



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:55 PM GMT

PDB ID : 1Z0E
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

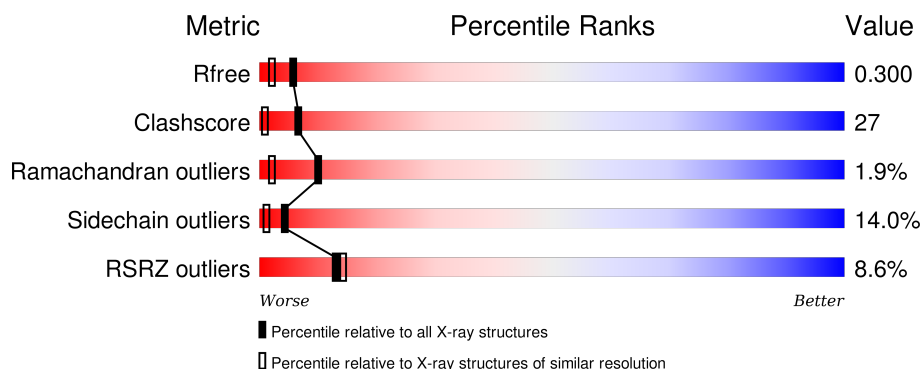
1 Overall quality at a glance

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}	91344	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div><div></div><div>7%</div><div>58%</div><div>24%</div><div>8%</div><div>5%</div><div>5%</div></div>

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.

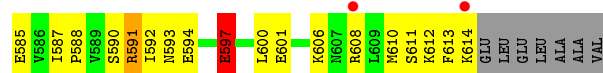
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

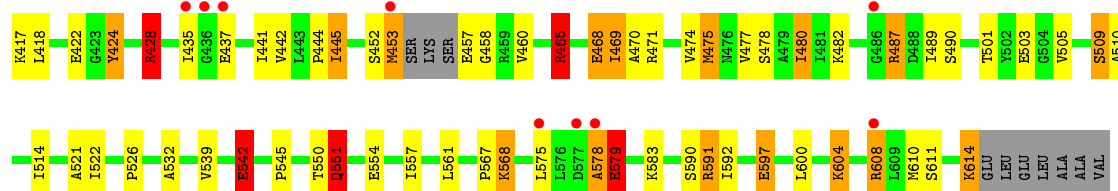
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1457	921	247	284	5			
1	B	195	Total	C	N	O	S	0	0	0
			1457	921	247	284	5			
1	C	194	Total	C	N	O	S	0	0	0
			1448	915	245	283	5			
1	D	195	Total	C	N	O	S	0	0	0
			1457	921	247	284	5			
1	E	195	Total	C	N	O	S	0	0	0
			1457	921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

- Molecule 2 is water.

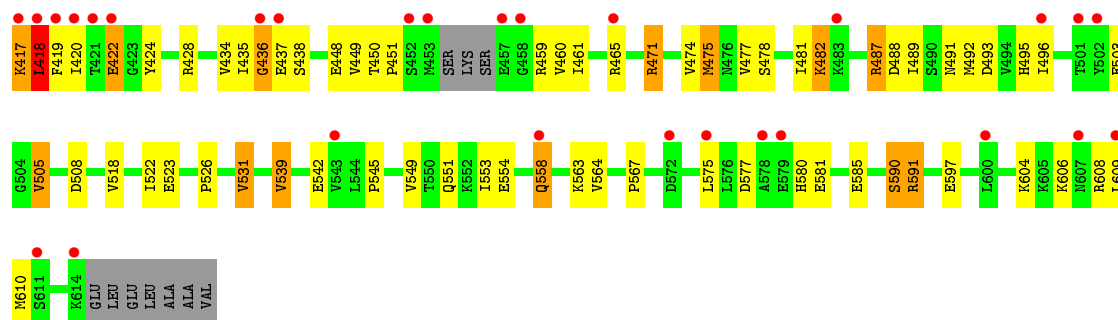
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	89	Total	O	0	0
			89	89		
2	B	65	Total	O	0	0
			65	65		
2	C	121	Total	O	0	0
			121	121		
2	D	106	Total	O	0	0
			106	106		
2	E	67	Total	O	0	0
			67	67		
2	F	104	Total	O	0	0
			104	104		



