119.99	111.50
1	A	587	ILE	N-CA-C	6.58	114.06	107.55
1	D	599	VAL	N-CA-C	6.58	117.66	111.48
1	D	505	VAL	CB-CA-C	-6.57	101.89	111.68
1	F	556	ALA	N-CA-C	6.55	118.42	111.28
1	C	459	ARG	N-CA-C	6.55	119.03	109.07
1	C	445	ILE	CB-CA-C	-6.52	100.28	110.52
1	E	589	VAL	N-CA-C	6.51	117.85	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	573	ASP	N-CA-C	-6.51	106.07	112.97
1	F	458	GLY	N-CA-C	6.48	120.10	111.03
1	A	612	LYS	N-CA-C	-6.43	105.97	113.88
1	E	566	ILE	CA-C-N	-6.43	113.33	119.76
1	E	566	ILE	C-N-CA	-6.43	113.33	119.76
1	A	604	LYS	CD-CE-NZ	6.41	132.42	111.90
1	A	586	VAL	CA-C-N	-6.39	115.57	122.85
1	A	586	VAL	C-N-CA	-6.39	115.57	122.85
1	F	485	THR	CA-C-O	6.33	121.61	117.94
1	A	442	VAL	N-CA-C	-6.33	101.41	109.58
1	E	481	ILE	N-CA-C	6.33	118.29	111.58
1	B	494	VAL	N-CA-C	6.32	117.67	108.58
1	B	452	SER	N-CA-C	6.29	120.67	113.19
1	D	522	ILE	N-CA-C	6.29	116.96	110.36
1	D	588	PRO	CA-C-N	-6.28	113.54	121.96
1	D	588	PRO	C-N-CA	-6.28	113.54	121.96
1	D	502	TYR	N-CA-C	6.28	121.05	107.49
1	C	418	LEU	N-CA-C	6.26	121.08	113.38
1	F	474	VAL	CA-C-O	-6.24	114.92	121.41
1	B	477	VAL	N-CA-C	6.23	120.86	111.89
1	A	469	ILE	N-CA-CB	-6.20	103.62	110.51
1	E	542	GLU	N-CA-C	6.20	119.25	110.50
1	C	530	SER	N-CA-C	-6.20	105.36	113.17
1	F	566	ILE	CA-C-N	-6.19	113.41	119.78
1	F	566	ILE	C-N-CA	-6.19	113.41	119.78
1	E	446	ILE	N-CA-C	-6.18	99.15	108.17
1	A	426	VAL	N-CA-C	6.17	117.27	108.93
1	E	612	LYS	CA-C-N	6.17	129.05	121.64
1	E	612	LYS	C-N-CA	6.17	129.05	121.64
1	E	505	VAL	N-CA-C	6.17	117.26	108.93
1	A	479	ALA	N-CA-C	-6.16	104.12	111.69
1	C	494	VAL	N-CA-C	6.15	116.67	107.51
1	F	482	LYS	N-CA-C	6.12	118.92	111.82
1	E	605	LYS	CA-C-N	6.12	128.39	120.44
1	E	605	LYS	C-N-CA	6.12	128.39	120.44
1	D	450	THR	CA-C-O	-6.10	114.38	120.66
1	B	550	THR	CA-C-O	-6.08	114.62	121.00
1	A	507	GLY	N-CA-C	-6.07	103.30	112.89
1	F	441	ILE	CB-CA-C	-6.04	99.62	110.48
1	C	431	GLY	N-CA-C	-6.03	102.17	112.30
1	D	441	ILE	CB-CA-C	-6.01	100.35	111.18
1	C	420	ILE	CB-CA-C	6.00	118.22	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	494	VAL	CA-C-N	-5.98	114.81	122.77
1	E	494	VAL	C-N-CA	-5.98	114.81	122.77
1	B	452	SER	CA-C-N	5.98	132.47	121.70
1	B	452	SER	C-N-CA	5.98	132.47	121.70
1	B	585	GLU	CA-CB-CG	5.97	126.05	114.10
1	D	480	ILE	N-CA-CB	5.97	117.54	110.55
1	F	474	VAL	N-CA-CB	5.97	116.89	110.62
1	A	465	ARG	CA-CB-CG	5.96	126.03	114.10
1	E	540	LYS	N-CA-C	-5.96	105.31	112.59
1	A	602	ASP	N-CA-C	5.96	118.87	110.23
1	A	599	VAL	N-CA-C	5.95	118.91	112.96
1	B	474	VAL	N-CA-C	5.95	116.61	110.36
1	C	491	ASN	CB-CA-C	-5.95	100.67	110.72
1	E	430	ASN	N-CA-C	5.94	119.09	107.57
1	E	538	SER	N-CA-C	-5.93	101.74	110.52
1	F	484	TYR	CB-CA-C	5.91	118.22	109.29
1	F	566	ILE	N-CA-C	5.90	115.68	109.01
1	E	465	ARG	CA-C-N	-5.89	113.84	122.86
1	E	465	ARG	C-N-CA	-5.89	113.84	122.86
1	E	467	GLN	N-CA-C	5.89	117.38	111.07
1	B	605	LYS	N-CA-CB	5.89	119.06	110.47
1	D	431	GLY	CA-C-N	-5.88	114.13	122.94
1	D	431	GLY	C-N-CA	-5.88	114.13	122.94
1	E	598	HIS	N-CA-C	5.85	119.39	112.72
1	C	587	ILE	N-CA-C	5.84	113.93	108.15
1	D	452	SER	N-CA-C	5.84	118.87	111.69
1	C	422	GLU	N-CA-C	5.83	116.79	108.74
1	D	467	GLN	N-CA-C	5.83	117.31	111.07
1	E	609	LEU	N-CA-C	-5.81	104.86	111.07
1	F	557	ILE	N-CA-CB	5.81	118.01	110.57
1	C	520	SER	N-CA-C	5.80	120.94	111.37
1	C	464	GLY	CA-C-N	-5.79	112.06	120.29
1	C	464	GLY	C-N-CA	-5.79	112.06	120.29
1	D	553	ILE	N-CA-C	-5.77	105.10	110.53
1	A	558	GLN	N-CA-C	-5.77	105.08	111.71
1	E	607	ASN	N-CA-C	-5.77	104.19	111.11
1	F	441	ILE	N-CA-C	5.76	117.36	108.44
1	A	564	VAL	CA-C-N	-5.75	115.54	122.90
1	A	564	VAL	C-N-CA	-5.75	115.54	122.90
1	B	447	ALA	N-CA-C	5.74	119.02	110.52
1	E	512	ILE	N-CA-C	5.74	118.22	111.05
1	C	460	VAL	N-CA-C	5.74	115.60	106.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	571	ILE	N-CA-CB	5.74	116.88	110.51
1	F	502	TYR	CA-C-N	5.73	128.98	120.90
1	F	502	TYR	C-N-CA	5.73	128.98	120.90
1	B	464	GLY	N-CA-C	5.73	122.61	112.53
1	C	614	LYS	CA-C-N	5.73	132.01	121.70
1	C	614	LYS	C-N-CA	5.73	132.01	121.70
1	B	496	ILE	N-CA-C	5.72	116.84	107.24
1	B	525	ILE	CA-C-O	5.71	124.89	119.98
1	E	591	ARG	CG-CD-NE	5.70	124.55	112.00
1	A	480	ILE	N-CA-CB	5.70	117.22	110.55
1	A	480	ILE	CA-CB-CG2	5.68	120.16	110.50
1	F	476	ASN	N-CA-C	5.67	122.88	110.80
1	F	509	SER	N-CA-C	-5.67	103.44	110.41
1	B	582	GLY	N-CA-C	-5.65	107.46	115.43
1	B	597	GLU	CA-C-N	-5.63	112.73	120.28
1	B	597	GLU	C-N-CA	-5.63	112.73	120.28
1	E	574	VAL	CB-CA-C	-5.63	103.35	111.34
1	E	562	LYS	N-CA-C	5.61	120.25	112.45
1	A	542	GLU	CA-C-N	-5.61	115.58	122.93
1	A	542	GLU	C-N-CA	-5.61	115.58	122.93
1	A	591	ARG	CB-CG-CD	-5.61	98.40	111.30
1	D	499	VAL	N-CA-C	-5.61	101.44	108.84
1	C	439	ALA	N-CA-C	5.60	117.59	109.07
1	A	494	VAL	N-CA-C	5.60	116.00	108.17
1	F	433	ALA	N-CA-C	5.58	115.61	108.24
1	E	550	THR	CA-C-O	-5.58	115.15	120.90
1	B	565	ILE	N-CA-C	-5.57	101.63	109.21
1	F	439	ALA	N-CA-C	5.57	117.00	108.42
1	F	566	ILE	CB-CA-C	-5.56	103.88	109.89
1	B	608	ARG	N-CA-CB	5.55	118.20	109.94
1	E	452	SER	N-CA-C	5.54	119.09	110.17
1	A	572	ASP	N-CA-C	-5.52	106.31	113.16
1	C	433	ALA	CA-C-N	-5.52	115.26	122.94
1	C	433	ALA	C-N-CA	-5.52	115.26	122.94
1	F	526	PRO	N-CA-C	5.50	119.66	111.41
1	B	422	GLU	CA-C-N	-5.49	114.78	122.85
1	B	422	GLU	C-N-CA	-5.49	114.78	122.85
1	F	499	VAL	N-CA-C	5.49	114.51	106.55
1	E	602	ASP	N-CA-C	5.49	118.65	110.14
1	F	496	ILE	CA-C-N	-5.48	113.61	122.81
1	F	496	ILE	C-N-CA	-5.48	113.61	122.81
1	A	516	THR	N-CA-C	5.47	117.68	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	580	HIS	N-CA-C	5.47	118.17	111.82
1	A	474	VAL	CB-CA-C	-5.47	101.35	111.79
1	E	541	GLY	N-CA-C	5.47	122.03	114.92
1	F	570	ASN	N-CA-C	-5.46	106.20	112.92
1	F	465	ARG	NE-CZ-NH1	-5.44	116.06	121.50
1	B	503	GLU	N-CA-C	-5.43	101.72	110.14
1	C	513	SER	CA-C-N	-5.43	113.72	120.56
1	C	513	SER	C-N-CA	-5.43	113.72	120.56
1	E	448	GLU	N-CA-C	5.43	118.25	108.48
1	D	519	ILE	N-CA-C	-5.40	104.34	111.09
1	F	571	ILE	CB-CA-C	-5.40	104.97	111.88
1	D	446	ILE	N-CA-C	5.39	116.35	108.53
1	A	453	MET	CB-CG-SD	5.39	128.88	112.70
1	D	608	ARG	CG-CD-NE	5.39	123.86	112.00
1	E	520	SER	N-CA-C	5.39	118.07	111.82
1	A	491	ASN	CB-CA-C	5.38	120.24	110.72
1	B	517	ALA	CA-C-N	5.35	127.40	120.56
1	B	517	ALA	C-N-CA	5.35	127.40	120.56
