



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:57 AM UTC

PDB ID : 1Z0E / pdb_00001z0e
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 : 2.05 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

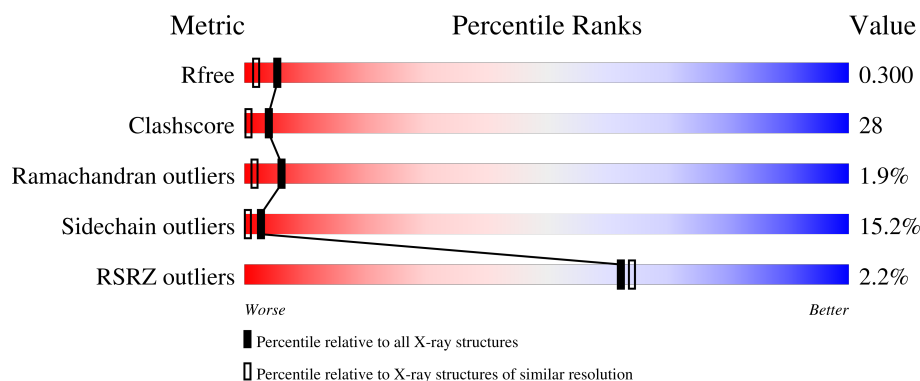
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	
1	B	205	
1	C	205	
1	D	205	
1	E	205	

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Mol	Chain	Length	Quality of chain
1	F	205	% 51% 26% 12% 6% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9285 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Putative protease La homolog type.

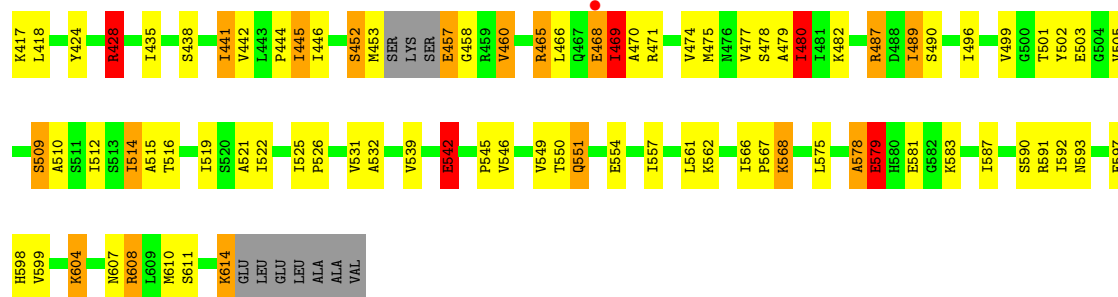
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1457	921	247	284	5			
1	B	195	Total	C	N	O	S	0	0	0
			1457	921	247	284	5			
1	C	194	Total	C	N	O	S	0	0	0
			1448	915	245	283	5			
1	D	195	Total	C	N	O	S	0	0	0
			1457	921	247	284	5			
1	E	195	Total	C	N	O	S	0	0	0
			1457	921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

- Molecule 2 is water.

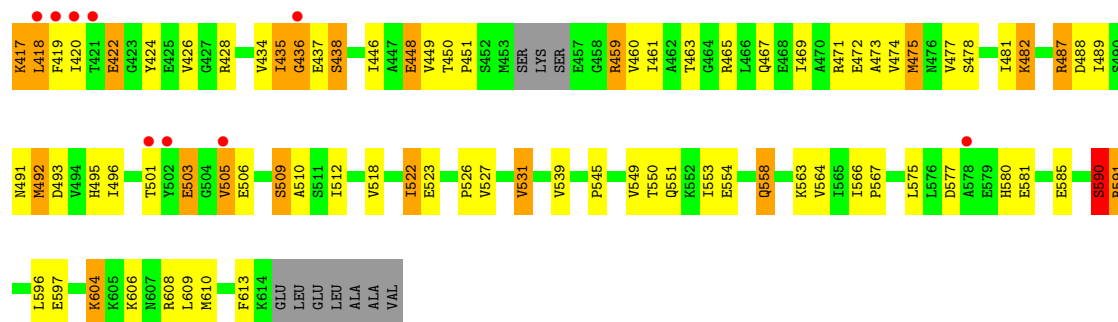
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	89	Total	O	0	0
			89	89		
2	B	65	Total	O	0	0
			65	65		
2	C	121	Total	O	0	0
			121	121		
2	D	106	Total	O	0	0
			106	106		
2	E	67	Total	O	0	0
			67	67		
2	F	104	Total	O	0	0
			104	104		



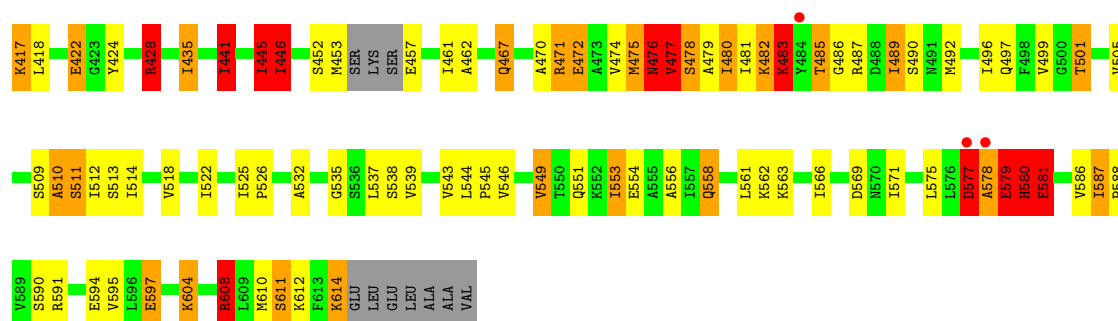
- Molecule 1: Putative protease La homolog type



- 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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.68Å 86.11Å 135.61Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	15.00 – 2.05 15.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.05) 96.5 (15.00-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.213 , 0.299 0.211 , 0.300	Depositor DCC
R_{free} test set	1009 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9285	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.70	12/1470 (0.8%)	1.59	21/1983 (1.1%)
1	B	1.48	9/1470 (0.6%)	1.42	15/1983 (0.8%)
1	C	1.83	25/1461 (1.7%)	1.61	20/1972 (1.0%)
1	D	1.77	22/1470 (1.5%)	1.57	23/1983 (1.2%)
1	E	1.50	7/1470 (0.5%)	1.45	19/1983 (1.0%)
1	F	1.71	19/1470 (1.3%)	1.63	25/1983 (1.3%)
All	All	1.67	94/8811 (1.1%)	1.55	123/11887 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	F	0	2
All	All	0	3