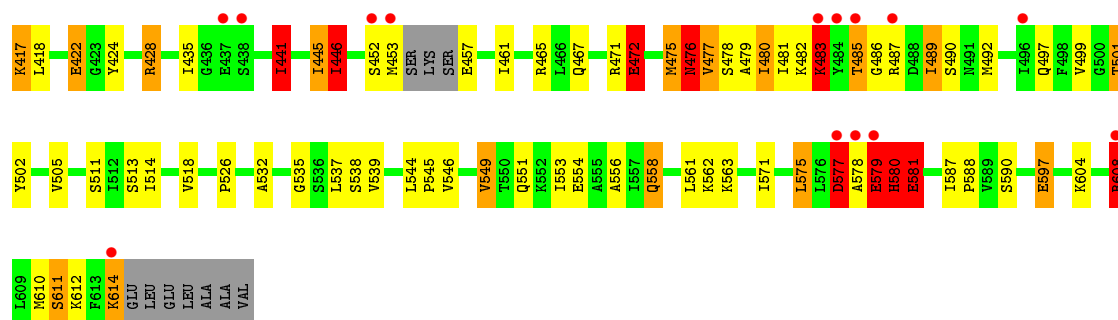
• Molecule 1: Putative protease La homolog type



• 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	48.68 Å 86.11 Å 135.61 Å 90.00° 94.70° 90.00°	Depositor
Resolution (Å)	15.00 – 2.05 14.92 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-2.05) 96.7 (14.92-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.05 Å)	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 (1.51%)	DCC
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 67688 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.35	7/1470 (0.5%)	1.21	8/1983 (0.4%)
1	B	1.17	2/1470 (0.1%)	1.07	3/1983 (0.2%)
1	C	1.49	12/1461 (0.8%)	1.30	12/1972 (0.6%)
1	D	1.51	14/1470 (1.0%)	1.23	6/1983 (0.3%)
1	E	1.22	5/1470 (0.3%)	1.13	5/1983 (0.3%)
1	F	1.37	7/1470 (0.5%)	1.27	12/1983 (0.6%)
All	All	1.36	47/8811 (0.5%)	1.20	46/11887 (0.4%)