1	F	539	VAL	N-CA-C	-5.35	104.19	111.89
1	B	554	GLU	N-CA-C	5.34	117.18	111.36
1	C	461	ILE	CB-CA-C	-5.34	103.76	111.34
1	B	471	ARG	CA-C-O	-5.33	115.20	120.90
1	B	463	THR	CA-CB-CG2	5.32	119.55	110.50
1	B	558	GLN	N-CA-C	5.32	118.56	111.75
1	D	608	ARG	CD-NE-CZ	5.32	131.84	124.40
1	F	478	SER	N-CA-C	5.29	122.07	110.80
1	F	576	LEU	N-CA-C	5.29	117.98	110.10
1	B	420	ILE	N-CA-C	5.28	117.16	108.97
1	A	613	PHE	N-CA-C	5.27	119.27	113.21
1	D	476	ASN	N-CA-C	5.26	118.86	112.23
1	D	613	PHE	CB-CA-C	-5.26	102.67	111.13
1	F	512	ILE	CB-CA-C	-5.25	104.38	112.05
1	D	479	ALA	N-CA-C	-5.23	105.02	111.40
1	B	498	PHE	N-CA-C	5.22	116.81	108.41
1	C	583	LYS	CD-CE-NZ	5.19	128.52	111.90
1	D	480	ILE	CB-CA-C	5.19	118.61	111.97
1	A	437	GLU	N-CA-C	5.16	119.15	111.87
1	B	527	VAL	N-CA-C	5.16	115.39	108.17
1	C	435	ILE	N-CA-CB	5.14	117.52	111.66
1	D	473	ALA	N-CA-C	-5.13	105.38	111.69
1	E	461	ILE	N-CA-C	-5.13	100.17	107.77
1	F	494	VAL	N-CA-C	5.13	114.97	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	480	ILE	CB-CG1-CD1	-5.12	103.05	113.80
1	A	550	THR	CA-C-N	-5.12	111.60	121.58
1	A	550	THR	C-N-CA	-5.12	111.60	121.58
1	A	590	SER	O-C-N	5.11	127.66	122.09
1	A	505	VAL	N-CA-C	5.11	115.67	108.36
1	C	487	ARG	CG-CD-NE	-5.09	100.80	112.00
1	B	446	ILE	CB-CG1-CD1	-5.09	103.11	113.80
1	C	420	ILE	N-CA-CB	-5.08	105.20	111.00
1	C	590	SER	N-CA-C	-5.07	107.77	114.31
1	D	595	VAL	CA-C-N	-5.07	112.06	120.68
1	D	595	VAL	C-N-CA	-5.07	112.06	120.68
1	D	581	GLU	N-CA-CB	5.07	118.80	110.39
1	F	501	THR	CA-C-N	-5.05	114.08	122.92
1	F	501	THR	C-N-CA	-5.05	114.08	122.92
1	C	582	GLY	N-CA-C	-5.04	106.84	115.61
1	E	422	GLU	CA-C-O	-5.04	115.22	121.06
1	E	492	MET	CG-SD-CE	-5.03	89.83	100.90
1	A	461	ILE	N-CA-C	5.03	113.99	106.85
1	C	426	VAL	O-C-N	5.03	127.80	122.67
1	D	607	ASN	O-C-N	5.03	127.52	122.09
1	A	608	ARG	N-CA-C	-5.02	105.52	111.69
1	C	491	ASN	N-CA-CB	5.02	118.51	110.73
1	D	469	ILE	CA-C-O	-5.02	116.05	121.27
1	D	549	VAL	N-CA-C	5.01	119.76	109.34
1	D	545	PRO	CB-CA-C	-5.01	104.39	110.95
1	E	487	ARG	CB-CA-C	5.00	117.71	109.90
1	B	478	SER	CA-CB-OG	-5.00	101.10	111.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	500	GLY	Peptide
1	B	606	LYS	Peptide
1	C	452	SER	Peptide
1	D	438	SER	Peptide
1	D	614	LYS	Peptide
1	E	424	TYR	Peptide
1	E	567	PRO	Peptide
1	F	484	TYR	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	101	0
1	B	1466	0	1529	186	0
1	C	1466	0	1529	134	0
1	D	1466	0	1529	99	0
1	E	1457	0	1523	177	0
1	F	1466	0	1529	141	0
2	A	159	0	0	13	0
2	B	164	0	0	32	0
2	C	208	0	0	36	0
2	D	190	0	0	17	0
2	E	145	0	0	32	0
2	F	226	0	0	35	0
All	All	9870	0	9162	815	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (815) 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:C:435:ILE:CD1	1:C:435:ILE:CG1	1.76	1.61
1:C:420:ILE:CB	1:C:420:ILE:CG2	1.78	1.60
1:F:522:ILE:CD1	1:F:522:ILE:CG1	1.79	1.58
1:B:463:THR:CB	1:B:463:THR:CG2	1.74	1.54
1:D:612:LYS:NZ	1:D:612:LYS:CE	1.70	1.54
1:A:605:LYS:CE	1:A:605:LYS:NZ	1.71	1.52
1:A:604:LYS:NZ	1:A:604:LYS:CE	1.73	1.50
1:A:583:LYS:NZ	1:A:583:LYS:CE	1.71	1.48
1:C:420:ILE:CD1	1:C:420:ILE:CG1	1.91	1.46
1:F:612:LYS:CE	1:F:612:LYS:NZ	1.82	1.42
1:C:502:TYR:CD1	2:C:701:HOH:O	1.68	1.33
1:E:576:LEU:HD22	1:E:580:HIS:CB	1.57	1.33
1:C:614:LYS:HG2	2:C:713:HOH:O	1.27	1.30
1:F:502:TYR:CE2	1:F:503:GLU:O	1.89	1.24
1:F:502:TYR:CD2	1:F:503:GLU:O	1.93	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:SER:N	2:B:633:HOH:O	1.71	1.21
1:C:497:GLN:HB2	2:C:826:HOH:O	1.04	1.21
1:E:426:VAL:HG11	2:E:647:HOH:O	1.39	1.20
1:E:576:LEU:HD22	1:E:580:HIS:HB3	1.22	1.17
1:E:451:PRO:HD3	2:E:639:HOH:O	1.46	1.16
1:E:450:THR:CG2	2:F:803:HOH:O	1.94	1.15
1:C:501:THR:HG21	2:D:676:HOH:O	1.43	1.15
1:E:450:THR:HG21	2:F:803:HOH:O	1.43	1.14
1:C:459:ARG:HB3	2:C:825:HOH:O	1.49	1.13
1:E:478:SER:HB3	1:E:489:ILE:HG12	1.23	1.13
1:E:437:GLU:HB2	2:E:735:HOH:O	1.44	1.12
1:A:470:ALA:O	1:A:474:VAL:HG23	1.47	1.12
1:E:422:GLU:OE2	1:E:423:GLY:N	1.84	1.09
1:B:453:MET:HG2	1:C:482:LYS:HZ2	1.02	1.08
1:D:428:ARG:CG	2:D:811:HOH:O	2.03	1.06
1:E:576:LEU:HD22	1:E:580:HIS:HB2	1.33	1.05
1:B:563:LYS:HG3	1:B:585:GLU:HB2	1.37	1.05
1:B:604:LYS:HB2	2:B:753:HOH:O	1.55	1.05
1:C:597:GLU:HB3	2:C:775:HOH:O	1.54	1.05
1:F:597:GLU:HB3	2:F:817:HOH:O	1.55	1.04
1:E:576:LEU:CD2	1:E:580:HIS:CB	2.36	1.03
1:D:428:ARG:HG2	2:D:811:HOH:O	1.56	1.02
1:F:502:TYR:CD2	1:F:505:VAL:HG23	1.94	1.02
1:B:563:LYS:HG2	1:B:587:ILE:HD11	1.43	1.01
1:B:453:MET:HG2	1:C:482:LYS:NZ	1.75	1.00
1:E:496:ILE:C	2:E:744:HOH:O	2.04	1.00
1:E:551:GLN:HB2	2:E:739:HOH:O	1.62	0.99
1:E:530:SER:HB3	1:E:562:LYS:HB2	1.43	0.99
1:E:418:LEU:HD13	1:E:419:PHE:HD2	1.27	0.97
1:E:601:GLU:HG2	1:E:602:ASP:H	1.27	0.96
1:E:450:THR:HG23	2:E:731:HOH:O	1.63	0.95
1:A:487:ARG:HG2	1:A:487:ARG:HH11	1.33	0.94
1:F:473:ALA:O	1:F:477:VAL:HG12	1.66	0.94
1:E:549:VAL:HB	2:E:734:HOH:O	1.69	0.92
1:B:585:GLU:HB3	2:B:653:HOH:O	1.70	0.91
1:A:438:SER:O	1:A:439:ALA:O	1.90	0.90
1:B:480:ILE:HG13	1:B:481:ILE:N	1.83	0.90
1:E:540:LYS:HG3	2:E:657:HOH:O	1.71	0.89
1:C:476:ASN:ND2	1:C:477:VAL:N	2.20	0.89
1:E:576:LEU:CD2	1:E:580:HIS:HB3	1.97	0.88
1:E:449:VAL:HG21	1:E:522:ILE:HG13	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:472:GLU:CG	1:C:473:ALA:N	2.36	0.87
1:B:523:GLU:HG3	1:B:609:LEU:HD22	1.56	0.87
1:B:549:VAL:HG23	2:B:643:HOH:O	1.73	0.86
1:D:428:ARG:HG2	1:D:428:ARG:HH11	1.38	0.86
1:D:611:SER:O	1:D:614:LYS:HG3	1.75	0.86
1:D:488:ASP:OD1	1:D:490:SER:HB2	1.75	0.86
1:A:477:VAL:O	1:A:481:ILE:HG23	1.74	0.86
1:C:445:ILE:CG2	2:C:645:HOH:O	2.24	0.85
1:A:469:ILE:HG21	2:A:777:HOH:O	1.76	0.85
1:B:451:PRO:HA	1:B:492:MET:HE2	1.58	0.85
1:D:465:ARG:HG3	1:D:465:ARG:HH11	1.42	0.85
1:C:420:ILE:CG2	1:C:420:ILE:CG1	2.55	0.85
1:D:459:ARG:NH2	2:D:678:HOH:O	2.04	0.85
1:E:496:ILE:N	2:E:744:HOH:O	2.10	0.84
1:B:489:ILE:HG13	1:B:492:MET:CG	2.07	0.84
1:F:563:LYS:HD2	1:F:587:ILE:HD11	1.59	0.84
1:A:568:LYS:HD3	2:A:725:HOH:O	1.77	0.83
1:B:529:GLN:HA	2:B:639:HOH:O	1.78	0.83
1:E:435:ILE:HG21	2:E:751:HOH:O	1.77	0.83
1:B:478:SER:HB3	1:B:482:LYS:HE3	1.60	0.83
1:D:489:ILE:HA	1:D:492:MET:HE3	1.60	0.83
1:C:445:ILE:HG22	2:C:645:HOH:O	1.79	0.82
1:D:568:LYS:O	1:D:571:ILE:HG13	1.79	0.82
1:E:577:ASP:O	1:E:581:GLU:HG2	1.80	0.82
1:B:484:TYR:CD2	1:B:613:PHE:CD2	2.68	0.81