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	496	ILE	CA-CB	10.61	1.67	1.54
1	F	556	ALA	CA-CB	9.08	1.67	1.53
1	C	566	ILE	C-O	-8.64	1.17	1.24
1	F	595	VAL	CA-CB	8.41	1.63	1.54
1	D	542	GLU	CB-CG	8.23	1.77	1.52
1	D	469	ILE	CA-CB	8.23	1.64	1.54
1	C	557	ILE	CA-CB	8.11	1.63	1.54
1	C	566	ILE	N-CA	8.06	1.54	1.46
1	D	578	ALA	C-O	7.80	1.33	1.24
1	F	587	ILE	CA-C	7.43	1.59	1.53
1	D	466	LEU	C-O	-7.41	1.14	1.24
1	F	511	SER	N-CA	-7.36	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	587	ILE	CA-C	7.25	1.59	1.53
1	A	433	ALA	CA-CB	7.11	1.65	1.53
1	C	473	ALA	CA-CB	-7.06	1.42	1.53
1	C	514	ILE	CA-CB	6.93	1.63	1.54
1	F	477	VAL	N-CA	6.81	1.54	1.46
1	D	521	ALA	CA-CB	6.72	1.64	1.53
1	F	496	ILE	C-O	6.66	1.30	1.24
1	F	543	VAL	CA-CB	6.61	1.61	1.54
1	C	444	PRO	C-O	6.51	1.31	1.23
1	D	516	THR	CA-CB	6.49	1.63	1.53
1	D	428	ARG	CB-CG	-6.44	1.33	1.52
1	A	519	ILE	CA-CB	6.37	1.61	1.54
1	C	587	ILE	CA-CB	-6.33	1.47	1.53
1	C	529	GLN	N-CA	6.27	1.54	1.46
1	D	593	ASN	C-O	-6.26	1.16	1.24
1	D	546	VAL	CA-CB	6.25	1.64	1.54
1	C	512	ILE	CA-CB	6.19	1.63	1.54
1	C	597	GLU	N-CA	-6.12	1.39	1.46
1	C	597	GLU	CD-OE2	6.12	1.36	1.25
1	F	566	ILE	CA-CB	6.00	1.61	1.54
1	F	510	ALA	C-O	-5.96	1.16	1.23
1	D	525	ILE	CA-CB	5.93	1.58	1.54
1	B	450	THR	CA-CB	5.92	1.63	1.53
1	B	527	VAL	CA-CB	5.92	1.61	1.54
1	D	512	ILE	CA-CB	5.91	1.62	1.54
1	B	442	VAL	CA-C	5.81	1.58	1.52
1	D	441	ILE	CA-CB	5.75	1.63	1.55
1	E	446	ILE	C-O	-5.67	1.18	1.24
1	D	496	ILE	CA-CB	5.66	1.61	1.54
1	B	514	ILE	CA-CB	5.66	1.61	1.54
1	D	519	ILE	CA-CB	5.64	1.61	1.54
1	B	420	ILE	CA-CB	5.59	1.62	1.54
1	F	581	GLU	CB-CG	5.59	1.69	1.52
1	C	564	VAL	CA-CB	5.58	1.61	1.54
1	D	542	GLU	CG-CD	5.53	1.65	1.52
1	A	531	VAL	C-O	5.52	1.30	1.24
1	A	512	ILE	N-CA	5.50	1.53	1.46
1	A	590	SER	C-O	-5.50	1.17	1.24
1	F	591	ARG	C-O	5.47	1.30	1.23
1	F	586	VAL	C-O	-5.47	1.18	1.24
1	E	531	VAL	CB-CG1	5.46	1.70	1.52
1	D	514	ILE	CA-CB	5.45	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	446	ILE	CA-CB	5.44	1.61	1.54
1	D	479	ALA	N-CA	-5.42	1.40	1.46
1	C	468	GLU	CD-OE2	5.42	1.35	1.25
1	D	515	ALA	CA-CB	5.39	1.61	1.53
1	F	470	ALA	CA-C	5.39	1.59	1.52
1	F	597	GLU	CG-CD	5.39	1.65	1.52
1	C	595	VAL	CA-CB	5.38	1.60	1.54
1	C	566	ILE	CA-CB	5.37	1.62	1.54
1	C	498	PHE	C-O	-5.37	1.17	1.23
1	E	463	THR	CA-CB	5.37	1.61	1.53
1	D	531	VAL	CA-C	5.36	1.59	1.52
1	F	553	ILE	CA-CB	5.36	1.61	1.54
1	A	599	VAL	CA-CB	5.35	1.61	1.54
1	A	584	ILE	CA-CB	5.34	1.62	1.54
1	E	448	GLU	N-CA	-5.34	1.39	1.46
1	B	557	ILE	CA-CB	5.33	1.60	1.54
1	C	556	ALA	CA-CB	5.30	1.61	1.53
1	C	511	SER	N-CA	-5.23	1.39	1.46
1	D	599	VAL	CA-CB	5.23	1.61	1.54
1	E	473	ALA	CA-CB	5.23	1.61	1.53
1	A	592	ILE	CA-CB	5.20	1.62	1.54
1	B	516	THR	CA-C	5.18	1.59	1.52
1	C	426	VAL	CA-C	5.17	1.58	1.52
1	C	421	THR	N-CA	5.17	1.52	1.46
1	F	475	MET	N-CA	5.16	1.52	1.46
1	A	568	LYS	CG-CD	5.12	1.67	1.52
1	F	483	LYS	CA-C	5.12	1.59	1.52
1	A	571	ILE	N-CA	5.10	1.52	1.46
1	B	460	VAL	CA-CB	5.10	1.60	1.54
1	C	608	ARG	CA-C	5.09	1.59	1.52
1	E	596	LEU	CG-CD2	5.08	1.69	1.52
1	C	468	GLU	CB-CG	5.07	1.67	1.52
1	A	600	LEU	C-O	5.06	1.30	1.23
1	E	527	VAL	CA-CB	5.05	1.60	1.54
1	D	587	ILE	C-N	5.04	1.40	1.33
1	C	565	ILE	N-CA	-5.04	1.40	1.46
1	B	496	ILE	CA-CB	5.04	1.61	1.54
1	C	508	ASP	CA-C	5.04	1.59	1.52
1	F	462	ALA	CA-CB	5.01	1.62	1.53
1	F	594	GLU	CA-C	5.00	1.59	1.52

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	446	ILE	CB-CA-C	-11.02	93.86	110.82
1	F	441	ILE	CB-CA-C	-10.51	96.58	111.40
1	D	452	SER	N-CA-C	8.09	122.42	112.23
1	F	483	LYS	N-CA-C	8.00	127.83	110.80
1	F	446	ILE	CB-CA-C	-7.93	98.81	110.62
1	D	598	HIS	N-CA-C	7.86	121.97	112.38
1	A	598	HIS	N-CA-C	7.62	120.66	111.82
1	B	502	TYR	N-CA-C	7.62	121.58	108.02
1	C	515	ALA	N-CA-C	7.18	118.75	111.07
1	B	469	ILE	N-CA-C	7.15	118.77	110.62
1	F	475	MET	N-CA-C	7.12	119.71	111.02
1	B	517	ALA	N-CA-C	-6.98	103.75	111.36
1	F	477	VAL	N-CA-C	6.98	123.85	109.34
1	A	525	ILE	CA-C-N	6.93	126.91	119.78
1	A	525	ILE	C-N-CA	6.93	126.91	119.78
1	A	571	ILE	CB-CA-C	-6.90	103.01	112.04
1	E	469	ILE	N-CA-C	6.89	117.65	110.62
1	D	581	GLU	N-CA-C	-6.83	99.32	109.15
1	F	581	GLU	CA-C-N	-6.79	110.48	122.97
1	F	581	GLU	C-N-CA	-6.79	110.48	122.97
1	E	512	ILE	N-CA-C	6.76	120.50	111.17
1	A	566	ILE	CA-C-N	-6.70	113.06	119.76
1	A	566	ILE	C-N-CA	-6.70	113.06	119.76
1	A	496	ILE	CA-CB-CG1	6.66	121.73	110.40
1	C	551	GLN	N-CA-C	-6.66	103.94	111.07
1	A	445	ILE	CB-CA-C	-6.59	100.67	110.82
1	A	471	ARG	CG-CD-NE	-6.58	97.51	112.00
1	C	475	MET	N-CA-C	6.54	118.96	111.11
1	A	446	ILE	CB-CG1-CD1	-6.53	100.09	113.80
1	F	608	ARG	CB-CA-C	6.50	123.65	110.38
1	C	597	GLU	CG-CD-OE1	-6.41	103.65	118.40
1	D	428	ARG	CG-CD-NE	-6.41	97.90	112.00
1	C	441	ILE	CB-CA-C	-6.40	99.49	110.30
1	E	590	SER	N-CA-C	-6.31	105.60	113.55
1	D	549	VAL	N-CA-C	6.24	116.92	110.36
1	A	581	GLU	CA-C-N	-6.21	112.80	122.86
1	A	581	GLU	C-N-CA	-6.21	112.80	122.86
1	E	472	GLU	N-CA-C	6.20	117.71	111.07
1	A	446	ILE	CB-CA-C	6.20	120.05	110.50
1	C	581	GLU	CA-C-N	-6.20	112.82	122.86
1	C	581	GLU	C-N-CA	-6.20	112.82	122.86
1	C	486	GLY	N-CA-C	6.18	127.83	113.18
1	E	509	SER	N-CA-C	6.16	118.93	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	492	MET	CB-CG-SD	-6.12	94.33	112.70
1	D	445	ILE	CB-CA-C	-6.11	101.52	110.62
1	F	578	ALA	N-CA-C	-6.06	102.11	110.35
1	B	474	VAL	N-CA-C	6.05	116.52	110.23
1	C	421	THR	N-CA-C	6.02	120.33	112.92
1	D	489	ILE	CB-CA-C	6.00	121.13	111.29
1	E	566	ILE	CA-C-N	-6.00	113.76	119.76
1	E	566	ILE	C-N-CA	-6.00	113.76	119.76
1	F	428	ARG	CA-C-N	-5.94	114.68	122.94
1	F	428	ARG	C-N-CA	-5.94	114.68	122.94
1	F	590	SER	CB-CA-C	-5.90	98.55	109.29
1	C	590	SER	CB-CA-C	-5.89	99.49	109.03
1	F	512	ILE	N-CA-C	5.88	117.32	110.62
1	C	446	ILE	CA-CB-CG1	5.82	120.29	110.40
1	D	525	ILE	CA-C-N	5.80	125.71	119.85
1	D	525	ILE	C-N-CA	5.80	125.71	119.85
1	E	492	MET	N-CA-C	5.80	118.22	109.23
1	F	476	ASN	CB-CA-C	5.77	121.91	110.42
1	F	482	LYS	CA-C-N	5.76	132.53	121.54
1	F	482	LYS	C-N-CA	5.76	132.53	121.54
1	A	587	ILE	CA-C-N	5.74	125.92	119.90
1	A	587	ILE	C-N-CA	5.74	125.92	119.90
1	D	438	SER	N-CA-C	5.65	118.53	111.24
1	B	599	VAL	N-CA-C	5.63	118.59	112.96
1	E	506	GLU	CA-C-N	-5.63	115.19	121.83
1	E	506	GLU	C-N-CA	-5.63	115.19	121.83
1	F	478	SER	N-CA-C	-5.61	105.31	111.82
1	B	492	MET	N-CA-C	5.61	117.70	109.24
1	C	585	GLU	CA-CB-CG	-5.55	102.99	114.10
1	F	467	GLN	N-CA-C	5.55	117.41	111.36
1	E	467	GLN	N-CA-C	5.54	117.32	111.28
1	A	613	PHE	CB-CA-C	-5.52	104.43	111.22
1	B	593	ASN	N-CA-C	5.50	118.03	111.71
1	E	426	VAL	N-CA-CB	5.48	117.05	110.31
1	D	479	ALA	N-CA-C	-5.46	105.22	111.07
1	F	569	ASP	N-CA-C	5.46	119.69	113.19
1	F	474	VAL	CA-C-N	5.46	128.38	120.79
1	F	474	VAL	C-N-CA	5.46	128.38	120.79
1	D	521	ALA	N-CA-C	-5.44	105.43	111.36
1	E	459	ARG	N-CA-C	5.42	117.08	108.79
1	B	585	GLU	N-CA-C	5.40	117.50	107.99
1	A	515	ALA	CA-C-N	5.39	127.51	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	ALA	C-N-CA	5.39	127.51	120.28
1	C	581	GLU	N-CA-C	-5.39	102.30	110.28
1	C	566	ILE	CB-CA-C	-5.35	104.11	109.89
1	B	525	ILE	CA-C-N	5.34	125.26	119.76
1	B	525	ILE	C-N-CA	5.34	125.26	119.76
1	B	445	ILE	CB-CA-C	-5.32	102.76	110.63
1	F	445	ILE	CB-CA-C	-5.31	102.71	110.62
1	F	471	ARG	N-CA-C	5.30	117.06	111.28
1	D	607	ASN	CA-C-N	5.30	127.65	120.44
1	D	607	ASN	C-N-CA	5.30	127.65	120.44
1	D	460	VAL	N-CA-C	-5.30	100.02	107.75
1	A	531	VAL	N-CA-C	5.29	114.37	106.85
1	E	438	SER	N-CA-C	5.29	122.06	110.80
1	E	604	LYS	N-CA-C	5.29	117.79	111.71
1	D	468	GLU	CA-C-N	5.25	127.66	120.46
1	D	468	GLU	C-N-CA	5.25	127.66	120.46
1	C	540	LYS	N-CA-C	5.21	119.62	113.16
1	F	525	ILE	CA-C-N	-5.21	114.87	120.03
1	F	525	ILE	C-N-CA	-5.21	114.87	120.03
1	D	566	ILE	CA-C-N	-5.20	114.40	119.76
1	D	566	ILE	C-N-CA	-5.20	114.40	119.76
1	E	613	PHE	CB-CA-C	-5.19	104.38	112.07
1	B	492	MET	CB-CG-SD	-5.14	97.28	112.70
1	C	435	ILE	N-CA-CB	5.13	117.15	110.99
1	D	480	ILE	CA-CB-CG2	5.13	119.22	110.50
1	B	469	ILE	CB-CA-C	-5.13	105.32	112.04
1	E	503	GLU	N-CA-C	-5.12	101.52	109.24
1	C	445	ILE	CB-CA-C	-5.11	102.94	110.82
1	A	496	ILE	N-CA-CB	5.11	118.46	111.41
1	E	522	ILE	N-CA-C	5.11	115.83	110.62
1	D	445	ILE	CA-CB-CG1	5.10	119.07	110.40
1	C	441	ILE	CG1-CB-CG2	5.10	125.99	110.70
1	A	596	LEU	N-CA-C	-5.10	105.62	111.07
1	B	480	ILE	N-CA-C	5.07	115.84	110.72
1	D	468	GLU	CB-CG-CD	5.05	121.18	112.60
1	C	474	VAL	N-CA-CB	5.04	116.44	110.55
1	B	557	ILE	CB-CA-C	5.04	118.62	112.02
1	D	579	GLU	N-CA-C	-5.03	100.09	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	438	SER	Peptide
1	F	579	GLU	Peptide
1	F	580	HIS	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	78	0
1	B	1457	0	1523	91	0
1	C	1448	0	1510	128	1
1	D	1457	0	1523	72	2
1	E	1457	0	1523	55	0
1	F	1457	0	1523	96	1
2	A	89	0	0	25	0
2	B	65	0	0	17	0
2	C	121	0	0	35	1
2	D	106	0	0	23	0
2	E	67	0	0	17	0
2	F	104	0	0	23	0
All	All	9285	0	9125	499	3