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 (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	542	GLU	CB-CG	13.16	1.77	1.52
1	C	597	GLU	CD-OE2	10.30	1.36	1.25
1	D	542	GLU	CG-CD	9.28	1.65	1.51
1	C	468	GLU	CD-OE2	9.08	1.35	1.25
1	F	597	GLU	CG-CD	9.05	1.65	1.51
1	F	581	GLU	CB-CG	8.98	1.69	1.52
1	E	531	VAL	CB-CG1	8.44	1.70	1.52
1	C	468	GLU	CB-CG	8.17	1.67	1.52
1	D	468	GLU	CG-CD	8.07	1.64	1.51
1	F	597	GLU	CD-OE1	7.85	1.34	1.25
1	F	556	ALA	CA-CB	7.27	1.67	1.52
1	D	428	ARG	CB-CG	-7.19	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	502	TYR	CD2-CE2	7.09	1.50	1.39
1	B	542	GLU	CG-CD	6.93	1.62	1.51
1	D	597	GLU	CD-OE2	6.83	1.33	1.25
1	D	468	GLU	CD-OE2	6.73	1.33	1.25
1	C	474	VAL	CB-CG1	6.72	1.67	1.52
1	C	449	VAL	CB-CG1	6.67	1.66	1.52
1	D	468	GLU	CD-OE1	6.67	1.32	1.25
1	D	424	TYR	CD1-CE1	-6.59	1.29	1.39
1	A	429	VAL	CB-CG1	6.44	1.66	1.52
1	C	472	GLU	CG-CD	6.43	1.61	1.51
1	C	468	GLU	CG-CD	6.40	1.61	1.51
1	A	597	GLU	CG-CD	6.33	1.61	1.51
1	C	503	GLU	CG-CD	6.30	1.61	1.51
1	F	502	TYR	CD2-CE2	6.26	1.48	1.39
1	E	539	VAL	CB-CG2	-6.10	1.40	1.52
1	A	433	ALA	CA-CB	5.96	1.65	1.52
1	F	590	SER	CB-OG	-5.90	1.34	1.42
1	C	503	GLU	CB-CG	5.89	1.63	1.52
1	C	590	SER	CB-OG	-5.86	1.34	1.42
1	C	539	VAL	CB-CG2	5.80	1.65	1.52
1	E	542	GLU	CG-CD	5.78	1.60	1.51
1	D	437	GLU	CG-CD	5.62	1.60	1.51
1	A	496	ILE	CA-CB	5.51	1.67	1.54
1	D	521	ALA	CA-CB	5.48	1.64	1.52
1	D	551	GLN	CG-CD	5.47	1.63	1.51
1	F	472	GLU	CD-OE1	5.46	1.31	1.25
1	E	585	GLU	CG-CD	5.42	1.60	1.51
1	E	542	GLU	CB-CG	5.39	1.62	1.52
1	D	468	GLU	CB-CG	5.37	1.62	1.52
1	A	597	GLU	CD-OE1	5.34	1.31	1.25
1	B	425	GLU	CB-CG	5.30	1.62	1.52
1	D	578	ALA	C-O	5.24	1.33	1.23
1	A	424	TYR	CD1-CE1	-5.23	1.31	1.39
1	D	422	GLU	CB-CG	5.16	1.61	1.52
1	A	469	ILE	CB-CG2	-5.01	1.37	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	600	LEU	CB-CG-CD1	-8.91	95.86	111.00
1	C	446	ILE	CB-CA-C	-8.87	93.86	111.60
1	A	591	ARG	NE-CZ-NH1	8.35	124.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	597	GLU	OE1-CD-OE2	8.22	133.17	123.30
1	F	441	ILE	CB-CA-C	-7.51	96.58	111.60
1	E	471	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	C	465	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	A	591	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	C	597	GLU	CG-CD-OE1	-7.32	103.65	118.30
1	E	508	ASP	CB-CG-OD1	-7.04	111.97	118.30
1	C	428	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	A	471	ARG	CG-CD-NE	-6.80	97.51	111.80
1	E	418	LEU	CA-CB-CG	6.76	130.84	115.30
1	B	471	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	C	441	ILE	CG1-CB-CG2	6.63	125.99	111.40
1	F	608	ARG	CB-CA-C	6.62	123.65	110.40
1	D	428	ARG	CG-CD-NE	-6.62	97.90	111.80
1	A	446	ILE	CG1-CB-CG2	-6.56	96.97	111.40
1	F	446	ILE	CB-CA-C	-6.40	98.81	111.60
1	F	483	LYS	N-CA-C	6.24	127.83	111.00
1	D	591	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	C	488	ASP	CB-CG-OD1	6.11	123.80	118.30
1	F	590	SER	CB-CA-C	-6.08	98.55	110.10
1	C	441	ILE	CB-CA-C	-6.06	99.49	111.60
1	F	465	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	E	492	MET	CB-CG-SD	-6.02	94.33	112.40
1	C	486	GLY	N-CA-C	5.89	127.83	113.10
1	F	575	LEU	CA-CB-CG	5.83	128.71	115.30
1	F	476	ASN	CB-CA-C	5.75	121.91	110.40
1	C	465	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	496	ILE	CA-CB-CG1	5.65	121.73	111.00
1	E	471	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	F	581	GLU	C-N-CA	-5.63	110.48	122.30
1	A	568	LYS	CD-CE-NZ	5.60	124.57	111.70
1	B	465	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	C	590	SER	CB-CA-C	-5.58	99.49	110.10
1	D	465	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	445	ILE	CB-CA-C	-5.46	100.67	111.60
1	F	441	ILE	CG1-CB-CG2	5.39	123.26	111.40
1	A	471	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	D	539	VAL	CG1-CB-CG2	5.24	119.29	110.90
1	F	492	MET	CG-SD-CE	-5.18	91.91	100.20
1	F	577	ASP	CB-CG-OD1	5.16	122.94	118.30
1	C	418	LEU	CB-CG-CD1	5.06	119.61	111.00
1	B	492	MET	CB-CG-SD	-5.04	97.28	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	445	ILE	CB-CA-C	-5.04	101.52	111.60

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 [i](#)

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	85	0
1	C	1448	0	1510	128	1
1	D	1457	0	1523	68	2
1	E	1457	0	1523	54	0
1	F	1457	0	1523	93	1
2	A	89	0	0	25	0
2	B	65	0	0	17	0
2	C	121	0	0	36	1
2	D	106	0	0	22	0
2	E	67	0	0	17	0
2	F	104	0	0	23	0
All	All	9285	0	9125	485	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 27.