1:F:562:LYS:HE3	2:F:680:HOH:O	1.80	0.81
1:B:450:THR:HG21	1:C:483:LYS:HB2	1.61	0.81
1:E:611:SER:O	1:E:614:LYS:HD3	1.80	0.80
1:D:571:ILE:HD11	1:D:588:PRO:HG3	1.60	0.80
1:C:420:ILE:HG13	2:C:774:HOH:O	1.80	0.80
1:B:418:LEU:HD23	2:B:658:HOH:O	1.82	0.80
1:C:476:ASN:HD22	1:C:477:VAL:N	1.76	0.80
1:F:469:ILE:HG21	2:F:815:HOH:O	1.82	0.80
1:F:485:THR:HA	2:F:762:HOH:O	1.81	0.80
1:B:484:TYR:CD2	1:B:613:PHE:HD2	1.99	0.80
1:B:478:SER:O	1:B:482:LYS:HD3	1.81	0.79
1:E:599:VAL:HG23	1:E:600:LEU:H	1.46	0.79
1:B:489:ILE:HG13	1:B:492:MET:HG3	1.65	0.79
1:D:422:GLU:HG2	1:D:423:GLY:N	1.98	0.79
1:E:425:GLU:H	1:E:526:PRO:HB2	1.48	0.79
1:B:563:LYS:HG3	1:B:585:GLU:CB	2.11	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:601:GLU:HG2	1:E:602:ASP:N	1.96	0.79
1:D:428:ARG:HG3	2:D:811:HOH:O	1.75	0.78
1:C:615:GLU:C	2:C:818:HOH:O	2.27	0.78
1:E:492:MET:HE1	1:E:522:ILE:HG12	1.66	0.78
1:B:531:VAL:HG22	1:B:563:LYS:HB2	1.66	0.78
1:C:424:TYR:HB3	1:C:526:PRO:HB2	1.65	0.78
1:D:558:GLN:NE2	2:D:744:HOH:O	2.16	0.78
1:E:496:ILE:CA	2:E:744:HOH:O	2.29	0.78
1:F:571:ILE:HD11	1:F:588:PRO:HG3	1.66	0.78
1:A:492:MET:HE1	1:A:522:ILE:HD13	1.66	0.77
1:C:472:GLU:HG2	1:C:473:ALA:H	1.47	0.77
1:E:425:GLU:H	1:E:526:PRO:CB	1.96	0.77
1:E:562:LYS:C	1:E:563:LYS:HG3	2.10	0.77
1:E:470:ALA:O	1:E:474:VAL:HG23	1.84	0.77
1:F:485:THR:HG23	1:F:523:GLU:OE2	1.84	0.77
1:B:480:ILE:CD1	1:B:613:PHE:HE2	1.97	0.76
1:B:430:ASN:ND2	2:B:639:HOH:O	2.18	0.76
1:B:568:LYS:O	1:B:571:ILE:HB	1.85	0.76
1:F:419:PHE:HB3	1:F:444:PRO:HG3	1.65	0.76
1:A:446:ILE:HD11	1:A:497:GLN:HB2	1.66	0.76
1:C:502:TYR:CE1	2:C:701:HOH:O	2.10	0.76
1:A:421:THR:HG22	1:A:561:LEU:HD21	1.67	0.76
1:C:476:ASN:HD22	1:C:477:VAL:H	1.34	0.75
1:E:427:GLY:O	1:E:447:ALA:N	2.15	0.75
1:D:568:LYS:HA	1:D:588:PRO:HB2	1.69	0.75
1:D:418:LEU:HD23	1:E:545:PRO:HB2	1.67	0.75
1:B:459:ARG:NH2	1:B:461:ILE:HD11	2.01	0.74
1:A:421:THR:HG22	1:A:561:LEU:CD2	2.16	0.74
1:B:480:ILE:HD11	1:B:613:PHE:CE2	2.21	0.74
1:E:485:THR:HG22	1:E:487:ARG:H	1.50	0.74
1:A:476:ASN:O	1:A:480:ILE:HG22	1.87	0.74
1:C:501:THR:HG22	2:D:653:HOH:O	1.86	0.74
1:C:474:VAL:CG2	1:C:496:ILE:HD11	2.18	0.74
1:C:428:ARG:HH11	1:C:428:ARG:HG3	1.53	0.74
1:C:614:LYS:HA	1:C:615:GLU:O	1.86	0.74
1:C:474:VAL:HG21	1:C:496:ILE:HD11	1.70	0.73
1:F:466:LEU:CD2	1:F:469:ILE:HD12	2.18	0.73
1:B:525:ILE:HG22	1:B:600:LEU:HD22	1.69	0.73
1:B:492:MET:O	2:B:631:HOH:O	2.06	0.73
1:A:443:LEU:HG	2:A:761:HOH:O	1.87	0.73
1:C:472:GLU:HG2	1:C:473:ALA:N	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:554:GLU:HG2	1:E:580:HIS:CD2	2.23	0.73
1:B:489:ILE:CD1	1:B:492:MET:HG2	2.19	0.73
1:B:482:LYS:HE2	1:B:489:ILE:H	1.54	0.73
1:C:445:ILE:HD11	2:C:787:HOH:O	1.87	0.72
1:B:543:VAL:O	2:B:744:HOH:O	2.06	0.72
1:C:531:VAL:HG22	1:C:563:LYS:HB2	1.70	0.72
1:E:478:SER:HB3	1:E:489:ILE:CG1	2.11	0.72
1:F:446:ILE:CD1	1:F:497:GLN:HB2	2.20	0.72
1:E:576:LEU:CD2	1:E:580:HIS:HB2	2.08	0.72
1:B:576:LEU:HB3	1:B:580:HIS:HB2	1.70	0.72
1:E:495:HIS:C	2:E:744:HOH:O	2.32	0.72
1:B:453:MET:CG	1:C:482:LYS:NZ	2.53	0.71
1:C:497:GLN:CB	2:C:826:HOH:O	1.83	0.71
1:C:420:ILE:HD12	1:C:420:ILE:HG23	1.72	0.71
1:A:553:ILE:HG21	1:A:576:LEU:HD11	1.72	0.71
1:B:417:LYS:HD2	1:B:419:PHE:CE1	2.24	0.71
1:E:466:LEU:HD12	2:E:718:HOH:O	1.91	0.71
1:F:469:ILE:O	1:F:472:GLU:HG3	1.90	0.71
1:E:553:ILE:HD11	1:E:566:ILE:HD11	1.73	0.71
1:E:595:VAL:O	1:E:599:VAL:HG22	1.91	0.71
1:A:475:MET:HE2	1:F:459:ARG:NH2	2.06	0.71
1:F:578:ALA:C	1:F:580:HIS:N	2.46	0.70
1:B:489:ILE:HG13	1:B:492:MET:HG2	1.73	0.70
1:C:577:ASP:OD2	1:C:580:HIS:HB2	1.92	0.70
1:E:551:GLN:CB	2:E:739:HOH:O	2.30	0.70
1:B:459:ARG:CZ	1:B:461:ILE:HD11	2.21	0.70
1:B:484:TYR:HD2	1:B:613:PHE:CE2	2.09	0.69
1:D:613:PHE:C	1:D:615:GLU:H	1.98	0.69
1:F:477:VAL:HG22	1:F:481:ILE:HG13	1.73	0.69
1:F:578:ALA:C	1:F:580:HIS:H	2.00	0.69
1:F:482:LYS:HG3	2:F:832:HOH:O	1.92	0.69
1:F:502:TYR:HD2	1:F:505:VAL:HG23	1.52	0.69
1:B:477:VAL:HG11	1:B:518:VAL:CG1	2.22	0.69
1:E:481:ILE:O	1:E:486:GLY:N	2.26	0.69
1:B:428:ARG:HA	1:B:445:ILE:O	1.93	0.69
1:E:601:GLU:O	1:E:606:LYS:HD2	1.92	0.69
1:A:481:ILE:HG13	1:A:482:LYS:N	2.07	0.68
1:B:463:THR:CG2	1:B:463:THR:HB	2.15	0.68
1:B:523:GLU:CG	1:B:609:LEU:HD22	2.23	0.68
1:E:562:LYS:O	1:E:563:LYS:HG3	1.93	0.68
1:B:571:ILE:HD13	1:B:571:ILE:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:538:SER:OG	1:D:542:GLU:HG2	1.93	0.68
1:F:476:ASN:ND2	2:F:666:HOH:O	2.25	0.68
1:B:545:PRO:HA	1:B:567:PRO:HG2	1.74	0.68
1:B:609:LEU:O	1:B:612:LYS:HB2	1.93	0.68
1:D:595:VAL:O	1:D:599:VAL:HG22	1.94	0.68
1:C:450:THR:HB	2:C:781:HOH:O	1.94	0.68
1:F:592:ILE:CG2	1:F:593:ASN:N	2.56	0.68
1:C:450:THR:CB	2:C:781:HOH:O	2.43	0.67
1:E:418:LEU:HD13	1:E:419:PHE:CD2	2.19	0.67
1:E:429:VAL:HG12	1:E:430:ASN:N	2.09	0.67
1:C:502:TYR:CE2	1:C:505:VAL:HG21	2.29	0.67
1:F:460:VAL:HG13	1:F:494:VAL:HG22	1.77	0.67
1:A:428:ARG:HD3	1:A:446:ILE:CG2	2.24	0.66
1:B:487:ARG:HD2	1:B:489:ILE:HD13	1.76	0.66
1:C:435:ILE:CD1	1:C:435:ILE:CB	2.72	0.66
1:E:528:ASP:HB3	1:E:531:VAL:HG23	1.78	0.66
1:F:554:GLU:OE1	2:F:807:HOH:O	2.13	0.66
1:A:475:MET:HE2	1:F:459:ARG:HH22	1.58	0.66
1:B:480:ILE:CD1	1:B:613:PHE:CE2	2.77	0.66
1:B:484:TYR:HD2	1:B:613:PHE:CD2	2.13	0.66
1:C:418:LEU:HD23	1:C:499:VAL:O	1.94	0.66
1:E:491:ASN:C	1:E:492:MET:HG2	2.20	0.66
1:A:424:TYR:HB3	1:A:526:PRO:HB3	1.79	0.66
1:A:574:VAL:HG12	1:A:574:VAL:O	1.97	0.65
1:B:501:THR:HG22	2:C:679:HOH:O	1.95	0.65
1:B:465:ARG:NE	2:B:747:HOH:O	2.27	0.65
1:C:467:GLN:OE1	1:C:471:ARG:NH2	2.29	0.65
1:B:453:MET:HB2	2:B:673:HOH:O	1.95	0.65
1:D:478:SER:HA	1:D:481:ILE:HD12	1.79	0.65
1:E:420:ILE:HG21	2:E:675:HOH:O	1.97	0.65
2:A:693:HOH:O	1:F:501:THR:HG21	1.95	0.65
1:C:420:ILE:CB	1:C:420:ILE:CD1	2.74	0.65
1:A:475:MET:CE	1:F:459:ARG:HH22	2.10	0.65
1:C:571:ILE:HD11	1:C:588:PRO:HG3	1.79	0.65
1:A:477:VAL:HA	1:A:480:ILE:HG23	1.79	0.64
1:B:551:GLN:CD	1:B:551:GLN:H	2.06	0.64
1:F:593:ASN:HB3	1:F:613:PHE:CD1	2.31	0.64
1:B:549:VAL:HG21	1:B:570:ASN:HB3	1.78	0.64
1:E:570:ASN:CG	2:E:734:HOH:O	2.39	0.64
1:C:446:ILE:HD11	1:D:544:LEU:HD13	1.80	0.64
1:D:562:LYS:HG2	2:D:632:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:ILE:HD11	1:A:522:ILE:HD11	1.78	0.64
1:C:428:ARG:HG3	1:C:428:ARG:NH1	2.13	0.64
1:F:532:ALA:HB2	1:F:561:LEU:HD13	1.80	0.64
1:A:475:MET:CE	1:F:459:ARG:NH2	2.61	0.64