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 28.

All (499) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:542:GLU:CG	1:D:542:GLU:CB	1.77	1.61
1:A:480:ILE:HG21	2:A:691:HOH:O	1.11	1.27
1:B:480:ILE:HG21	2:B:682:HOH:O	1.37	1.24
1:C:418:LEU:N	2:C:725:HOH:O	1.62	1.23
1:C:502:TYR:HB2	2:C:726:HOH:O	1.12	1.22
1:C:457:GLU:HA	1:C:457:GLU:OE1	1.45	1.13
1:C:502:TYR:CD1	2:C:726:HOH:O	2.01	1.12
1:D:551:GLN:HG2	2:D:716:HOH:O	1.48	1.11
1:B:491:ASN:HB2	2:B:636:HOH:O	1.50	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:ILE:HD11	2:B:628:HOH:O	1.51	1.08
1:A:469:ILE:HG21	2:A:684:HOH:O	1.54	1.06
1:C:597:GLU:HG2	1:C:610:MET:HE2	1.37	1.06
1:F:435:ILE:HG22	1:F:505:VAL:HG22	1.31	1.06
1:F:551:GLN:HG2	2:F:710:HOH:O	1.53	1.06
1:A:487:ARG:HG3	1:A:487:ARG:HH11	0.98	1.06
1:D:597:GLU:HG2	1:D:610:MET:HE2	1.08	1.05
1:A:445:ILE:HD11	2:A:640:HOH:O	1.57	1.03
1:C:502:TYR:CB	2:C:726:HOH:O	1.72	1.02
1:E:597:GLU:HG2	1:E:610:MET:HE2	1.41	1.02
1:A:597:GLU:HG2	1:A:610:MET:HE2	1.41	1.01
1:C:445:ILE:HB	2:C:727:HOH:O	1.62	0.99
1:E:465:ARG:HD2	2:E:670:HOH:O	1.62	0.99
1:D:501:THR:HB	2:E:647:HOH:O	1.62	0.98
1:A:428:ARG:HD2	1:A:446:ILE:HB	1.44	0.98
1:D:487:ARG:HG3	1:D:487:ARG:HH11	1.24	0.98
1:F:479:ALA:O	1:F:483:LYS:HB3	1.64	0.98
1:F:478:SER:HB2	1:F:489:ILE:HD12	1.46	0.97
1:F:472:GLU:HB3	2:F:711:HOH:O	1.63	0.97
1:A:487:ARG:HG3	1:A:487:ARG:NH1	1.76	0.97
1:C:445:ILE:HD12	2:C:718:HOH:O	1.64	0.95
1:E:591:ARG:HB3	2:E:680:HOH:O	1.66	0.95
1:D:435:ILE:HG22	1:D:505:VAL:HG22	1.45	0.95
1:C:597:GLU:CG	1:C:610:MET:HE2	1.95	0.94
1:C:611:SER:O	1:C:614:LYS:HE2	1.69	0.93
1:B:482:LYS:HG3	2:B:681:HOH:O	1.68	0.93
1:A:577:ASP:HB3	2:A:697:HOH:O	1.68	0.92
1:C:445:ILE:CD1	2:C:718:HOH:O	2.18	0.92
1:F:435:ILE:HG23	1:F:441:ILE:HG12	1.49	0.91
1:F:477:VAL:HB	2:F:647:HOH:O	1.70	0.91
1:C:422:GLU:HB2	2:C:739:HOH:O	1.69	0.91
1:F:608:ARG:HE	1:F:612:LYS:NZ	1.68	0.90
1:A:571:ILE:HD11	1:A:588:PRO:HB3	1.53	0.90
1:A:593:ASN:O	1:A:597:GLU:HG3	1.70	0.90
1:F:597:GLU:CG	1:F:610:MET:HE2	2.02	0.90
1:B:489:ILE:HG22	2:B:686:HOH:O	1.71	0.89
1:D:480:ILE:CD1	1:D:592:ILE:HG21	2.01	0.89
1:B:418:LEU:HD13	2:C:711:HOH:O	1.73	0.88
1:F:475:MET:C	1:F:476:ASN:O	2.15	0.88
1:D:452:SER:O	1:D:453:MET:SD	2.32	0.88
1:B:463:THR:HG23	2:C:657:HOH:O	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:597:GLU:HG3	1:F:610:MET:HE2	1.53	0.87
1:C:465:ARG:CD	1:C:503:GLU:HG2	2.06	0.86
1:E:422:GLU:HB3	2:E:673:HOH:O	1.75	0.86
1:B:568:LYS:HE2	1:B:590:SER:HB2	1.58	0.86
1:C:445:ILE:HD13	1:C:445:ILE:N	1.90	0.86
1:D:597:GLU:CG	1:D:610:MET:HE2	2.01	0.85
1:C:481:ILE:HG21	1:C:489:ILE:CD1	2.07	0.85
1:C:422:GLU:CB	2:C:739:HOH:O	2.21	0.85
1:D:579:GLU:CD	2:D:711:HOH:O	2.20	0.84
1:C:463:THR:OG1	1:D:468:GLU:HG3	1.78	0.84
1:C:578:ALA:HA	1:C:581:GLU:OE1	1.78	0.83
1:A:542:GLU:HG2	2:F:669:HOH:O	1.79	0.83
1:F:579:GLU:HB3	1:F:580:HIS:ND1	1.94	0.83
1:E:597:GLU:HG2	1:E:610:MET:CE	2.08	0.82
1:C:502:TYR:HB3	1:C:505:VAL:HG21	1.61	0.82
1:C:438:SER:HA	1:C:551:GLN:OE1	1.80	0.82
1:D:597:GLU:HG2	1:D:610:MET:CE	2.03	0.81
1:C:467:GLN:OE1	1:C:471:ARG:NH2	2.14	0.81
1:C:445:ILE:CG2	2:C:727:HOH:O	2.29	0.81
1:C:469:ILE:O	1:C:472:GLU:HG3	1.81	0.80
1:F:435:ILE:CG2	1:F:505:VAL:HG22	2.12	0.80
1:E:422:GLU:CB	2:E:673:HOH:O	2.30	0.80
1:D:597:GLU:HB3	2:D:622:HOH:O	1.80	0.79
1:B:448:GLU:OE2	1:B:450:THR:HG23	1.82	0.79
1:C:550:THR:O	1:C:554:GLU:HG3	1.83	0.79
1:B:435:ILE:O	1:B:436:GLY:O	2.01	0.78
1:B:568:LYS:HE2	1:B:590:SER:CB	2.13	0.78
1:D:480:ILE:HD11	1:D:592:ILE:HG21	1.64	0.78
1:F:445:ILE:CG2	2:F:713:HOH:O	2.31	0.78
1:C:578:ALA:HA	1:C:581:GLU:CD	2.09	0.78
1:F:597:GLU:HB3	2:F:622:HOH:O	1.85	0.77
1:A:475:MET:SD	1:F:461:ILE:HD13	2.24	0.77
1:D:487:ARG:HH11	1:D:487:ARG:CG	1.97	0.77
1:B:480:ILE:CG2	2:B:682:HOH:O	2.09	0.77
1:A:608:ARG:HG3	1:A:608:ARG:HH11	1.50	0.77
1:C:481:ILE:HG21	1:C:489:ILE:HD11	1.65	0.77
1:C:468:GLU:OE2	1:C:472:GLU:HB3	1.85	0.76
1:C:480:ILE:CG2	2:C:732:HOH:O	2.34	0.76
1:D:542:GLU:OE2	1:D:591:ARG:HG3	1.84	0.76
1:F:597:GLU:HG3	1:F:610:MET:CE	2.15	0.75
1:A:487:ARG:HD2	2:A:710:HOH:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:590:SER:HB3	1:E:591:ARG:HG3	1.69	0.75
1:C:501:THR:HB	2:D:649:HOH:O	1.87	0.75
1:C:554:GLU:HB3	2:C:731:HOH:O	1.88	0.74
1:D:568:LYS:HG2	1:D:590:SER:HB3	1.69	0.74
1:D:489:ILE:HG21	1:D:522:ILE:CD1	2.17	0.74
1:C:479:ALA:O	1:C:483:LYS:N	2.21	0.74
1:F:467:GLN:OE1	1:F:471:ARG:NH2	2.20	0.74
1:C:428:ARG:HG3	2:C:740:HOH:O	1.86	0.74
1:D:489:ILE:HG21	1:D:522:ILE:HD13	1.69	0.74
1:A:568:LYS:O	1:A:571:ILE:HG12	1.87	0.73
1:F:475:MET:O	1:F:476:ASN:O	2.06	0.73
1:A:608:ARG:HH11	1:A:608:ARG:CG	2.02	0.73
1:D:583:LYS:HE2	2:D:630:HOH:O	1.88	0.73
1:A:501:THR:HG22	2:B:641:HOH:O	1.89	0.72
1:C:477:VAL:O	1:C:477:VAL:HG22	1.87	0.72
1:C:502:TYR:HD1	2:C:726:HOH:O	1.53	0.72
1:A:453:MET:CB	2:A:662:HOH:O	2.37	0.72
1:F:480:ILE:HG23	2:F:691:HOH:O	1.88	0.72
1:B:463:THR:CG2	2:C:657:HOH:O	2.34	0.72
1:E:591:ARG:CG	2:E:680:HOH:O	2.38	0.71
1:C:459:ARG:NH2	1:D:475:MET:HE1	2.05	0.71
1:C:502:TYR:HB3	1:C:505:VAL:CG2	2.20	0.71
1:C:591:ARG:HB3	1:C:593:ASN:OD1	1.89	0.71
1:F:476:ASN:O	1:F:478:SER:N	2.23	0.71
1:A:571:ILE:CD1	1:A:588:PRO:HB3	2.21	0.71
1:D:457:GLU:HG3	1:D:490:SER:O	1.91	0.71
2:A:637:HOH:O	1:F:501:THR:HG21	1.91	0.70
1:F:485:THR:OG1	1:F:486:GLY:N	2.21	0.70
1:A:417:LYS:HD2	2:A:707:HOH:O	1.90	0.70
1:C:452:SER:O	1:C:453:MET:HB2	1.90	0.70
1:B:575:LEU:O	1:B:575:LEU:HG	1.92	0.70
1:C:437:GLU:OE1	1:C:437:GLU:HA	1.91	0.69
1:D:435:ILE:CG2	1:D:505:VAL:HG22	2.22	0.69