All (485) 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:CB	1:D:542:GLU:CG	1.77	1.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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:D:487:ARG:HG3	1:D:487:ARG:HH11	1.24	0.98
1:A:428:ARG:HD2	1:A:446:ILE:HB	1.44	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:F:597:GLU:HG3	1:F:610:MET:HE1	1.48	0.95
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:593:ASN:O	1:A:597:GLU:HG3	1.70	0.90
1:A:571:ILE:HD11	1:A:588:PRO:HB3	1.53	0.90
1:B:489:ILE:HG22	2:B:686:HOH:O	1.71	0.89
1:D:597:GLU:HG2	1:D:610:MET:CE	2.03	0.89
1:D:480:ILE:CD1	1:D:592:ILE:HG21	2.01	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:LEU:HD13	2:C:711:HOH:O	1.73	0.88
1:D:452:SER:O	1:D:453:MET:SD	2.32	0.88
1:D:597:GLU:HG2	1:D:610:MET:HE1	1.54	0.87
1:B:463:THR:HG23	2:C:657:HOH:O	1.74	0.87
1:E:422:GLU:HB3	2:E:673:HOH:O	1.75	0.86
1:C:465:ARG:CD	1:C:503:GLU:HG2	2.06	0.86
1:B:568:LYS:HE2	1:B:590:SER:HB2	1.58	0.86
1:C:445:ILE:N	1:C:445:ILE:HD13	1.90	0.86
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:C:463:THR:OG1	1:D:468:GLU:HG3	1.78	0.84
1:F:475:MET:C	1:F:476:ASN:O	2.15	0.83
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: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:579:GLU:CD	2:D:711:HOH:O	2.20	0.79
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:E:597:GLU:HG2	1:E:610:MET:HE1	1.64	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: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:C:481:ILE:HG21	1:C:489:ILE:HD11	1.65	0.77
1:A:608:ARG:HH11	1:A:608:ARG:HG3	1.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:489:ILE:HG21	1:D:522:ILE:HD13	1.69	0.74
1:C:428:ARG:HG3	2:C:740:HOH:O	1.86	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:D:583:LYS:HE2	2:D:630:HOH:O	1.88	0.73
1:A:608:ARG:CG	1:A:608:ARG:HH11	2.02	0.73
1:C:578:ALA:HA	1:C:581:GLU:CD	2.09	0.73
1:C:459:ARG:NH2	1:D:475:MET:HE1	2.02	0.73
1:C:502:TYR:HD1	2:C:726:HOH:O	1.53	0.72
1:C:477:VAL:HG22	1:C:477:VAL:O	1.87	0.72
1:A:501:THR:HG22	2:B:641:HOH:O	1.89	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: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
1:F:485:THR:OG1	1:F:486:GLY:N	2.21	0.70
2:A:637:HOH:O	1:F:501:THR:HG21	1.91	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:C:597:GLU:HG2	1:C:610:MET:CE	2.21	0.70
1:B:575:LEU:O	1:B:575:LEU:HG	1.92	0.70
1:C:485:THR:OG1	1:C:486:GLY:N	2.23	0.69
1:D:435:ILE:CG2	1:D:505:VAL:HG22	2.22	0.69
1:C:437:GLU:HA	1:C:437:GLU:OE1	1.91	0.69
1:C:463:THR:HG23	2:D:648:HOH:O	1.92	0.69
1:D:480:ILE:HD13	1:D:592:ILE:HG21	1.76	0.68
1:C:480:ILE:HG23	2:C:732:HOH:O	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:481:ILE:HG21	1:C:489:ILE:HD13	1.76	0.68
1:A:597:GLU:HG2	1:A:610:MET:CE	2.23	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
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:CG	1:A:487:ARG:HH11	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:F:435:ILE:HG22	1:F:505:VAL:CG2	2.18	0.66
1:B:422:GLU:HG3	1:B:423:GLY:H	1.59	0.66