1:D:445:ILE:HD12	1:D:513:SER:HB2	1.79	0.64
1:E:499:VAL:HG22	2:E:727:HOH:O	1.98	0.63
1:C:545:PRO:HG3	1:C:569:ASP:HB2	1.79	0.63
1:F:483:LYS:O	1:F:484:TYR:CD1	2.52	0.63
1:C:597:GLU:HG2	2:C:775:HOH:O	1.97	0.63
1:D:548:GLY:HA2	1:D:551:GLN:HE22	1.63	0.63
1:E:614:LYS:HA	2:E:666:HOH:O	1.97	0.63
1:B:488:ASP:O	1:B:489:ILE:HD13	1.98	0.63
1:B:489:ILE:CG1	1:B:492:MET:HG2	2.27	0.63
1:E:608:ARG:O	1:E:612:LYS:HG2	1.98	0.63
1:A:428:ARG:HD3	1:A:446:ILE:HG22	1.81	0.63
1:E:596:LEU:O	1:E:597:GLU:C	2.42	0.63
1:A:424:TYR:HB3	1:A:526:PRO:CB	2.29	0.63
1:C:597:GLU:CG	2:C:775:HOH:O	2.47	0.63
1:C:550:THR:HG23	2:C:816:HOH:O	1.97	0.63
1:A:570:ASN:ND2	1:A:573:ASP:OD2	2.29	0.62
1:C:467:GLN:HB2	1:C:471:ARG:HH21	1.64	0.62
1:B:604:LYS:N	2:B:753:HOH:O	2.25	0.62
1:C:472:GLU:HG3	1:C:473:ALA:N	2.13	0.62
1:E:531:VAL:HA	1:E:563:LYS:O	2.00	0.62
1:D:428:ARG:HG2	1:D:428:ARG:NH1	2.14	0.62
1:D:435:ILE:HG23	1:D:505:VAL:HG22	1.81	0.61
1:F:563:LYS:HG2	1:F:585:GLU:HB3	1.82	0.61
1:E:519:ILE:HD13	1:E:596:LEU:HD11	1.82	0.61
1:F:421:THR:HB	2:F:769:HOH:O	2.00	0.61
1:F:579:GLU:N	2:F:802:HOH:O	2.04	0.61
1:A:481:ILE:CD1	1:A:485:THR:HG22	2.30	0.61
1:E:495:HIS:NE2	1:F:479:ALA:HB2	2.15	0.61
1:B:483:LYS:HD3	1:B:484:TYR:CE1	2.36	0.61
1:C:477:VAL:HG22	1:C:481:ILE:CD1	2.31	0.61
1:D:484:TYR:HB3	1:D:612:LYS:O	2.00	0.61
1:F:577:ASP:O	1:F:578:ALA:O	2.17	0.61
1:A:477:VAL:O	1:A:481:ILE:CG2	2.47	0.61
1:D:565:ILE:HD11	1:D:598:HIS:HB3	1.82	0.61
1:F:467:GLN:OE1	2:F:784:HOH:O	2.16	0.61
1:F:517:ALA:HB3	2:F:701:HOH:O	2.00	0.61
1:A:470:ALA:O	1:A:474:VAL:CG2	2.37	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:PRO:O	1:A:570:ASN:HB2	2.01	0.61
1:D:443:LEU:HD21	1:D:466:LEU:HD13	1.81	0.61
1:B:487:ARG:HD2	1:B:488:ASP:O	2.01	0.60
1:D:480:ILE:HD11	1:D:613:PHE:HE1	1.66	0.60
1:D:571:ILE:CD1	1:D:588:PRO:HG3	2.31	0.60
1:E:496:ILE:HD11	1:E:518:VAL:CG2	2.31	0.60
1:E:599:VAL:HG23	1:E:600:LEU:N	2.16	0.60
1:E:611:SER:O	1:E:614:LYS:CD	2.48	0.60
1:F:511:SER:OG	1:F:514:ILE:HD12	2.00	0.60
1:C:577:ASP:OD2	1:C:580:HIS:CB	2.50	0.60
1:F:472:GLU:O	1:F:473:ALA:C	2.44	0.60
1:B:478:SER:C	1:B:482:LYS:HD3	2.26	0.60
1:B:418:LEU:HD11	2:C:808:HOH:O	2.01	0.60
1:B:563:LYS:CG	1:B:587:ILE:HD11	2.26	0.60
1:C:485:THR:OG1	1:C:486:GLY:N	2.34	0.60
1:B:509:SER:O	1:B:510:ALA:C	2.45	0.60
1:B:558:GLN:HE21	1:B:558:GLN:N	1.99	0.60
1:E:551:GLN:CD	1:E:551:GLN:H	2.10	0.60
1:E:575:LEU:HB2	2:E:635:HOH:O	2.02	0.59
1:B:482:LYS:HD2	2:B:784:HOH:O	2.01	0.59
1:A:438:SER:O	1:A:439:ALA:C	2.45	0.59
1:A:449:VAL:HG12	1:A:494:VAL:HG22	1.83	0.59
1:B:610:MET:C	2:B:648:HOH:O	2.45	0.59
1:F:547:GLY:O	1:F:552:LYS:HE3	2.02	0.59
1:B:508:ASP:HA	2:B:633:HOH:O	2.01	0.59
1:C:550:THR:HA	2:C:816:HOH:O	2.01	0.59
1:B:525:ILE:CG2	1:B:600:LEU:HD22	2.31	0.59
1:C:472:GLU:CG	1:C:473:ALA:H	2.09	0.59
1:C:477:VAL:HG22	1:C:481:ILE:HD12	1.83	0.59
1:E:528:ASP:HB3	1:E:531:VAL:CG2	2.33	0.59
1:C:420:ILE:CG2	1:C:420:ILE:CA	2.78	0.59
1:E:425:GLU:N	1:E:526:PRO:CB	2.65	0.59
1:E:440:GLY:N	2:E:739:HOH:O	2.36	0.59
1:E:540:LYS:CD	2:E:657:HOH:O	2.51	0.59
1:F:558:GLN:HG3	2:F:842:HOH:O	2.01	0.58
1:A:429:VAL:HG22	1:A:527:VAL:HG11	1.85	0.58
1:A:432:LEU:HG	1:A:532:ALA:HB1	1.84	0.58
1:A:428:ARG:HA	1:A:445:ILE:O	2.02	0.58
1:A:487:ARG:HG2	1:A:487:ARG:NH1	2.08	0.58
1:A:420:ILE:HB	1:A:529:GLN:HG3	1.86	0.58
1:E:553:ILE:HD11	1:E:566:ILE:CD1	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:514:ILE:O	1:F:518:VAL:HG23	2.03	0.58
1:F:612:LYS:HG2	2:F:699:HOH:O	2.03	0.58
1:A:428:ARG:CD	1:A:446:ILE:CG2	2.82	0.58
1:F:571:ILE:O	1:F:574:VAL:HG23	2.04	0.58
1:B:592:ILE:HG23	1:B:593:ASN:N	2.16	0.58
2:C:755:HOH:O	1:D:540:LYS:HE3	2.04	0.57
1:B:451:PRO:CA	1:B:492:MET:HE2	2.32	0.57
1:B:467:GLN:HG3	2:B:762:HOH:O	2.05	0.57
1:E:428:ARG:HG2	1:E:429:VAL:N	2.20	0.57
1:B:592:ILE:CG2	1:B:593:ASN:N	2.67	0.57
1:E:588:PRO:HG2	2:E:760:HOH:O	2.05	0.57
1:F:435:ILE:HG23	1:F:505:VAL:HG22	1.85	0.57
1:A:468:GLU:OE1	2:A:649:HOH:O	2.18	0.57
1:B:492:MET:HE2	1:B:492:MET:HA	1.87	0.57
1:C:502:TYR:CD2	1:C:505:VAL:HG21	2.39	0.57
1:B:508:ASP:C	2:B:633:HOH:O	2.28	0.57
1:F:475:MET:HB2	2:F:705:HOH:O	2.04	0.57
1:A:555:ALA:O	1:A:558:GLN:HB3	2.05	0.57
1:D:422:GLU:HG2	1:D:423:GLY:H	1.67	0.57
1:F:483:LYS:O	1:F:484:TYR:HD1	1.88	0.57
1:F:469:ILE:CG2	2:F:815:HOH:O	2.48	0.57
1:A:589:VAL:HG21	1:A:595:VAL:HG23	1.87	0.56
1:B:513:SER:HB2	2:B:769:HOH:O	2.05	0.56
1:A:492:MET:HE1	1:A:522:ILE:CD1	2.35	0.56
1:B:449:VAL:HG13	1:B:521:ALA:HB1	1.86	0.56
1:B:457:GLU:HG2	2:B:689:HOH:O	2.05	0.56
1:B:609:LEU:O	1:B:609:LEU:HD12	2.05	0.56
1:A:435:ILE:HG12	1:A:441:ILE:HG23	1.87	0.56
1:A:549:VAL:HG13	1:A:553:ILE:CD1	2.35	0.56
1:B:593:ASN:O	1:B:610:MET:HE1	2.06	0.56
1:A:481:ILE:HD11	1:A:487:ARG:HB2	1.87	0.56
1:B:545:PRO:HA	1:B:567:PRO:CB	2.36	0.56
1:D:472:GLU:HB2	2:D:777:HOH:O	2.06	0.56
1:F:487:ARG:HB3	1:F:492:MET:HE3	1.87	0.56
1:B:489:ILE:HG12	1:B:522:ILE:HD12	1.87	0.56
1:C:428:ARG:HG2	1:C:446:ILE:HG23	1.86	0.56
1:E:525:ILE:HG21	1:E:600:LEU:HD13	1.87	0.56
1:F:538:SER:O	1:F:541:GLY:N	2.31	0.56
1:B:457:GLU:CD	2:B:689:HOH:O	2.49	0.55
1:C:420:ILE:CD1	1:C:420:ILE:HG23	2.36	0.55
1:F:446:ILE:HD12	1:F:497:GLN:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:VAL:HG22	1:B:518:VAL:HG21	1.88	0.55
1:B:512:ILE:O	1:B:513:SER:C	2.50	0.55
1:C:428:ARG:HD3	1:C:446:ILE:HG12	1.87	0.55
1:A:428:ARG:CD	1:A:446:ILE:HG23	2.37	0.55
1:B:419:PHE:HA	1:B:428:ARG:NH2	2.21	0.55
1:B:480:ILE:HD12	1:B:613:PHE:HE2	1.71	0.55
1:B:577:ASP:O	1:B:578:ALA:C	2.50	0.55
1:C:469:ILE:O	1:C:472:GLU:HG2	2.07	0.55
1:D:474:VAL:HG22	1:D:518:VAL:HG21	1.88	0.55
1:E:610:MET:O	1:E:613:PHE:HB2	2.07	0.55
1:B:545:PRO:HA	1:B:567:PRO:CG	2.37	0.55
1:E:434:VAL:HG12	1:E:439:ALA:O	2.06	0.55
1:E:484:TYR:CB	1:E:613:PHE:HD1	2.20	0.55
1:D:441:ILE:HD11	1:D:505:VAL:HG13	1.89	0.55
1:A:558:GLN:HB3	2:A:636:HOH:O	2.06	0.54
1:B:449:VAL:HG21	1:B:522:ILE:HD13	1.89	0.54
1:E:540:LYS:CG	2:E:657:HOH:O	2.41	0.54
1:B:477:VAL:O	1:B:477:VAL:HG13	2.05	0.54
1:C:516:THR:HG23	1:C:596:LEU:CD2	2.37	0.54
1:E:527:VAL:HG13	1:E:599:VAL:HB	1.89	0.54
1:A:611:SER:O	1:A:614:LYS:HD3	2.07	0.54
1:B:444:PRO:HD2	1:B:499:VAL:O	2.07	0.54
1:B:600:LEU:HB2	1:B:606:LYS:HG3	1.88	0.54
1:B:428:ARG:HH11	1:B:446:ILE:HD11	1.72	0.54
1:B:465:ARG:HD3	2:B:687:HOH:O	2.07	0.54