1:C:463:THR:HG23	2:D:648:HOH:O	1.92	0.69
1:C:485:THR:OG1	1:C:486:GLY:N	2.23	0.69
1:C:480:ILE:HG23	2:C:732:HOH:O	1.91	0.68
1:D:480:ILE:HD13	1:D:592:ILE:HG21	1.76	0.68
1:C:481:ILE:HG21	1:C:489:ILE:HD13	1.76	0.68
1:D:532:ALA:HB2	1:D:561:LEU:HD13	1.73	0.68
1:F:480:ILE:CG2	2:F:691:HOH:O	2.40	0.68
1:C:571:ILE:HD11	1:C:588:PRO:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:GLU:HG2	1:B:610:MET:HE2	1.75	0.67
1:D:608:ARG:HD2	2:D:727:HOH:O	1.95	0.67
1:F:457:GLU:N	2:F:673:HOH:O	2.26	0.67
1:A:482:LYS:HE2	1:A:489:ILE:H	1.59	0.67
1:F:579:GLU:HB3	1:F:580:HIS:CE1	2.30	0.66
1:A:487:ARG:HH11	1:A:487:ARG:CG	1.88	0.66
1:C:597:GLU:OE1	2:C:625:HOH:O	2.13	0.66
1:F:428:ARG:HG3	2:F:670:HOH:O	1.95	0.66
1:B:422:GLU:HG3	1:B:423:GLY:H	1.59	0.66
1:F:435:ILE:HG22	1:F:505:VAL:CG2	2.18	0.66
1:C:465:ARG:HD2	1:C:503:GLU:CD	2.20	0.66
1:A:571:ILE:HD11	1:A:588:PRO:CB	2.26	0.66
1:D:579:GLU:OE2	2:D:630:HOH:O	2.13	0.66
1:F:477:VAL:HG23	1:F:480:ILE:HD13	1.78	0.66
1:F:445:ILE:HG22	2:F:713:HOH:O	1.92	0.66
1:C:501:THR:HG21	2:D:668:HOH:O	1.95	0.66
1:D:435:ILE:HD13	1:D:441:ILE:HG23	1.77	0.65
1:A:417:LYS:HB2	2:A:707:HOH:O	1.96	0.65
2:A:648:HOH:O	1:F:418:LEU:CD2	2.44	0.65
1:B:549:VAL:HG11	1:B:573:ASP:HB2	1.78	0.65
1:A:459:ARG:HG2	1:A:493:ASP:OD1	1.96	0.65
1:C:465:ARG:HD3	1:C:503:GLU:HG2	1.78	0.65
1:E:531:VAL:HG22	1:E:563:LYS:HB2	1.78	0.64
1:B:449:VAL:HG12	1:B:494:VAL:HG22	1.79	0.64
1:F:581:GLU:HG2	1:F:581:GLU:O	1.97	0.64
1:F:422:GLU:HG3	2:F:638:HOH:O	1.96	0.64
1:B:611:SER:HA	1:B:614:LYS:HD3	1.77	0.64
1:F:478:SER:CB	1:F:489:ILE:HD12	2.23	0.64
1:A:441:ILE:HD11	1:A:505:VAL:HG11	1.78	0.64
1:B:435:ILE:HG22	1:B:505:VAL:HG22	1.80	0.64
1:A:453:MET:HB2	2:A:662:HOH:O	1.98	0.64
1:F:577:ASP:HB2	1:F:578:ALA:O	1.98	0.64
1:C:457:GLU:OE1	1:C:457:GLU:CA	2.32	0.63
1:F:477:VAL:HG22	1:F:481:ILE:HG13	1.80	0.63
1:E:418:LEU:HA	1:F:545:PRO:HG2	1.80	0.63
1:F:446:ILE:CD1	1:F:497:GLN:HB2	2.29	0.63
1:C:578:ALA:O	1:C:579:GLU:HB2	1.97	0.63
1:C:597:GLU:HG2	1:C:610:MET:CE	2.21	0.63
1:E:419:PHE:HA	1:E:428:ARG:NH2	2.13	0.63
1:A:459:ARG:CB	1:A:459:ARG:HH11	2.11	0.63
1:A:610:MET:HE3	2:A:664:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:597:GLU:HB3	2:F:719:HOH:O	1.98	0.62
1:D:487:ARG:HG3	1:D:487:ARG:NH1	2.04	0.62
1:F:608:ARG:HE	1:F:612:LYS:HZ1	1.44	0.62
1:E:435:ILE:HG22	1:E:505:VAL:HG13	1.82	0.62
1:B:448:GLU:HG2	2:C:720:HOH:O	1.98	0.62
1:E:523:GLU:HG3	1:E:609:LEU:HD22	1.82	0.62
1:E:471:ARG:NE	2:E:677:HOH:O	2.32	0.61
1:C:480:ILE:HD12	1:C:592:ILE:HG21	1.81	0.61
1:C:479:ALA:HB1	1:C:483:LYS:HG2	1.81	0.61
1:F:422:GLU:HG2	2:F:690:HOH:O	1.99	0.61
1:C:419:PHE:HB3	1:C:444:PRO:HG3	1.83	0.61
1:C:435:ILE:HG23	1:C:505:VAL:HG22	1.82	0.61
1:C:481:ILE:CG2	1:C:489:ILE:HD13	2.31	0.61
1:C:445:ILE:HD13	1:C:445:ILE:H	1.62	0.60
1:F:571:ILE:HD11	1:F:588:PRO:HG3	1.83	0.60
1:D:428:ARG:NE	2:D:713:HOH:O	2.28	0.60
1:C:597:GLU:HG3	1:C:610:MET:HE2	1.82	0.60
1:A:435:ILE:HG23	1:A:505:VAL:HG22	1.81	0.60
1:C:465:ARG:HD2	1:C:503:GLU:OE2	2.01	0.60
1:F:597:GLU:HG2	1:F:610:MET:HE2	1.84	0.60
1:E:471:ARG:CZ	2:E:677:HOH:O	2.49	0.60
1:A:597:GLU:HG2	1:A:610:MET:CE	2.23	0.60
1:C:463:THR:OG1	1:D:468:GLU:CG	2.49	0.60
1:C:477:VAL:O	1:C:477:VAL:CG2	2.49	0.60
1:C:477:VAL:HG22	1:C:481:ILE:HG13	1.85	0.59
1:D:579:GLU:OE1	2:D:711:HOH:O	2.16	0.59
1:B:593:ASN:HD22	1:B:613:PHE:HB3	1.68	0.59
1:C:465:ARG:HD2	1:C:503:GLU:HG2	1.84	0.59
1:C:438:SER:CA	1:C:551:GLN:OE1	2.51	0.59
1:F:435:ILE:CG2	1:F:441:ILE:HG12	2.28	0.59
1:F:478:SER:HB2	1:F:489:ILE:CD1	2.28	0.59
1:A:593:ASN:O	1:A:597:GLU:CG	2.49	0.59
1:E:591:ARG:CB	2:E:680:HOH:O	2.32	0.59
1:B:532:ALA:HB2	1:B:561:LEU:HD13	1.85	0.58
1:E:460:VAL:CG2	1:E:474:VAL:HG11	2.33	0.58
1:B:531:VAL:HG22	1:B:563:LYS:HB2	1.85	0.58
1:D:545:PRO:HA	1:D:567:PRO:HG2	1.84	0.58
1:D:579:GLU:CG	2:D:711:HOH:O	2.48	0.58
1:B:461:ILE:CG2	1:C:475:MET:HG2	2.34	0.58
1:C:461:ILE:HD13	1:D:475:MET:SD	2.43	0.58
1:D:435:ILE:HD13	1:D:441:ILE:CG2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:LYS:HG2	1:A:488:ASP:HA	1.84	0.57
1:C:591:ARG:NH2	1:C:594:GLU:OE2	2.37	0.57
1:A:482:LYS:HE2	1:A:489:ILE:N	2.19	0.57
1:A:488:ASP:OD2	1:A:490:SER:HB2	2.03	0.57
1:F:480:ILE:HD13	1:F:537:LEU:HD21	1.87	0.57
1:C:433:ALA:HB3	1:C:441:ILE:HD11	1.87	0.57
1:D:550:THR:O	1:D:554:GLU:HG3	2.05	0.57
1:F:562:LYS:HE2	2:F:638:HOH:O	2.04	0.57
1:B:435:ILE:CG2	1:B:505:VAL:HG22	2.35	0.57
1:F:578:ALA:O	1:F:579:GLU:HB2	2.03	0.57
1:C:465:ARG:CD	1:C:503:GLU:CG	2.82	0.56
1:C:480:ILE:HG21	2:C:732:HOH:O	1.98	0.56
1:A:452:SER:O	1:A:453:MET:CB	2.53	0.56
1:C:480:ILE:CD1	1:C:592:ILE:HG21	2.35	0.56
1:C:593:ASN:HB3	1:C:613:PHE:CD1	2.40	0.56
1:C:445:ILE:HG21	2:C:727:HOH:O	1.98	0.56
1:C:479:ALA:O	1:C:483:LYS:HG3	2.05	0.56
1:C:446:ILE:CD1	1:C:499:VAL:HG22	2.36	0.56
1:A:428:ARG:CD	1:A:446:ILE:HB	2.29	0.56
1:B:568:LYS:HG3	1:B:589:VAL:O	2.06	0.56
1:A:550:THR:HG23	2:A:685:HOH:O	2.06	0.55
1:A:597:GLU:HB2	2:A:622:HOH:O	2.06	0.55
1:E:481:ILE:HG22	1:E:487:ARG:O	2.07	0.55
1:B:480:ILE:HD12	1:B:484:TYR:CD2	2.42	0.55
1:D:471:ARG:NH2	2:D:723:HOH:O	2.40	0.55
1:A:563:LYS:HG2	1:A:585:GLU:HB3	1.88	0.55
1:C:459:ARG:HH22	1:D:475:MET:HE1	1.70	0.54
1:C:578:ALA:O	1:C:579:GLU:CB	2.55	0.54
1:F:477:VAL:HG22	1:F:477:VAL:O	2.06	0.54
1:A:608:ARG:CG	1:A:608:ARG:NH1	2.66	0.54
1:B:422:GLU:HB3	2:B:635:HOH:O	2.06	0.54
1:B:452:SER:C	2:B:666:HOH:O	2.50	0.54
1:D:478:SER:HB2	2:D:722:HOH:O	2.07	0.54
1:F:578:ALA:HA	1:F:581:GLU:OE1	2.08	0.54
1:D:465:ARG:NE	1:D:503:GLU:OE2	2.40	0.54
1:F:424:TYR:HB3	1:F:526:PRO:HB2	1.89	0.54