1:F:477:VAL:HG23	1:F:480:ILE:HD13	1.78	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: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:C:578:ALA:O	1:C:579:GLU:HB2	1.97	0.64
1:F:581:GLU:O	1:F:581:GLU:HG2	1.97	0.64
1:B:449:VAL:HG12	1:B:494:VAL:HG22	1.79	0.64
1:F:422:GLU:HG3	2:F:638:HOH:O	1.96	0.64
1:F:478:SER:CB	1:F:489:ILE:HD12	2.23	0.64
1:B:611:SER:HA	1:B:614:LYS:HD3	1.77	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:F:577:ASP:HB2	1:F:578:ALA:O	1.98	0.64
1:A:453:MET:HB2	2:A:662:HOH:O	1.98	0.64
1:C:457:GLU:CA	1:C:457:GLU:OE1	2.32	0.63
1:F:477:VAL:HG22	1:F:481:ILE:HG13	1.80	0.63
1:F:446:ILE:CD1	1:F:497:GLN:HB2	2.29	0.63
1:E:418:LEU:HA	1:F:545:PRO:HG2	1.80	0.63
1:E:419:PHE:HA	1:E:428:ARG:NH2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ARG:HH11	1:A:459:ARG:CB	2.11	0.63
1:F:597:GLU:HB3	2:F:719:HOH:O	1.98	0.62
1:D:487:ARG:NH1	1:D:487:ARG:HG3	2.04	0.62
1:D:579:GLU:CG	2:D:711:HOH:O	2.48	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:465:ARG:HD2	1:C:503:GLU:CD	2.20	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:A:597:GLU:HG2	1:A:610:MET:HE1	1.83	0.60
1:D:428:ARG:NE	2:D:713:HOH:O	2.28	0.60
1:C:465:ARG:HD2	1:C:503:GLU:OE2	2.01	0.60
1:A:435:ILE:HG23	1:A:505:VAL:HG22	1.81	0.60
1:E:471:ARG:CZ	2:E:677:HOH:O	2.49	0.60
1:C:463:THR:OG1	1:D:468:GLU:CG	2.49	0.60
1:E:597:GLU:HG2	1:E:610:MET:HE2	1.83	0.60
1:C:477:VAL:CG2	1:C:477:VAL:O	2.49	0.60
1:C:477:VAL:HG22	1:C:481:ILE:HG13	1.85	0.59
1:F:608:ARG:HE	1:F:612:LYS:HZ1	1.47	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:F:435:ILE:CG2	1:F:441:ILE:HG12	2.28	0.59
1:C:438:SER:CA	1:C:551:GLN:OE1	2.51	0.59
1:F:478:SER:HB2	1:F:489:ILE:CD1	2.28	0.59
1:E:591:ARG:CB	2:E:680:HOH:O	2.32	0.59
1:A:593:ASN:O	1:A:597:GLU:CG	2.49	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:F:578:ALA:O	1:F:579:GLU:HB2	2.03	0.58
1:D:545:PRO:HA	1:D:567:PRO:HG2	1.84	0.58
1:B:461:ILE:CG2	1:C:475:MET:HG2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:435:ILE:HD13	1:D:441:ILE:CG2	2.34	0.58
1:C:461:ILE:HD13	1:D:475:MET:SD	2.43	0.58
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:F:480:ILE:HD13	1:F:537:LEU:HD21	1.87	0.57
1:A:488:ASP:OD2	1:A:490:SER:HB2	2.03	0.57
1:F:562:LYS:HE2	2:F:638:HOH:O	2.04	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:B:435:ILE:CG2	1:B:505:VAL:HG22	2.35	0.57
1:F:608:ARG:HE	1:F:612:LYS:HZ2	1.48	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:B:492:MET:HE2	1:B:492:MET:CA	2.34	0.56
1:C:480:ILE:CD1	1:C:592:ILE:HG21	2.35	0.56
1:A:452:SER:O	1:A:453:MET:CB	2.53	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:A:610:MET:HE3	2:A:664:HOH:O	2.06	0.56
1:B:568:LYS:HG3	1:B:589:VAL:O	2.06	0.56
1:A:597:GLU:HB2	2:A:622:HOH:O	2.06	0.55
1:A:550:THR:HG23	2:A:685: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: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:F:578:ALA:HA	1:F:581:GLU:OE1	2.08	0.54
1:D:478:SER:HB2	2:D:722:HOH:O	2.07	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:C:475:MET:HE3	2:C:703:HOH:O	2.07	0.54