1:D:424:TYR:HB3	1:D:526:PRO:HB2	1.89	0.54
1:F:429:VAL:HG22	1:F:527:VAL:HG11	1.89	0.54
1:F:466:LEU:HD23	1:F:469:ILE:HD12	1.89	0.54
1:D:548:GLY:O	1:D:552:LYS:HG3	2.07	0.54
1:A:489:ILE:HG12	1:A:492:MET:HE3	1.88	0.54
1:A:570:ASN:HA	1:A:573:ASP:OD2	2.08	0.54
1:B:428:ARG:NH1	1:B:446:ILE:HD11	2.22	0.54
1:B:484:TYR:CD2	1:B:613:PHE:CE2	2.94	0.54
1:C:532:ALA:HB2	1:C:561:LEU:HD13	1.90	0.54
1:F:553:ILE:HG23	1:F:584:ILE:HG21	1.89	0.54
1:B:535:GLY:HA2	1:B:567:PRO:HG3	1.89	0.54
1:C:435:ILE:HD13	1:C:435:ILE:HG21	1.89	0.54
1:C:435:ILE:CD1	1:C:435:ILE:HG21	2.38	0.54
1:E:422:GLU:OE2	1:E:422:GLU:C	2.50	0.54
1:B:451:PRO:HB3	1:B:492:MET:HE1	1.89	0.54
1:B:558:GLN:HE21	1:B:558:GLN:H	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:MET:C	1:A:612:LYS:H	2.16	0.53
1:B:424:TYR:HA	1:B:527:VAL:O	2.08	0.53
1:C:511:SER:N	2:C:719:HOH:O	2.37	0.53
1:D:478:SER:HB3	1:D:489:ILE:HD12	1.89	0.53
1:C:577:ASP:OD2	1:C:580:HIS:ND1	2.41	0.53
1:E:425:GLU:N	1:E:526:PRO:HB2	2.20	0.53
1:E:606:LYS:O	1:E:610:MET:HG2	2.08	0.53
1:A:457:GLU:HG2	1:A:490:SER:O	2.08	0.53
1:B:489:ILE:HG23	1:B:489:ILE:O	2.08	0.53
1:A:509:SER:O	1:A:510:ALA:C	2.51	0.53
1:D:445:ILE:CD1	1:D:513:SER:HB2	2.39	0.53
1:F:592:ILE:HG23	1:F:593:ASN:N	2.22	0.53
1:C:464:GLY:O	1:C:467:GLN:HG2	2.09	0.53
1:F:433:ALA:O	1:F:440:GLY:HA2	2.09	0.53
1:F:543:VAL:HG12	1:F:567:PRO:HB3	1.90	0.53
1:B:469:ILE:HG22	1:B:514:ILE:HD12	1.90	0.53
1:B:489:ILE:CG1	1:B:492:MET:CG	2.82	0.53
1:F:475:MET:HG3	2:F:723:HOH:O	2.08	0.53
1:E:428:ARG:HG3	1:E:446:ILE:HG13	1.91	0.53
1:E:592:ILE:O	1:E:595:VAL:HB	2.07	0.53
1:E:492:MET:HE1	1:E:522:ILE:CG1	2.37	0.53
1:E:568:LYS:O	1:E:571:ILE:HG12	2.08	0.53
1:E:576:LEU:CD2	1:E:580:HIS:CG	2.92	0.53
1:D:444:PRO:HD2	1:D:502:TYR:OH	2.08	0.53
1:C:577:ASP:OD2	1:C:580:HIS:CG	2.62	0.52
1:D:538:SER:OG	1:D:542:GLU:CG	2.56	0.52
1:E:484:TYR:CB	1:E:613:PHE:CD1	2.92	0.52
1:C:500:GLY:N	2:C:641:HOH:O	2.33	0.52
1:D:465:ARG:HG3	1:D:465:ARG:NH1	2.16	0.52
1:A:568:LYS:O	1:A:571:ILE:HD12	2.09	0.52
1:E:430:ASN:O	1:E:533:MET:N	2.42	0.52
1:E:539:VAL:HG12	1:E:539:VAL:O	2.08	0.52
1:E:614:LYS:N	2:E:666:HOH:O	2.41	0.52
1:E:430:ASN:HB2	1:E:532:ALA:HA	1.91	0.52
1:F:483:LYS:HG2	1:F:484:TYR:CE1	2.43	0.52
1:D:535:GLY:N	2:D:749:HOH:O	2.08	0.52
1:E:570:ASN:OD1	2:E:734:HOH:O	2.19	0.52
1:F:472:GLU:HG3	1:F:473:ALA:H	1.75	0.52
1:C:516:THR:HG23	1:C:596:LEU:HD23	1.92	0.52
1:A:591:ARG:NE	2:A:753:HOH:O	2.42	0.52
1:C:566:ILE:O	1:C:588:PRO:HA	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:420:ILE:HB	1:D:529:GLN:HG3	1.91	0.52
2:A:628:HOH:O	1:F:501:THR:HG22	2.10	0.52
1:E:472:GLU:O	1:E:473:ALA:C	2.52	0.51
1:A:481:ILE:CD1	1:A:485:THR:CG2	2.87	0.51
1:C:597:GLU:CB	2:C:775:HOH:O	2.27	0.51
1:E:422:GLU:OE2	1:E:422:GLU:CA	2.59	0.51
1:E:499:VAL:O	1:E:502:TYR:HE1	1.94	0.51
1:F:445:ILE:HD12	1:F:513:SER:HB2	1.91	0.51
1:C:477:VAL:O	1:C:478:SER:C	2.52	0.51
1:D:444:PRO:C	1:D:445:ILE:HG13	2.34	0.51
1:F:488:ASP:OD2	1:F:490:SER:OG	2.25	0.51
1:B:435:ILE:HD11	1:B:502:TYR:HB3	1.90	0.51
1:E:579:GLU:O	1:E:580:HIS:ND1	2.44	0.51
1:B:457:GLU:HG3	1:B:458:GLY:H	1.75	0.51
1:C:472:GLU:OE1	1:C:509:SER:HA	2.11	0.51
1:C:497:GLN:C	2:C:826:HOH:O	2.52	0.51
1:D:597:GLU:HG2	1:D:610:MET:HE2	1.92	0.51
1:F:531:VAL:HG22	1:F:563:LYS:HB2	1.93	0.51
1:B:585:GLU:CG	2:B:653:HOH:O	2.58	0.51
1:D:548:GLY:HA2	1:D:551:GLN:NE2	2.25	0.51
1:E:421:THR:O	1:E:421:THR:HG22	2.11	0.51
1:E:438:SER:O	1:E:439:ALA:HB2	2.10	0.51
1:E:568:LYS:C	1:E:570:ASN:H	2.18	0.51
1:B:459:ARG:HH11	1:B:459:ARG:HB3	1.76	0.51
1:E:445:ILE:HG22	1:E:446:ILE:N	2.26	0.51
1:E:565:ILE:HG12	1:E:587:ILE:HB	1.92	0.51
1:F:418:LEU:HG	1:F:499:VAL:O	2.10	0.51
1:A:421:THR:HG22	1:A:561:LEU:HD23	1.92	0.51
1:B:477:VAL:HG11	1:B:518:VAL:HG11	1.93	0.51
1:C:592:ILE:O	1:C:595:VAL:HB	2.10	0.51
1:D:540:LYS:O	1:D:540:LYS:HG2	2.11	0.51
1:F:445:ILE:HD11	2:F:813:HOH:O	2.10	0.51
1:B:479:ALA:HA	2:B:775:HOH:O	2.10	0.51
1:F:446:ILE:HD11	1:F:497:GLN:HB2	1.91	0.51
1:B:545:PRO:HA	1:B:567:PRO:HB2	1.93	0.50
1:D:568:LYS:CA	1:D:588:PRO:HB2	2.40	0.50
1:A:545:PRO:HG3	1:A:569:ASP:HB3	1.93	0.50
1:D:591:ARG:HB2	1:D:593:ASN:OD1	2.10	0.50
1:D:613:PHE:O	1:D:615:GLU:N	2.36	0.50
1:E:451:PRO:HA	1:E:492:MET:HA	1.92	0.50
1:E:496:ILE:HD11	1:E:518:VAL:HG22	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:499:VAL:O	1:E:502:TYR:CE1	2.65	0.50
1:F:570:ASN:ND2	1:F:573:ASP:OD2	2.40	0.50
1:A:421:THR:O	1:A:530:SER:HB3	2.10	0.50
1:B:438:SER:CA	1:B:551:GLN:HG2	2.42	0.50
1:E:417:LYS:HD2	1:E:419:PHE:O	2.11	0.50
1:E:614:LYS:CA	2:E:666:HOH:O	2.56	0.50
1:C:435:ILE:CD1	1:C:435:ILE:CG2	2.90	0.50
1:C:562:LYS:O	1:C:584:ILE:HG13	2.11	0.50
1:B:474:VAL:CG2	1:B:496:ILE:HD11	2.41	0.50
1:C:537:LEU:HG	1:C:538:SER:O	2.11	0.50
1:D:477:VAL:HG21	1:D:519:ILE:HG13	1.93	0.50
1:F:432:LEU:HD21	1:F:556:ALA:HB2	1.92	0.50
1:C:592:ILE:HG23	1:C:593:ASN:N	2.27	0.50
1:D:502:TYR:HB3	1:D:505:VAL:HG21	1.94	0.50
1:B:613:PHE:O	1:B:614:LYS:HB3	2.12	0.50
1:A:477:VAL:HG22	1:A:519:ILE:HD11	1.93	0.49
1:B:583:LYS:O	1:B:584:ILE:HB	2.12	0.49
1:C:593:ASN:HB3	1:C:613:PHE:CD1	2.47	0.49
1:F:417:LYS:HG3	1:F:418:LEU:N	2.26	0.49
1:F:475:MET:HB2	2:F:751:HOH:O	2.12	0.49
1:A:446:ILE:HD13	1:A:446:ILE:H	1.78	0.49
1:B:512:ILE:HG13	1:B:513:SER:H	1.78	0.49
1:D:532:ALA:HB2	1:D:561:LEU:HD13	1.95	0.49
1:B:477:VAL:HG13	1:B:481:ILE:HD12	1.95	0.49
1:D:417:LYS:HG2	2:D:768:HOH:O	2.12	0.49
1:E:584:ILE:HG12	1:E:585:GLU:N	2.27	0.49
1:F:577:ASP:C	1:F:578:ALA:O	2.55	0.49
1:A:481:ILE:HD12	1:A:485:THR:HG22	1.93	0.49
1:B:438:SER:HB2	1:B:551:GLN:HG2	1.93	0.49
1:D:563:LYS:HE2	1:D:585:GLU:OE2	2.13	0.49
1:D:571:ILE:HD11	1:D:588:PRO:CG	2.37	0.49
1:E:420:ILE:HD12	1:E:425:GLU:OE1	2.12	0.49
1:B:489:ILE:HD12	1:B:492:MET:HG2	1.91	0.49
1:F:591:ARG:N	1:F:594:GLU:OE1	2.43	0.49
1:A:428:ARG:HD3	1:A:446:ILE:HG23	1.94	0.49
1:B:453:MET:CG	1:C:482:LYS:HZ2	1.95	0.49
1:E:444:PRO:O	1:E:499:VAL:HG23	2.12	0.49
1:A:464:GLY:HA3	2:A:652:HOH:O	2.13	0.49
1:D:484:TYR:HB2	2:D:778:HOH:O	2.12	0.49
1:D:614:LYS:O	1:D:615:GLU:HB2	2.12	0.48
1:E:577:ASP:OD2	1:E:577:ASP:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:ARG:HD2	1:A:593:ASN:OD1	2.12	0.48
1:B:461:ILE:N	1:B:494:VAL:O	2.36	0.48
1:C:424:TYR:CE1	1:C:528:ASP:HB2	2.48	0.48
1:E:591:ARG:N	1:E:594:GLU:OE1	2.46	0.48
1:B:427:GLY:O	1:B:447:ALA:N	2.43	0.48