1:F:608:ARG:HE	1:F:612:LYS:HZ2	1.51	0.54
1:A:470:ALA:O	1:A:474:VAL:HG23	2.07	0.54
1:B:489:ILE:O	1:B:492:MET:HE2	2.08	0.54
1:E:435:ILE:O	1:E:436:GLY:C	2.51	0.54
1:E:451:PRO:HD3	2:E:667:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:578:ALA:C	1:F:579:GLU:O	2.50	0.54
1:C:424:TYR:HB3	1:C:526:PRO:HB2	1.90	0.54
1:D:562:LYS:NZ	2:D:708:HOH:O	2.40	0.53
1:F:579:GLU:O	1:F:580:HIS:HB2	2.09	0.53
1:B:502:TYR:HB2	1:B:505:VAL:CG2	2.39	0.53
1:A:417:LYS:N	1:B:569:ASP:O	2.41	0.53
1:A:487:ARG:NH1	1:A:487:ARG:CG	2.55	0.53
1:D:604:LYS:HZ1	1:D:608:ARG:HG3	1.73	0.53
1:A:540:LYS:HD2	2:A:705:HOH:O	2.08	0.53
1:A:613:PHE:HB2	2:A:664:HOH:O	2.06	0.53
1:A:597:GLU:CB	2:A:622:HOH:O	2.57	0.53
1:D:470:ALA:HA	1:D:514:ILE:HD13	1.90	0.53
1:C:446:ILE:CD1	1:C:499:VAL:CG2	2.87	0.53
1:E:496:ILE:HD11	1:E:518:VAL:CG2	2.39	0.53
1:A:579:GLU:HG3	2:A:697:HOH:O	2.09	0.52
1:C:472:GLU:CD	2:C:640:HOH:O	2.52	0.52
1:C:492:MET:HE1	1:C:522:ILE:HD11	1.89	0.52
1:F:563:LYS:HD3	1:F:587:ILE:HD11	1.92	0.52
1:F:597:GLU:CB	2:F:622:HOH:O	2.50	0.52
1:F:578:ALA:O	1:F:579:GLU:CB	2.56	0.52
1:C:476:ASN:CB	2:C:659:HOH:O	2.57	0.52
1:D:578:ALA:O	1:D:579:GLU:HB3	2.09	0.52
1:C:445:ILE:CB	2:C:727:HOH:O	2.30	0.52
1:F:604:LYS:NZ	1:F:604:LYS:CB	2.73	0.52
1:B:435:ILE:HG22	1:B:505:VAL:CG2	2.40	0.52
1:D:604:LYS:NZ	1:D:608:ARG:HG3	2.25	0.52
1:C:428:ARG:CG	2:C:740:HOH:O	2.53	0.51
1:C:481:ILE:CG2	1:C:489:ILE:CD1	2.83	0.51
1:C:422:GLU:HB3	2:C:739:HOH:O	1.98	0.51
1:C:465:ARG:HD2	1:C:503:GLU:CG	2.40	0.51
1:E:448:GLU:HG3	2:E:683:HOH:O	2.10	0.51
1:B:451:PRO:O	1:B:453:MET:N	2.29	0.51
1:F:446:ILE:HD11	1:F:497:GLN:HB2	1.92	0.51
1:D:579:GLU:HG2	2:D:711:HOH:O	2.08	0.51
1:D:597:GLU:HG3	2:D:640:HOH:O	2.10	0.51
1:C:445:ILE:HG23	1:C:498:PHE:CD1	2.46	0.51
1:C:463:THR:CG2	2:D:648:HOH:O	2.55	0.51
1:C:563:LYS:HD3	1:C:587:ILE:HD11	1.92	0.51
1:C:611:SER:O	1:C:614:LYS:CE	2.51	0.51
1:B:551:GLN:CD	1:B:551:GLN:H	2.19	0.51
1:C:479:ALA:HB3	2:C:720:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:THR:HB	2:B:663:HOH:O	2.12	0.50
1:B:471:ARG:NE	2:B:668:HOH:O	2.40	0.50
1:F:445:ILE:HD12	1:F:514:ILE:HG13	1.92	0.50
1:A:545:PRO:HG2	1:F:499:VAL:HG12	1.93	0.50
1:E:448:GLU:CG	2:E:683:HOH:O	2.60	0.50
1:E:422:GLU:HB2	2:E:673:HOH:O	2.04	0.50
1:F:554:GLU:O	1:F:558:GLN:NE2	2.44	0.50
1:A:545:PRO:HG2	1:F:499:VAL:CG1	2.41	0.50
1:E:496:ILE:HD11	1:E:518:VAL:HG23	1.93	0.50
1:E:478:SER:O	1:E:482:LYS:HE2	2.11	0.50
1:A:539:VAL:HG12	2:F:723:HOH:O	2.12	0.50
1:B:422:GLU:CG	1:B:423:GLY:H	2.25	0.50
1:C:445:ILE:CD1	1:C:445:ILE:N	2.67	0.50
1:C:501:THR:CG2	2:D:668:HOH:O	2.54	0.50
1:A:448:GLU:HB3	1:B:540:LYS:HZ1	1.77	0.50
1:B:476:ASN:O	1:B:480:ILE:HG23	2.11	0.50
1:B:501:THR:O	1:B:501:THR:HG22	2.12	0.50
2:A:648:HOH:O	1:F:418:LEU:HD22	2.08	0.49
1:B:460:VAL:CG2	1:B:474:VAL:HG11	2.42	0.49
1:D:441:ILE:HD11	1:D:505:VAL:CG2	2.42	0.49
1:D:424:TYR:HB3	1:D:526:PRO:HB2	1.95	0.49
1:B:452:SER:CA	2:B:666:HOH:O	2.61	0.49
1:A:568:LYS:HE2	1:A:590:SER:HB3	1.95	0.49
1:C:433:ALA:HB3	1:C:441:ILE:CD1	2.43	0.49
1:C:600:LEU:HB2	1:C:606:LYS:HD2	1.93	0.49
1:D:551:GLN:H	1:D:551:GLN:CD	2.20	0.49
1:F:477:VAL:HG13	1:F:481:ILE:HD12	1.94	0.49
1:B:482:LYS:HG2	1:B:487:ARG:O	2.13	0.48
1:D:487:ARG:CG	1:D:487:ARG:NH1	2.66	0.48
1:E:478:SER:OG	1:E:489:ILE:HD11	2.13	0.48
1:F:435:ILE:HG23	1:F:441:ILE:CG1	2.35	0.48
1:D:509:SER:O	1:D:510:ALA:C	2.56	0.48
1:B:592:ILE:O	1:B:595:VAL:HB	2.13	0.48
1:E:424:TYR:HB3	1:E:526:PRO:HB2	1.95	0.48
1:C:580:HIS:HA	1:C:583:LYS:HG3	1.95	0.48
1:B:568:LYS:HE2	1:B:590:SER:HA	1.96	0.48
1:E:597:GLU:CG	1:E:610:MET:HE2	2.27	0.48
1:E:417:LYS:HD3	1:E:417:LYS:N	2.28	0.48
1:F:514:ILE:O	1:F:518:VAL:HG23	2.12	0.48
1:B:422:GLU:O	1:B:529:GLN:HB2	2.14	0.47
1:B:489:ILE:HG23	2:B:681:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:435:ILE:HG22	1:D:505:VAL:CG2	2.32	0.47
1:D:489:ILE:HG21	1:D:522:ILE:HD11	1.94	0.47
1:A:537:LEU:HD11	1:A:541:GLY:HA2	1.95	0.47
1:E:545:PRO:HA	1:E:567:PRO:HG2	1.95	0.47
1:B:492:MET:HB2	1:B:492:MET:HE3	1.14	0.47
1:A:452:SER:O	1:A:453:MET:HB2	2.13	0.47
2:A:637:HOH:O	1:F:501:THR:CG2	2.57	0.47
1:B:422:GLU:CB	2:B:635:HOH:O	2.62	0.47
1:B:482:LYS:HG2	1:B:488:ASP:HA	1.95	0.47
1:C:577:ASP:OD1	1:C:577:ASP:N	2.43	0.47
1:A:441:ILE:HD11	1:A:505:VAL:CG1	2.44	0.47
1:A:494:VAL:HG12	1:A:496:ILE:HD13	1.97	0.47
1:B:480:ILE:HD12	1:B:484:TYR:HD2	1.80	0.47
1:D:435:ILE:CG2	1:D:441:ILE:HD13	2.45	0.47
1:D:480:ILE:HD11	1:D:592:ILE:CG2	2.39	0.47
1:F:480:ILE:CD1	1:F:537:LEU:HD21	2.45	0.47
1:E:438:SER:O	1:E:551:GLN:HG2	2.15	0.47
1:C:511:SER:HB3	1:C:514:ILE:HD12	1.96	0.47
1:E:449:VAL:HG21	1:E:522:ILE:HD13	1.96	0.47
1:B:568:LYS:HE2	1:B:590:SER:CA	2.44	0.47
1:C:465:ARG:CG	1:C:503:GLU:HG2	2.44	0.47
1:D:442:VAL:HG12	1:D:444:PRO:HD3	1.97	0.47
1:B:422:GLU:CG	1:B:423:GLY:N	2.77	0.46
1:B:502:TYR:CB	1:B:505:VAL:HG23	2.45	0.46
1:C:501:THR:HG22	2:D:638:HOH:O	2.15	0.46
1:E:435:ILE:HG22	1:E:505:VAL:CG1	2.45	0.46
1:B:418:LEU:CD1	2:C:711:HOH:O	2.45	0.46
1:A:446:ILE:HD11	2:A:647:HOH:O	2.15	0.46
1:C:578:ALA:HA	1:C:581:GLU:OE2	2.15	0.46
1:E:460:VAL:HG22	1:E:474:VAL:HG11	1.96	0.46
1:F:614:LYS:HZ3	1:F:614:LYS:HB3	1.81	0.46
1:C:489:ILE:HA	1:C:492:MET:HE2	1.97	0.46
1:F:422:GLU:CG	2:F:690:HOH:O	2.61	0.46
1:F:577:ASP:O	1:F:579:GLU:O	2.33	0.46
1:C:445:ILE:HD11	2:C:718:HOH:O	1.99	0.46
1:E:554:GLU:O	1:E:558:GLN:NE2	2.49	0.46
1:C:424:TYR:CD1	1:C:601:GLU:HB2	2.50	0.46
1:A:488:ASP:HB3	1:A:491:ASN:ND2	2.31	0.46
1:C:463:THR:HG21	1:D:469:ILE:CD1	2.45	0.45
1:A:494:VAL:HG12	1:A:496:ILE:CD1	2.46	0.45