1:A:470:ALA:O	1:A:474:VAL:HG23	2.07	0.54
1:D:597:GLU:HG2	1:D:610:MET:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:451:PRO:HD3	2:E:667:HOH:O	2.08	0.54
1:C:424:TYR:HB3	1:C:526:PRO:HB2	1.90	0.54
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:487:ARG:CG	1:A:487:ARG:NH1	2.55	0.53
1:A:417:LYS:N	1:B:569:ASP:O	2.41	0.53
1:A:613:PHE:HB2	2:A:664:HOH:O	2.06	0.53
1:A:540:LYS:HD2	2:A:705:HOH:O	2.08	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:D:578:ALA:O	1:D:579:GLU:HB3	2.09	0.53
1:C:459:ARG:HH22	1:D:475:MET:HE1	1.72	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: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: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:481:ILE:CG2	1:C:489:ILE:CD1	2.83	0.51
1:C:428:ARG:CG	2:C:740:HOH:O	2.53	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:F:446:ILE:HD11	1:F:497:GLN:HB2	1.92	0.51
1:B:451:PRO:O	1:B:453:MET:N	2.29	0.51
1:F:597:GLU:CG	1:F:610:MET:CE	2.86	0.51
1:D:597:GLU:HG3	2:D:640:HOH:O	2.10	0.51
1:D:579:GLU:HG2	2:D:711:HOH:O	2.08	0.51
1:C:445:ILE:HG23	1:C:498:PHE:CD1	2.46	0.51
1:C:611:SER:O	1:C:614:LYS:CE	2.51	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:479:ALA:HB3	2:C:720:HOH:O	2.11	0.51
1:F:445:ILE:HD12	1:F:514:ILE:HG13	1.92	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:448:GLU:CG	2:E:683:HOH:O	2.60	0.50
1:A:545:PRO:HG2	1:F:499:VAL:HG12	1.93	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:597:GLU:HG2	1:A:610:MET:HE2	1.94	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:A:448:GLU:HB3	1:B:540:LYS:HZ1	1.76	0.50
1:E:478:SER:O	1:E:482:LYS:HE2	2.11	0.50
1:B:422:GLU:CG	1:B:423:GLY:H	2.25	0.50
1:A:539:VAL:HG12	2:F:723:HOH:O	2.12	0.50
1:C:445:ILE:N	1:C:445:ILE:CD1	2.67	0.50
1:C:501:THR:CG2	2:D:668:HOH:O	2.54	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
1:F:578:ALA:C	1:F:579:GLU:O	2.50	0.49
2:A:648:HOH:O	1:F:418:LEU:HD22	2.08	0.49
1:C:597:GLU:CG	1:C:610:MET:CE	2.90	0.49
1:E:435:ILE:O	1:E:436:GLY:C	2.51	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:F:477:VAL:HG13	1:F:481:ILE:HD12	1.94	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:F:435:ILE:HG23	1:F:441:ILE:CG1	2.35	0.48
1:D:487:ARG:NH1	1:D:487:ARG:CG	2.66	0.48
1:B:482:LYS:HG2	1:B:487:ARG:O	2.13	0.48
1:E:478:SER:OG	1:E:489:ILE:HD11	2.13	0.48
1:B:452:SER:C	2:B:666:HOH:O	2.50	0.48
1:C:472:GLU:CD	2:C:640:HOH:O	2.52	0.48
1:E:424:TYR:HB3	1:E:526:PRO:HB2	1.95	0.48
1:B:592:ILE:O	1:B:595:VAL:HB	2.13	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:F:514:ILE:O	1:F:518:VAL:HG23	2.12	0.48
1:B:422:GLU:CG	1:B:423:GLY:N	2.77	0.48
1:E:417:LYS:N	1:E:417:LYS:HD3	2.28	0.48
1:C:597:GLU:HG2	1:C:610:MET:HE2	1.92	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:B:489:ILE:HG23	2:B:681:HOH:O	2.13	0.47
1:D:489:ILE:HG21	1:D:522:ILE:HD11	1.94	0.47
1:B:422:GLU:O	1:B:529:GLN:HB2	2.14	0.47
1:E:545:PRO:HA	1:E:567:PRO:HG2	1.95	0.47
1:A:537:LEU:HD11	1:A:541:GLY:HA2	1.95	0.47