1:D:556:ALA:O	1:D:557:ILE:C	2.54	0.48
1:E:450:THR:HG23	2:F:803:HOH:O	1.89	0.48
1:E:601:GLU:CG	1:E:602:ASP:H	2.13	0.48
1:E:448:GLU:CD	2:E:731:HOH:O	2.56	0.48
1:E:592:ILE:O	1:E:595:VAL:N	2.46	0.48
1:B:480:ILE:HD11	1:B:613:PHE:CZ	2.48	0.48
1:B:508:ASP:CA	2:B:633:HOH:O	2.56	0.48
1:E:564:VAL:HG12	1:E:584:ILE:CD1	2.43	0.48
1:D:577:ASP:O	1:D:580:HIS:N	2.42	0.48
1:E:451:PRO:HA	1:E:492:MET:HB3	1.95	0.48
1:F:424:TYR:HB3	1:F:526:PRO:HB2	1.96	0.48
1:F:566:ILE:HG13	1:F:567:PRO:O	2.13	0.48
1:D:419:PHE:CE1	1:D:559:ALA:HB1	2.49	0.48
1:C:563:LYS:HD2	2:C:802:HOH:O	2.14	0.47
1:E:425:GLU:N	1:E:526:PRO:HB3	2.27	0.47
1:A:578:ALA:HA	1:A:581:GLU:HB2	1.96	0.47
1:C:471:ARG:O	1:C:475:MET:HB2	2.13	0.47
1:C:512:ILE:HD11	1:C:534:THR:O	2.13	0.47
1:E:579:GLU:O	1:E:580:HIS:CG	2.67	0.47
1:A:569:ASP:O	1:F:417:LYS:N	2.47	0.47
1:B:487:ARG:CD	1:B:489:ILE:HD13	2.42	0.47
1:C:445:ILE:HG21	2:C:645:HOH:O	1.99	0.47
1:E:531:VAL:HG13	1:E:563:LYS:HB2	1.95	0.47
1:B:489:ILE:CD1	1:B:492:MET:CG	2.90	0.47
1:C:476:ASN:O	1:C:478:SER:N	2.47	0.47
1:F:489:ILE:HD13	1:F:489:ILE:N	2.28	0.47
1:F:553:ILE:HG12	1:F:564:VAL:HG11	1.96	0.47
1:B:438:SER:CB	1:B:551:GLN:HG2	2.45	0.47
1:E:422:GLU:CD	1:E:423:GLY:N	2.71	0.47
1:E:444:PRO:HD2	1:E:499:VAL:HB	1.95	0.47
1:B:482:LYS:HA	1:B:487:ARG:O	2.14	0.47
1:C:420:ILE:CG2	1:C:420:ILE:CD1	2.92	0.47
1:C:484:TYR:HD1	1:C:484:TYR:HA	1.58	0.47
1:D:489:ILE:CA	1:D:492:MET:HE3	2.39	0.47
1:C:424:TYR:HA	1:C:527:VAL:O	2.14	0.47
1:C:476:ASN:ND2	1:C:477:VAL:CA	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:565:ILE:HG21	1:E:595:VAL:HG22	1.95	0.47
1:F:445:ILE:CG2	2:F:701:HOH:O	2.62	0.47
1:C:509:SER:O	1:C:510:ALA:C	2.57	0.47
1:F:472:GLU:OE1	1:F:510:ALA:N	2.48	0.47
1:D:424:TYR:CE1	1:D:528:ASP:HB2	2.50	0.47
1:D:431:GLY:N	1:D:443:LEU:O	2.45	0.47
1:F:431:GLY:HA3	2:F:813:HOH:O	2.14	0.47
1:D:445:ILE:HD13	1:D:514:ILE:HG12	1.97	0.46
1:E:497:GLN:NE2	1:F:539:VAL:HG22	2.30	0.46
1:D:469:ILE:HG22	1:D:514:ILE:HD12	1.96	0.46
1:E:562:LYS:N	1:E:562:LYS:HD2	2.26	0.46
1:B:424:TYR:CE1	1:B:528:ASP:HB2	2.51	0.46
1:D:510:ALA:O	1:D:511:SER:C	2.58	0.46
1:D:597:GLU:H	1:D:597:GLU:HG3	1.37	0.46
1:E:431:GLY:HA2	1:E:513:SER:OG	2.16	0.46
1:F:477:VAL:HG22	1:F:481:ILE:CG1	2.44	0.46
1:C:420:ILE:HD13	1:C:420:ILE:HA	1.96	0.46
1:A:428:ARG:CD	1:A:446:ILE:HG22	2.42	0.46
1:B:478:SER:HB2	2:B:759:HOH:O	2.15	0.46
1:E:611:SER:C	1:E:613:PHE:H	2.21	0.46
1:F:597:GLU:CG	2:F:817:HOH:O	2.60	0.46
1:A:589:VAL:HG12	2:A:765:HOH:O	2.15	0.46
1:C:538:SER:HB3	1:C:544:LEU:HD11	1.98	0.46
1:F:552:LYS:O	1:F:553:ILE:C	2.58	0.46
1:A:510:ALA:O	1:A:511:SER:C	2.59	0.46
1:F:509:SER:O	1:F:510:ALA:C	2.59	0.46
1:F:538:SER:C	1:F:540:LYS:N	2.72	0.46
1:F:555:ALA:HA	2:F:781:HOH:O	2.15	0.46
1:C:463:THR:CG2	2:D:773:HOH:O	2.63	0.46
1:D:492:MET:HE1	1:D:522:ILE:HG12	1.98	0.46
1:D:568:LYS:HG3	2:D:626:HOH:O	2.15	0.46
1:E:561:LEU:C	1:E:562:LYS:HD2	2.41	0.46
1:B:484:TYR:HD1	1:B:484:TYR:HA	1.62	0.46
1:E:429:VAL:HG23	1:E:517:ALA:HB2	1.97	0.46
1:E:484:TYR:CG	1:E:613:PHE:HD1	2.34	0.46
1:C:494:VAL:HG23	2:C:626:HOH:O	2.15	0.46
1:F:550:THR:HG22	2:F:838:HOH:O	2.16	0.46
1:B:464:GLY:O	1:B:467:GLN:NE2	2.42	0.45
1:B:609:LEU:HD12	1:B:609:LEU:C	2.41	0.45
1:D:553:ILE:O	1:D:556:ALA:HB3	2.16	0.45
1:E:568:LYS:O	1:E:570:ASN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:TYR:CE1	1:A:528:ASP:HB2	2.51	0.45
1:B:457:GLU:OE2	1:B:490:SER:OG	2.35	0.45
1:C:428:ARG:HH11	1:C:428:ARG:CG	2.26	0.45
1:F:611:SER:O	1:F:614:LYS:HE2	2.16	0.45
1:B:433:ALA:HB3	1:B:441:ILE:CG1	2.46	0.45
1:E:429:VAL:CG1	1:E:430:ASN:N	2.77	0.45
1:F:466:LEU:HB3	1:F:498:PHE:CE2	2.50	0.45
1:A:446:ILE:O	1:A:446:ILE:HG12	2.17	0.45
1:A:489:ILE:HG12	1:A:492:MET:CE	2.46	0.45
1:E:424:TYR:HB3	1:E:526:PRO:HB2	1.97	0.45
1:E:477:VAL:O	1:E:481:ILE:HG13	2.16	0.45
1:B:460:VAL:HG11	1:B:471:ARG:HA	1.98	0.45
1:B:476:ASN:O	1:B:479:ALA:HB3	2.17	0.45
1:B:563:LYS:CG	1:B:585:GLU:CB	2.91	0.45
1:E:605:LYS:HE2	1:E:605:LYS:HB3	1.81	0.45
1:B:440:GLY:H	1:B:551:GLN:HB3	1.80	0.45
1:B:459:ARG:HH11	1:B:459:ARG:CB	2.28	0.45
1:D:461:ILE:HD12	1:D:461:ILE:N	2.31	0.45
1:F:465:ARG:C	1:F:466:LEU:HG	2.41	0.45
1:F:566:ILE:HB	1:F:567:PRO:HD2	1.98	0.45
1:A:568:LYS:HB2	2:A:725:HOH:O	2.16	0.45
1:B:591:ARG:NH2	2:B:677:HOH:O	2.50	0.45
1:C:522:ILE:HG23	2:C:750:HOH:O	2.16	0.45
1:F:596:LEU:HA	1:F:596:LEU:HD23	1.70	0.45
1:A:481:ILE:HD12	1:A:485:THR:CG2	2.47	0.45
1:C:502:TYR:HE1	2:C:625:HOH:O	1.97	0.45
1:C:546:VAL:HG12	2:C:733:HOH:O	2.16	0.45
1:C:576:LEU:HD22	1:C:580:HIS:HB3	1.99	0.45
1:E:418:LEU:HA	1:F:545:PRO:HG2	1.99	0.45
1:E:598:HIS:O	1:E:599:VAL:HG13	2.17	0.45
1:B:432:LEU:HD11	1:B:564:VAL:HG23	1.99	0.45
1:B:607:ASN:O	1:B:608:ARG:C	2.59	0.45
1:F:475:MET:O	1:F:478:SER:HB3	2.16	0.45
1:F:538:SER:HB2	1:F:544:LEU:HD11	1.97	0.45
1:A:578:ALA:O	1:A:579:GLU:C	2.60	0.45
1:B:557:ILE:O	1:B:560:GLY:N	2.48	0.45
1:C:525:ILE:HD13	1:C:606:LYS:N	2.32	0.44
1:E:613:PHE:HB3	2:E:745:HOH:O	2.15	0.44
1:F:489:ILE:HD12	1:F:489:ILE:HA	1.50	0.44
1:B:523:GLU:CB	1:B:609:LEU:HD22	2.46	0.44
1:B:551:GLN:CD	1:B:551:GLN:N	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:ILE:HA	1:B:588:PRO:HD2	1.61	0.44
1:C:465:ARG:HA	1:C:465:ARG:HD2	1.78	0.44
1:C:563:LYS:HE2	1:C:585:GLU:OE1	2.17	0.44
1:D:553:ILE:HG22	1:D:557:ILE:CD1	2.48	0.44
1:E:531:VAL:HG21	1:E:599:VAL:HG12	1.99	0.44
1:C:476:ASN:O	1:C:477:VAL:C	2.60	0.44
1:D:480:ILE:HD11	1:D:613:PHE:CE1	2.49	0.44
1:B:517:ALA:O	1:B:520:SER:HB3	2.17	0.44
1:C:563:LYS:HG2	1:C:585:GLU:HB2	2.00	0.44
1:D:449:VAL:HG12	1:D:494:VAL:HA	1.99	0.44
1:E:474:VAL:HA	1:E:477:VAL:HG12	1.99	0.44
1:A:596:LEU:HD23	1:A:596:LEU:HA	1.78	0.44
1:C:428:ARG:CG	1:C:446:ILE:HG23	2.48	0.44
1:C:463:THR:HG23	1:C:464:GLY:N	2.33	0.44
1:E:563:LYS:HG2	1:E:585:GLU:HB3	1.99	0.44
1:F:512:ILE:O	1:F:516:THR:OG1	2.28	0.44
1:B:419:PHE:CE2	2:B:679:HOH:O	2.56	0.44
1:B:537:LEU:HD13	1:B:592:ILE:HD13	1.99	0.44
1:D:453:MET:HE3	1:D:453:MET:HB3	1.67	0.44
1:E:435:ILE:H	1:E:435:ILE:HG13	1.35	0.44
1:B:445:ILE:HD12	1:B:498:PHE:CD1	2.52	0.44
1:D:471:ARG:O	1:D:475:MET:HB2	2.16	0.44
1:D:571:ILE:HD13	1:D:571:ILE:HG21	1.77	0.44
1:F:571:ILE:HD13	1:F:571:ILE:HA	1.73	0.44
1:B:594:GLU:O	1:B:595:VAL:C	2.59	0.44
1:C:499:VAL:CG1	1:D:545:PRO:HG2	2.47	0.44
1:D:486:GLY:O	1:D:487:ARG:C	2.60	0.44