1:F:614:LYS:HD2	2:F:717:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:GLN:OE1	1:D:509:SER:HB3	2.17	0.45
1:C:580:HIS:CD2	2:C:731:HOH:O	2.70	0.45
1:E:475:MET:HB2	1:E:475:MET:HE2	1.51	0.45
1:A:459:ARG:HG2	1:A:459:ARG:H	1.56	0.45
1:A:568:LYS:CE	1:A:590:SER:HB3	2.46	0.45
1:B:429:VAL:HG22	1:B:527:VAL:HG11	1.99	0.45
1:B:448:GLU:CD	1:C:483:LYS:HE2	2.41	0.45
1:B:488:ASP:OD2	1:B:490:SER:HB2	2.17	0.45
1:F:492:MET:HE1	1:F:522:ILE:HG12	1.99	0.45
1:D:460:VAL:CG2	1:D:474:VAL:HG11	2.47	0.45
1:F:579:GLU:CB	1:F:580:HIS:ND1	2.75	0.45
1:B:502:TYR:CB	1:B:505:VAL:CG2	2.95	0.45
1:E:591:ARG:CD	2:E:680:HOH:O	2.64	0.45
1:B:450:THR:O	1:B:492:MET:HB3	2.16	0.45
1:E:450:THR:HG23	1:E:493:ASP:HB2	1.99	0.45
1:B:561:LEU:C	1:B:562:LYS:HE2	2.42	0.44
1:B:562:LYS:CA	1:B:562:LYS:HE2	2.47	0.44
1:D:499:VAL:O	1:D:502:TYR:OH	2.34	0.44
1:B:489:ILE:HD12	2:B:639:HOH:O	2.17	0.44
1:B:568:LYS:HE3	2:B:626:HOH:O	2.18	0.44
1:B:429:VAL:HG13	1:B:533:MET:HE3	2.00	0.44
1:B:502:TYR:HB2	1:B:505:VAL:HG23	2.00	0.44
1:E:591:ARG:HG2	2:E:680:HOH:O	2.11	0.44
1:F:509:SER:O	1:F:510:ALA:C	2.61	0.44
1:C:468:GLU:HG3	2:C:662:HOH:O	2.17	0.44
1:D:471:ARG:NE	2:D:719:HOH:O	1.90	0.44
1:F:445:ILE:HB	2:F:713:HOH:O	2.18	0.44
1:C:465:ARG:CD	1:C:503:GLU:OE2	2.65	0.44
1:C:479:ALA:C	1:C:483:LYS:HG3	2.43	0.44
1:D:480:ILE:CD1	1:D:592:ILE:CG2	2.86	0.44
1:D:557:ILE:HG21	1:D:583:LYS:HE3	1.99	0.44
1:F:604:LYS:HB2	1:F:604:LYS:HZ2	1.81	0.44
1:B:557:ILE:HD13	1:B:580:HIS:HB3	1.99	0.44
1:B:576:LEU:HD13	1:B:580:HIS:O	2.18	0.44
1:A:509:SER:HB3	1:F:497:GLN:OE1	2.17	0.43
1:B:429:VAL:CG1	1:B:533:MET:HE3	2.48	0.43
1:B:577:ASP:C	1:B:577:ASP:OD1	2.60	0.43
1:A:576:LEU:HD23	2:A:685:HOH:O	2.18	0.43
1:B:424:TYR:CD1	1:B:601:GLU:HB2	2.53	0.43
1:C:446:ILE:HD13	1:C:446:ILE:H	1.83	0.43
1:C:591:ARG:HG2	2:C:660:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:509:SER:O	1:E:510:ALA:C	2.60	0.43
1:E:591:ARG:HD3	2:E:639:HOH:O	2.17	0.43
1:F:535:GLY:HA2	1:F:546:VAL:CG1	2.48	0.43
1:B:480:ILE:HA	1:B:483:LYS:HG2	1.99	0.43
1:B:523:GLU:OE2	1:B:609:LEU:HD13	2.18	0.43
1:C:446:ILE:HD13	1:C:446:ILE:N	2.33	0.43
1:D:441:ILE:HD11	1:D:505:VAL:HG21	1.98	0.43
1:E:419:PHE:HA	1:E:428:ARG:HH22	1.80	0.43
1:A:429:VAL:HG22	1:A:527:VAL:HG11	2.00	0.43
1:B:491:ASN:C	1:B:492:MET:HG3	2.42	0.43
1:B:419:PHE:CE1	1:B:559:ALA:HB1	2.54	0.43
1:A:532:ALA:HB2	1:A:561:LEU:HD13	2.00	0.43
1:C:476:ASN:HB2	2:C:659:HOH:O	2.18	0.43
1:C:545:PRO:HA	1:C:567:PRO:HG2	1.99	0.43
1:F:549:VAL:O	1:F:553:ILE:HG13	2.18	0.43
1:F:477:VAL:O	1:F:477:VAL:CG2	2.67	0.43
1:B:424:TYR:HB3	1:B:526:PRO:CB	2.49	0.43
1:B:560:GLY:O	1:B:562:LYS:HE3	2.18	0.43
1:C:501:THR:CG2	2:D:649:HOH:O	2.66	0.43
1:C:514:ILE:O	1:C:518:VAL:HG23	2.19	0.43
1:F:477:VAL:N	2:F:647:HOH:O	2.52	0.43
1:F:532:ALA:HB2	1:F:561:LEU:HD13	2.01	0.42
1:F:537:LEU:HD23	2:F:647:HOH:O	2.19	0.42
1:A:482:LYS:CG	1:A:488:ASP:HA	2.49	0.42
1:B:505:VAL:HB	2:B:671:HOH:O	2.18	0.42
1:B:576:LEU:HD22	1:B:580:HIS:HB2	2.01	0.42
1:E:418:LEU:HD23	1:F:544:LEU:HB3	2.01	0.42
1:C:463:THR:HG1	1:D:468:GLU:HG3	1.83	0.42
1:F:604:LYS:NZ	1:F:604:LYS:HB2	2.34	0.42
1:A:577:ASP:O	1:A:578:ALA:C	2.62	0.42
1:B:460:VAL:HG21	1:B:474:VAL:HG11	2.00	0.42
1:B:502:TYR:HB2	1:B:505:VAL:HG21	2.02	0.42
1:C:446:ILE:HD12	1:C:499:VAL:CG2	2.49	0.42
1:E:449:VAL:HG11	1:E:522:ILE:CD1	2.50	0.42
1:F:452:SER:O	1:F:453:MET:HB2	2.19	0.42
1:C:534:THR:O	1:C:567:PRO:HD3	2.19	0.42
1:D:428:ARG:NH2	2:D:713:HOH:O	2.51	0.42
1:B:448:GLU:O	1:B:448:GLU:HG3	2.16	0.42
1:E:448:GLU:HB3	1:F:539:VAL:HG23	2.02	0.42
1:A:573:ASP:OD2	1:F:417:LYS:N	2.52	0.42
1:E:564:VAL:HG13	1:E:564:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:ALA:N	2:A:657:HOH:O	2.53	0.42
1:B:449:VAL:O	1:B:449:VAL:HG23	2.19	0.42
1:A:487:ARG:CD	2:A:710:HOH:O	2.58	0.42
1:C:463:THR:CG2	1:D:469:ILE:CD1	2.98	0.42
1:C:465:ARG:HG3	1:C:503:GLU:HG2	2.01	0.42
1:E:450:THR:CG2	1:E:493:ASP:HB2	2.50	0.42
1:F:478:SER:CB	1:F:489:ILE:CD1	2.95	0.41
1:F:597:GLU:HG2	2:F:637:HOH:O	2.20	0.41
1:A:485:THR:O	1:A:485:THR:HG23	2.19	0.41
1:A:594:GLU:HA	1:A:597:GLU:HG3	2.01	0.41
1:B:606:LYS:O	1:B:610:MET:HG2	2.19	0.41
1:C:477:VAL:HG23	1:C:480:ILE:HG12	2.01	0.41
1:B:452:SER:HB3	1:B:458:GLY:HA2	2.03	0.41
1:B:548:GLY:O	1:B:552:LYS:HG3	2.20	0.41
1:E:606:LYS:O	1:E:610:MET:HG2	2.20	0.41
1:A:427:GLY:O	1:A:446:ILE:HA	2.21	0.41
1:B:562:LYS:HE2	1:B:562:LYS:HA	2.02	0.41
1:C:532:ALA:HB2	1:C:561:LEU:HD13	2.03	0.41
1:F:446:ILE:HD12	1:F:497:GLN:HB2	2.00	0.41
1:A:443:LEU:HD21	1:A:466:LEU:HD13	2.03	0.41
1:D:453:MET:HE3	1:D:453:MET:HB3	1.93	0.41
1:D:469:ILE:HD12	1:D:469:ILE:HA	1.90	0.41
1:D:611:SER:O	1:D:614:LYS:HD2	2.21	0.41
1:E:554:GLU:HG2	1:E:580:HIS:CE1	2.56	0.41
1:E:577:ASP:O	1:E:581:GLU:HB2	2.21	0.41
1:C:612:LYS:NZ	2:C:729:HOH:O	2.53	0.41
1:F:511:SER:HB3	1:F:514:ILE:HD12	2.03	0.41
1:B:424:TYR:HB3	1:B:526:PRO:HB2	2.03	0.40
1:E:438:SER:HA	2:E:649:HOH:O	2.20	0.40
1:A:477:VAL:HA	1:A:480:ILE:HG23	2.03	0.40
1:F:611:SER:O	1:F:614:LYS:NZ	2.51	0.40
1:A:446:ILE:O	1:A:446:ILE:HD13	2.20	0.40
1:B:469:ILE:H	1:B:469:ILE:HG12	1.63	0.40
2:A:642:HOH:O	1:F:501:THR:HB	2.20	0.40
1:B:470:ALA:O	1:B:474:VAL:HG23	2.22	0.40
1:C:553:ILE:HG12	1:C:564:VAL:HG11	2.02	0.40
1:E:450:THR:HA	1:E:451:PRO:HD2	1.90	0.40
1:E:461:ILE:HD12	1:E:495:HIS:NE2	2.36	0.40
1:E:549:VAL:O	1:E:553:ILE:HG13	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:486:GLY:O	1:F:578:ALA:CB[1_455]	1.82	0.38
1:C:585:GLU:OE2	1:D:597:GLU:OE1[2_546]	2.13	0.07
1:D:568:LYS:CD	2:C:738:HOH:O[2_556]	2.16	0.04