1:D:531:VAL:HG13	1:D:563:LYS:HB2	1.99	0.44
1:A:468:GLU:HG3	2:A:706:HOH:O	2.18	0.44
1:B:545:PRO:HB2	1:B:570:ASN:ND2	2.33	0.44
1:D:530:SER:O	1:D:562:LYS:N	2.51	0.44
1:A:480:ILE:HD13	1:A:481:ILE:N	2.33	0.43
1:A:580:HIS:ND1	1:A:580:HIS:N	2.65	0.43
1:B:489:ILE:O	1:B:489:ILE:CG2	2.66	0.43
1:E:601:GLU:O	1:E:606:LYS:CD	2.63	0.43
1:B:427:GLY:O	1:B:446:ILE:HA	2.17	0.43
1:C:420:ILE:CD1	1:C:420:ILE:HA	2.48	0.43
1:F:512:ILE:HD11	1:F:534:THR:O	2.18	0.43
1:C:463:THR:HG22	1:D:509:SER:HB3	2.00	0.43
1:E:484:TYR:HB3	1:E:613:PHE:CD1	2.54	0.43
1:A:476:ASN:O	1:A:480:ILE:CG2	2.63	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:ILE:HD11	1:B:492:MET:SD	2.59	0.43
1:D:613:PHE:C	1:D:615:GLU:N	2.66	0.43
1:E:508:ASP:HB2	2:E:697:HOH:O	2.18	0.43
1:F:445:ILE:CD1	1:F:513:SER:HB2	2.48	0.43
1:F:457:GLU:CG	2:F:772:HOH:O	2.67	0.43
1:F:593:ASN:HB3	1:F:613:PHE:HD1	1.80	0.43
1:B:450:THR:HG22	1:C:483:LYS:HE3	2.00	0.43
1:B:484:TYR:HD2	1:B:613:PHE:HE2	1.61	0.43
1:B:570:ASN:HD22	1:B:570:ASN:HA	1.64	0.43
1:D:419:PHE:HD1	1:D:421:THR:HG23	1.84	0.43
1:D:608:ARG:HG3	1:D:608:ARG:HH11	1.83	0.43
1:E:465:ARG:NH2	1:E:503:GLU:HG2	2.33	0.43
1:F:612:LYS:CG	2:F:699:HOH:O	2.63	0.43
1:B:604:LYS:CB	2:B:753:HOH:O	2.34	0.43
1:F:417:LYS:HE3	1:F:417:LYS:HB2	1.42	0.43
1:F:563:LYS:HE2	2:F:698:HOH:O	2.19	0.43
1:A:542:GLU:OE2	1:A:591:ARG:HG3	2.18	0.43
1:B:565:ILE:HA	1:B:587:ILE:O	2.19	0.43
1:D:483:LYS:HD2	2:D:754:HOH:O	2.19	0.43
1:E:429:VAL:HG12	1:E:430:ASN:H	1.82	0.43
1:E:605:LYS:HG3	2:E:699:HOH:O	2.18	0.43
1:B:418:LEU:CD1	1:C:544:LEU:HB3	2.49	0.43
1:C:446:ILE:HD12	2:C:826:HOH:O	2.18	0.43
1:D:442:VAL:HG23	2:D:654:HOH:O	2.18	0.43
1:F:494:VAL:HG23	1:F:496:ILE:HG13	2.00	0.43
1:A:424:TYR:HB3	1:A:526:PRO:HB2	2.01	0.42
1:A:553:ILE:O	1:A:554:GLU:C	2.59	0.42
1:B:512:ILE:O	1:B:516:THR:N	2.38	0.42
1:B:596:LEU:HD22	1:B:600:LEU:HD11	2.02	0.42
1:F:477:VAL:HA	1:F:480:ILE:HD12	2.01	0.42
1:F:614:LYS:HA	2:F:836:HOH:O	2.19	0.42
1:A:489:ILE:O	1:A:489:ILE:CG2	2.66	0.42
1:E:601:GLU:CG	1:E:602:ASP:N	2.73	0.42
1:F:516:THR:HG23	1:F:596:LEU:CD2	2.49	0.42
1:A:488:ASP:OD1	1:A:489:ILE:N	2.52	0.42
1:C:418:LEU:CD2	1:C:500:GLY:HA3	2.49	0.42
1:C:437:GLU:OE2	1:C:437:GLU:N	2.52	0.42
1:E:432:LEU:HD23	1:E:432:LEU:HA	1.66	0.42
1:F:548:GLY:O	1:F:552:LYS:HG3	2.19	0.42
1:E:480:ILE:O	1:E:484:TYR:HD2	2.02	0.42
1:F:457:GLU:HG2	2:F:772:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:522:ILE:CD1	1:F:522:ILE:CB	2.85	0.42
1:F:561:LEU:HA	2:F:645:HOH:O	2.19	0.42
1:D:542:GLU:HG2	1:D:542:GLU:H	1.24	0.42
1:E:606:LYS:O	1:E:607:ASN:C	2.61	0.42
1:F:424:TYR:CD1	1:F:601:GLU:HB2	2.54	0.42
1:B:592:ILE:HD12	1:B:592:ILE:HA	1.70	0.42
1:F:424:TYR:HA	1:F:527:VAL:O	2.19	0.42
1:F:580:HIS:O	1:F:581:GLU:C	2.62	0.42
1:B:579:GLU:OE1	1:B:579:GLU:HA	2.19	0.42
1:E:437:GLU:HB3	1:E:438:SER:H	1.58	0.42
1:B:418:LEU:HD21	2:C:733:HOH:O	2.20	0.42
1:B:494:VAL:HG23	2:B:631:HOH:O	2.20	0.42
1:B:525:ILE:HD13	1:B:525:ILE:HG21	1.84	0.42
1:C:444:PRO:HD2	2:C:625:HOH:O	2.18	0.42
1:D:426:VAL:HB	2:D:745:HOH:O	2.19	0.42
1:E:564:VAL:HG12	1:E:584:ILE:HD13	2.01	0.42
1:C:429:VAL:HG22	1:C:527:VAL:HG11	2.02	0.42
1:C:445:ILE:CD1	1:C:513:SER:HB2	2.50	0.42
1:E:481:ILE:HG22	1:E:487:ARG:HB3	2.02	0.42
1:E:434:VAL:HA	1:E:439:ALA:O	2.19	0.41
1:B:418:LEU:HD13	1:C:545:PRO:HD2	2.02	0.41
1:B:438:SER:HB2	1:B:551:GLN:CG	2.50	0.41
1:C:435:ILE:HB	2:C:824:HOH:O	2.20	0.41
1:D:512:ILE:HG13	1:D:513:SER:N	2.35	0.41
1:F:518:VAL:HG12	1:F:522:ILE:HD12	2.02	0.41
1:F:550:THR:O	1:F:554:GLU:HB2	2.20	0.41
1:A:438:SER:HB2	1:A:439:ALA:H	1.72	0.41
1:A:511:SER:HA	1:A:535:GLY:O	2.20	0.41
1:B:576:LEU:HB2	1:B:581:GLU:HG2	2.02	0.41
1:D:525:ILE:HA	1:D:526:PRO:HD3	1.92	0.41
1:F:571:ILE:HG22	1:F:572:ASP:N	2.35	0.41
1:A:547:GLY:HA3	1:F:501:THR:CG2	2.50	0.41
1:B:481:ILE:O	1:B:482:LYS:C	2.64	0.41
1:E:420:ILE:HG13	1:E:428:ARG:CZ	2.50	0.41
1:E:435:ILE:CG2	2:E:751:HOH:O	2.51	0.41
1:E:568:LYS:C	1:E:570:ASN:N	2.78	0.41
1:A:570:ASN:HA	1:A:570:ASN:HD22	1.76	0.41
1:C:435:ILE:N	1:C:439:ALA:O	2.49	0.41
1:C:545:PRO:HG3	1:C:569:ASP:CB	2.47	0.41
1:E:450:THR:HG22	2:F:808:HOH:O	2.20	0.41
1:F:509:SER:O	1:F:511:SER:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:552:LYS:C	1:F:554:GLU:N	2.78	0.41
1:A:435:ILE:CG2	1:A:505:VAL:HG22	2.51	0.41
1:A:435:ILE:HG23	1:A:505:VAL:HG22	2.02	0.41
1:B:474:VAL:HG21	1:B:496:ILE:HD11	2.02	0.41
1:B:611:SER:C	1:B:613:PHE:N	2.77	0.41
1:C:473:ALA:HA	1:C:510:ALA:HA	2.02	0.41
1:D:418:LEU:HD13	1:D:500:GLY:CA	2.50	0.41
1:E:484:TYR:HB3	1:E:613:PHE:HD1	1.83	0.41
1:F:562:LYS:HD3	1:F:562:LYS:HA	1.69	0.41
1:B:419:PHE:CD2	2:B:679:HOH:O	2.74	0.41
1:B:502:TYR:HA	2:B:782:HOH:O	2.20	0.41
1:B:523:GLU:HG3	1:B:609:LEU:CD2	2.40	0.41
1:D:457:GLU:HB3	1:D:490:SER:O	2.20	0.41
1:E:465:ARG:HH22	1:E:503:GLU:HG2	1.85	0.41
1:E:549:VAL:HG11	1:E:573:ASP:HB2	2.01	0.41
1:F:473:ALA:O	1:F:474:VAL:C	2.64	0.41
1:A:441:ILE:O	1:A:441:ILE:HG12	2.21	0.41
1:A:526:PRO:HB2	1:A:601:GLU:HB2	2.02	0.41
1:A:595:VAL:HG12	1:A:596:LEU:N	2.36	0.41
1:B:439:ALA:O	1:B:440:GLY:C	2.64	0.41
1:B:500:GLY:HA3	1:B:502:TYR:CE1	2.55	0.41
1:B:571:ILE:HD13	1:B:571:ILE:C	2.46	0.41
1:C:459:ARG:HD2	2:C:825:HOH:O	2.21	0.41
1:D:505:VAL:HG12	1:D:506:GLU:N	2.36	0.41
1:E:424:TYR:HA	1:E:527:VAL:O	2.21	0.41
1:E:444:PRO:HB2	1:E:499:VAL:HG21	2.02	0.41
1:E:473:ALA:HB3	1:E:514:ILE:HG21	2.02	0.41
1:E:498:PHE:CD2	1:E:498:PHE:N	2.88	0.41
1:E:605:LYS:NZ	2:E:658:HOH:O	2.54	0.41
1:B:419:PHE:HA	1:B:428:ARG:HH22	1.85	0.41
1:B:420:ILE:C	1:B:421:THR:CG2	2.94	0.41
1:C:523:GLU:HB2	1:C:525:ILE:HG13	2.03	0.41
1:E:467:GLN:HB2	1:E:471:ARG:NH1	2.36	0.41
1:E:479:ALA:O	1:E:480:ILE:C	2.63	0.41
1:F:445:ILE:HG21	2:F:701:HOH:O	2.20	0.41
1:F:465:ARG:HH11	1:F:465:ARG:HG3	1.85	0.41
1:F:474:VAL:O	1:F:477:VAL:HG13	2.20	0.41
1:F:474:VAL:CG2	1:F:496:ILE:HD11	2.51	0.41
1:F:496:ILE:HD13	1:F:496:ILE:HG21	1.62	0.41
1:A:571:ILE:O	1:A:574:VAL:HB	2.21	0.40
1:D:495:HIS:HE1	1:E:475:MET:HE2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:418:LEU:HD13	1:E:419:PHE:H	1.87	0.40
1:F:597:GLU:CB	2:F:817:HOH:O	2.35	0.40
1:F:614:LYS:HB2	1:F:615:GLU:H	1.47	0.40
1:A:469:ILE:HG12	2:A:758:HOH:O	2.20	0.40
1:C:563:LYS:HG2	1:C:585:GLU:CB	2.51	0.40
1:E:574:VAL:HG12	1:E:575:LEU:N	2.36	0.40
1:F:592:ILE:HG22	1:F:593:ASN:N	2.35	0.40
1:E:481:ILE:HG23	1:E:485:THR:HB	2.03	0.40
1:E:532:ALA:HB2	1:E:561:LEU:HD12	2.03	0.40
1:B:420:ILE:HG21	2:B:700:HOH:O	2.21	0.40
1:B:519:ILE:HG21	1:B:596:LEU:HD21	2.03	0.40
1:B:556:ALA:HA	1:B:561:LEU:HD12	2.04	0.40
1:F:537:LEU:HD12	1:F:542:GLU:O	2.22	0.40
1:A:536:SER:HB2	1:A:544:LEU:HB2	2.04	0.40
1:B:609:LEU:HA	1:B:612:LYS:HG3	2.02	0.40
1:C:587:ILE:HA	1:C:588:PRO:HD2	1.96	0.40
1:C:591:ARG:HE	1:C:591:ARG:HB2	1.59	0.40
1:D:463:THR:HG22	1:E:468:GLU:HB2	2.02	0.40
1:E:545:PRO:HA	1:E:567:PRO:HG2	2.02	0.40
1:F:428:ARG:HD2	1:F:446:ILE:HG23	2.03	0.40
1:F:592:ILE:HG22	1:F:593:ASN:H	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	191/205 (93%)	175 (92%)	13 (7%)	3 (2%)	7	34
1	B	192/205 (94%)	146 (76%)	29 (15%)	17 (9%)	0	3
1	C	192/205 (94%)	163 (85%)	22 (12%)	7 (4%)	2	16
1	D	192/205 (94%)	163 (85%)	21 (11%)	8 (4%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	191/205 (93%)	149 (78%)	26 (14%)	16 (8%)	0	3
1	F	192/205 (94%)	165 (86%)	21 (11%)	6 (3%)	3	19
All	All	1150/1230 (94%)	961 (84%)	132 (12%)	57 (5%)	1	10

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	ALA
1	B	438	SER
1	B	440	GLY
1	B	528	ASP
1	B	529	GLN
1	B	571	ILE
1	B	592	ILE
1	B	606	LYS
1	B	607	ASN
1	B	614	LYS
1	C	479	ALA
1	D	489	ILE
1	D	510	ALA
1	E	437	GLU
1	E	439	ALA
1	E	601	GLU
1	F	510	ALA
1	B	505	VAL
1	B	576	LEU
1	B	610	MET
1	D	436	GLY
1	E	484	TYR
1	E	558	GLN
1	E	580	HIS
1	E	599	VAL
1	F	476	ASN
1	F	578	ALA
1	F	614	LYS
1	A	438	SER
1	B	513	SER
1	C	482	LYS
1	D	487	ARG
1	E	425	GLU
1	C	476	ASN

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Mol	Chain	Res	Type
1	C	578	ALA
1	D	509	SER
1	E	568	LYS
1	E	569	ASP
1	E	575	LEU
1	B	595	VAL
1	B	611	SER
1	C	483	LYS
1	D	557	ILE
1	D	614	LYS
1	E	472	GLU
1	E	584	ILE
1	E	611	SER
1	F	475	MET
1	B	424	TYR
1	B	584	ILE
1	C	592	ILE
1	E	524	GLY
1	F	465	ARG
1	C	524	GLY
1	D	588	PRO
1	E	427	GLY
1	A	499	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	160/168 (95%)	124 (78%)	36 (22%)	1	5
1	B	161/168 (96%)	116 (72%)	45 (28%)	0	2
1	C	161/168 (96%)	126 (78%)	35 (22%)	1	6
1	D	161/168 (96%)	135 (84%)	26 (16%)	2	12
1	E	160/168 (95%)	118 (74%)	42 (26%)	0	3
1	F	161/168 (96%)	126 (78%)	35 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	964/1008 (96%)	745 (77%)	219 (23%)	1 5

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	418	LEU
1	A	422	GLU
1	A	435	ILE
1	A	438	SER
1	A	441	ILE
1	A	446	ILE
1	A	453	MET
1	A	457	GLU
1	A	465	ARG
1	A	477	VAL
1	A	480	ILE
1	A	481	ILE
1	A	485	THR
1	A	487	ARG
1	A	489	ILE
1	A	491	ASN
1	A	495	HIS
1	A	501	THR
1	A	506	GLU
1	A	539	VAL
1	A	540	LYS
1	A	542	GLU
1	A	562	LYS
1	A	568	LYS
1	A	570	ASN
1	A	571	ILE
1	A	574	VAL
1	A	579	GLU
1	A	584	ILE
1	A	597	GLU
1	A	598	HIS
1	A	599	VAL
1	A	608	ARG
1	A	610	MET
1	A	611	SER
1	A	614	LYS
1	B	417	LYS

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Mol	Chain	Res	Type
1	B	418	LEU
1	B	419	PHE
1	B	420	ILE
1	B	421	THR
1	B	422	GLU
1	B	441	ILE
1	B	443	LEU
1	B	446	ILE
1	B	448	GLU
1	B	449	VAL
1	B	459	ARG
1	B	463	THR
1	B	465	ARG
1	B	467	GLN
1	B	475	MET
1	B	477	VAL
1	B	480	ILE
1	B	482	LYS
1	B	485	THR
1	B	487	ARG
1	B	489	ILE
1	B	490	SER
1	B	491	ASN
1	B	492	MET
1	B	496	ILE
1	B	502	TYR
1	B	505	VAL
1	B	518	VAL
1	B	539	VAL
1	B	540	LYS
1	B	551	GLN
1	B	558	GLN
1	B	563	LYS
1	B	569	ASP
1	B	571	ILE
1	B	579	GLU
1	B	591	ARG
1	B	592	ILE
1	B	593	ASN
1	B	605	LYS
1	B	608	ARG
1	B	609	LEU

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Mol	Chain	Res	Type
1	B	610	MET
1	B	614	LYS
1	C	417	LYS
1	C	419	PHE
1	C	428	ARG
1	C	435	ILE
1	C	437	GLU
1	C	441	ILE
1	C	446	ILE
1	C	463	THR
1	C	476	ASN
1	C	477	VAL
1	C	480	ILE
1	C	482	LYS
1	C	485	THR
1	C	487	ARG
1	C	489	ILE
1	C	494	VAL
1	C	501	THR
1	C	502	TYR
1	C	509	SER
1	C	513	SER
1	C	514	ILE
1	C	539	VAL
1	C	540	LYS
1	C	542	GLU
1	C	549	VAL
1	C	554	GLU
1	C	571	ILE
1	C	577	ASP
1	C	585	GLU
1	C	591	ARG
1	C	593	ASN
1	C	597	GLU
1	C	608	ARG
1	C	614	LYS
1	C	615	GLU
1	D	424	TYR
1	D	428	ARG
1	D	435	ILE
1	D	441	ILE
1	D	453	MET

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Mol	Chain	Res	Type
1	D	459	ARG
1	D	465	ARG
1	D	471	ARG
1	D	480	ILE
1	D	482	LYS
1	D	487	ARG
1	D	501	THR
1	D	503	GLU
1	D	513	SER
1	D	529	GLN
1	D	542	GLU
1	D	551	GLN
1	D	565	ILE
1	D	568	LYS
1	D	583	LYS
1	D	591	ARG
1	D	597	GLU
1	D	601	GLU
1	D	604	LYS
1	D	608	ARG
1	D	611	SER
1	E	418	LEU
1	E	420	ILE
1	E	422	GLU
1	E	426	VAL
1	E	434	VAL
1	E	435	ILE
1	E	438	SER
1	E	446	ILE
1	E	448	GLU
1	E	459	ARG
1	E	466	LEU
1	E	475	MET
1	E	478	SER
1	E	480	ILE
1	E	482	LYS
1	E	488	ASP
1	E	490	SER
1	E	492	MET
1	E	501	THR
1	E	503	GLU
1	E	505	VAL

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Mol	Chain	Res	Type
1	E	522	ILE
1	E	523	GLU
1	E	531	VAL
1	E	540	LYS
1	E	543	VAL
1	E	549	VAL
1	E	551	GLN
1	E	558	GLN
1	E	562	LYS
1	E	566	ILE
1	E	571	ILE
1	E	583	LYS
1	E	584	ILE
1	E	585	GLU
1	E	587	ILE
1	E	597	GLU
1	E	600	LEU
1	E	605	LYS
1	E	608	ARG
1	E	612	LYS
1	E	614	LYS
1	F	417	LYS
1	F	418	LEU
1	F	420	ILE
1	F	435	ILE
1	F	437	GLU
1	F	438	SER
1	F	445	ILE
1	F	446	ILE
1	F	457	GLU
1	F	459	ARG
1	F	465	ARG
1	F	472	GLU
1	F	478	SER
1	F	482	LYS
1	F	485	THR
1	F	487	ARG
1	F	489	ILE
1	F	494	VAL
1	F	501	THR
1	F	509	SER
1	F	513	SER

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Mol	Chain	Res	Type
1	F	519	ILE
1	F	539	VAL
1	F	540	LYS
1	F	562	LYS
1	F	571	ILE
1	F	579	GLU
1	F	583	LYS
1	F	584	ILE
1	F	592	ILE
1	F	593	ASN
1	F	605	LYS
1	F	609	LEU
1	F	614	LYS
1	F	615	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	430	ASN
1	B	551	GLN
1	B	558	GLN
1	B	598	HIS
1	C	476	ASN
1	C	551	GLN
1	C	593	ASN
1	D	551	GLN
1	D	558	GLN
1	E	430	ASN
1	E	497	GLN
1	E	607	ASN
1	F	476	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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%)	-0.74	0	100	100	2, 6, 29, 44	0
1	B	196/205 (95%)	-0.49	2 (1%)	79	59	2, 15, 49, 67	0
1	C	196/205 (95%)	-0.78	0	100	100	2, 5, 28, 48	0
1	D	196/205 (95%)	-0.78	0	100	100	2, 5, 25, 42	0
1	E	195/205 (95%)	-0.54	0	100	100	2, 13, 44, 61	0
1	F	196/205 (95%)	-0.73	0	100	100	2, 7, 34, 68	0
All	All	1174/1230 (95%)	-0.68	2 (0%)	91	83	2, 9, 38, 68	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	420	ILE	2.1
1	B	418	LEU	2.1

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.