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%)	183 (96%)	8 (4%)	0	100	100
1	B	191/205 (93%)	181 (95%)	5 (3%)	5 (3%)	4	0
1	C	190/205 (93%)	179 (94%)	5 (3%)	6 (3%)	3	0
1	D	191/205 (93%)	183 (96%)	6 (3%)	2 (1%)	12	6
1	E	191/205 (93%)	181 (95%)	9 (5%)	1 (0%)	24	16
1	F	191/205 (93%)	177 (93%)	6 (3%)	8 (4%)	2	0
All	All	1145/1230 (93%)	1084 (95%)	39 (3%)	22 (2%)	6	2

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	436	GLY
1	B	452	SER
1	C	579	GLU
1	F	476	ASN
1	F	477	VAL
1	F	482	LYS
1	F	483	LYS
1	F	577	ASP
1	F	580	HIS
1	B	437	GLU
1	B	486	GLY
1	C	578	ALA
1	D	579	GLU

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Mol	Chain	Res	Type
1	E	436	GLY
1	F	581	GLU
1	C	436	GLY
1	C	483	LYS
1	C	486	GLY
1	F	579	GLU
1	C	485	THR
1	D	458	GLY
1	B	435	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%)	138 (86%)	22 (14%)	3	1
1	B	160/168 (95%)	138 (86%)	22 (14%)	3	1
1	C	159/168 (95%)	130 (82%)	29 (18%)	2	0
1	D	160/168 (95%)	139 (87%)	21 (13%)	4	1
1	E	160/168 (95%)	133 (83%)	27 (17%)	2	0
1	F	160/168 (95%)	135 (84%)	25 (16%)	2	0
All	All	959/1008 (95%)	813 (85%)	146 (15%)	3	0

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	417	LYS
1	A	435	ILE
1	A	441	ILE
1	A	446	ILE
1	A	457	GLU
1	A	459	ARG
1	A	469	ILE
1	A	480	ILE
1	A	485	THR

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Mol	Chain	Res	Type
1	A	487	ARG
1	A	489	ILE
1	A	501	THR
1	A	503	GLU
1	A	509	SER
1	A	539	VAL
1	A	540	LYS
1	A	568	LYS
1	A	575	LEU
1	A	579	GLU
1	A	605	LYS
1	A	608	ARG
1	A	611	SER
1	B	435	ILE
1	B	448	GLU
1	B	452	SER
1	B	457	GLU
1	B	459	ARG
1	B	463	THR
1	B	480	ILE
1	B	482	LYS
1	B	489	ILE
1	B	492	MET
1	B	501	THR
1	B	502	TYR
1	B	506	GLU
1	B	539	VAL
1	B	540	LYS
1	B	562	LYS
1	B	568	LYS
1	B	597	GLU
1	B	604	LYS
1	B	608	ARG
1	B	611	SER
1	B	614	LYS
1	C	418	LEU
1	C	420	ILE
1	C	428	ARG
1	C	435	ILE
1	C	437	GLU
1	C	438	SER
1	C	441	ILE

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Mol	Chain	Res	Type
1	C	445	ILE
1	C	446	ILE
1	C	457	GLU
1	C	463	THR
1	C	465	ARG
1	C	469	ILE
1	C	472	GLU
1	C	476	ASN
1	C	478	SER
1	C	480	ILE
1	C	485	THR
1	C	489	ILE
1	C	490	SER
1	C	501	THR
1	C	508	ASP
1	C	538	SER
1	C	558	GLN
1	C	562	LYS
1	C	580	HIS
1	C	581	GLU
1	C	591	ARG
1	C	597	GLU
1	D	417	LYS
1	D	418	LEU
1	D	428	ARG
1	D	445	ILE
1	D	457	GLU
1	D	465	ARG
1	D	469	ILE
1	D	477	VAL
1	D	480	ILE
1	D	482	LYS
1	D	487	ARG
1	D	509	SER
1	D	539	VAL
1	D	542	GLU
1	D	551	GLN
1	D	568	LYS
1	D	575	LEU
1	D	579	GLU
1	D	604	LYS
1	D	608	ARG

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Mol	Chain	Res	Type
1	D	614	LYS
1	E	417	LYS
1	E	418	LEU
1	E	420	ILE
1	E	422	GLU
1	E	434	VAL
1	E	435	ILE
1	E	437	GLU
1	E	459	ARG
1	E	475	MET
1	E	477	VAL
1	E	482	LYS
1	E	487	ARG
1	E	488	ASP
1	E	491	ASN
1	E	492	MET
1	E	501	THR
1	E	503	GLU
1	E	505	VAL
1	E	539	VAL
1	E	550	THR
1	E	558	GLN
1	E	575	LEU
1	E	585	GLU
1	E	590	SER
1	E	591	ARG
1	E	604	LYS
1	E	608	ARG
1	F	417	LYS
1	F	422	GLU
1	F	428	ARG
1	F	435	ILE
1	F	441	ILE
1	F	445	ILE
1	F	446	ILE
1	F	472	GLU
1	F	480	ILE
1	F	485	THR
1	F	487	ARG
1	F	489	ILE
1	F	490	SER
1	F	501	THR

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Mol	Chain	Res	Type
1	F	513	SER
1	F	538	SER
1	F	549	VAL
1	F	558	GLN
1	F	575	LEU
1	F	577	ASP
1	F	581	GLU
1	F	604	LYS
1	F	608	ARG
1	F	611	SER
1	F	614	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	491	ASN
1	A	551	GLN
1	B	593	ASN
1	E	607	ASN
1	F	558	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.12	1 (0%) 87 89	26, 33, 52, 60	0
1	B	195/205 (95%)	0.28	7 (3%) 46 46	29, 39, 60, 78	0
1	C	194/205 (94%)	-0.21	5 (2%) 57 59	23, 30, 54, 65	0
1	D	195/205 (95%)	-0.24	1 (0%) 87 89	24, 31, 48, 60	0
1	E	195/205 (95%)	0.40	9 (4%) 37 37	30, 38, 57, 77	0
1	F	195/205 (95%)	-0.10	3 (1%) 72 73	26, 33, 56, 60	0
All	All	1169/1230 (95%)	0.00	26 (2%) 62 64	23, 35, 56, 78	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	502	TYR	4.8
1	B	418	LEU	4.2
1	E	418	LEU	4.1
1	E	419	PHE	3.8
1	B	420	ILE	3.7
1	C	484	TYR	3.4
1	E	420	ILE	3.3
1	E	421	THR	3.2
1	B	421	THR	3.0
1	B	502	TYR	3.0
1	B	453	MET	3.0
1	E	436	GLY	2.9
1	C	483	LYS	2.8
1	F	577	ASP	2.8
1	E	578	ALA	2.8
1	C	476	ASN	2.7
1	F	484	TYR	2.6
1	B	419	PHE	2.6
1	E	505	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	501	THR	2.5
1	F	578	ALA	2.4
1	C	578	ALA	2.3
1	C	453	MET	2.2
1	A	578	ALA	2.2
1	B	504	GLY	2.1
1	D	468	GLU	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.