1:B:482:LYS:HG2	1:B:488:ASP:HA	1.95	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:C:577:ASP:OD1	1:C:577:ASP:N	2.43	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:F:480:ILE:CD1	1:F:537:LEU:HD21	2.45	0.47
1:D:480:ILE:HD11	1:D:592:ILE:CG2	2.39	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: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:C:465:ARG:CG	1:C:503:GLU:HG2	2.44	0.47
1:B:568:LYS:HE2	1:B:590:SER:CA	2.44	0.47
1:D:442:VAL:HG12	1:D:444:PRO:HD3	1.97	0.47
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:C:578:ALA:HA	1:C:581:GLU:OE2	2.15	0.46
1:A:446:ILE:HD11	2:A:647:HOH:O	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:F:577:ASP:O	1:F:579:GLU:O	2.33	0.46
1:F:422:GLU:CG	2:F:690:HOH:O	2.61	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:B:551:GLN:H	1:B:551:GLN:CD	2.19	0.46
1:A:488:ASP:HB3	1:A:491:ASN:ND2	2.31	0.46
1:C:489:ILE:CD1	1:C:492:MET:HE1	2.46	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:614:LYS:HD2	2:F:717:HOH:O	2.17	0.45
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:A:568:LYS:CE	1:A:590:SER:HB3	2.46	0.45
1:A:459:ARG:HG2	1:A:459:ARG:H	1.56	0.45
1:E:475:MET:HB2	1:E:475:MET:HE2	1.71	0.45
1:B:429:VAL:HG22	1:B:527:VAL:HG11	1.99	0.45
1:B:488:ASP:OD2	1:B:490:SER:HB2	2.17	0.45
1:F:579:GLU:CB	1:F:580:HIS:ND1	2.75	0.45
1:D:460:VAL:CG2	1:D:474:VAL:HG11	2.47	0.45
1:E:591:ARG:CD	2:E:680:HOH:O	2.64	0.45
1:B:502:TYR:CB	1:B:505:VAL:CG2	2.95	0.45
1:B:450:THR:O	1:B:492:MET:HB3	2.16	0.45
1:B:448:GLU:O	1:B:448:GLU:HG3	2.16	0.45
1:E:450:THR:HG23	1:E:493:ASP:HB2	1.99	0.45
1:C:597:GLU:HG2	1:C:610:MET:HE1	1.99	0.44
1:B:562:LYS:CA	1:B:562:LYS:HE2	2.47	0.44
1:B:489:ILE:HD12	2:B:639:HOH:O	2.17	0.44
1:D:551:GLN:CD	1:D:551:GLN:H	2.20	0.44
1:B:568:LYS:HE3	2:B:626:HOH:O	2.18	0.44
1:E:591:ARG:HG2	2:E:680:HOH:O	2.11	0.44
1:B:502:TYR:HB2	1:B:505:VAL:HG23	2.00	0.44
1:C:468:GLU:HG3	2:C:662:HOH:O	2.17	0.44
1:F:445:ILE:HB	2:F:713:HOH:O	2.18	0.44
1:D:471:ARG:NE	2:D:719:HOH:O	1.90	0.44
1:D:480:ILE:CD1	1:D:592:ILE:CG2	2.86	0.44
1:C:465:ARG:CD	1:C:503:GLU:OE2	2.65	0.44
1:D:557:ILE:HG21	1:D:583:LYS:HE3	1.99	0.44
1:F:604:LYS:HZ2	1:F:604:LYS:HB2	1.81	0.44
1:D:509:SER:O	1:D:510:ALA:C	2.56	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:E:591:ARG:HD3	2:E:639:HOH:O	2.17	0.43
1:C:591:ARG:HG2	2:C:660:HOH:O	2.19	0.43
1:C:446:ILE:H	1:C:446:ILE:HD13	1.83	0.43
1:A:576:LEU:HD23	2:A:685:HOH:O	2.18	0.43
1:F:535:GLY:HA2	1:F:546:VAL:CG1	2.48	0.43
1:B:424:TYR:CD1	1:B:601:GLU:HB2	2.53	0.43
1:B:480:ILE:HA	1:B:483:LYS:HG2	1.99	0.43
1:D:441:ILE:HD11	1:D:505:VAL:HG21	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:419:PHE:HA	1:E:428:ARG:HH22	1.80	0.43
1:C:446:ILE:HD13	1:C:446:ILE:N	2.33	0.43
1:B:523:GLU:OE2	1:B:609:LEU:HD13	2.18	0.43
1:A:429:VAL:HG22	1:A:527:VAL:HG11	2.00	0.43
1:B:419:PHE:CE1	1:B:559:ALA:HB1	2.54	0.43
1:C:476:ASN:HB2	2:C:659:HOH:O	2.18	0.43
1:A:532:ALA:HB2	1:A:561:LEU:HD13	2.00	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:CG2	1:F:477:VAL:O	2.67	0.43
1:C:597:GLU:CG	1:C:610:MET:HE2	2.48	0.43
1:B:560:GLY:O	1:B:562:LYS:HE3	2.18	0.43
1:B:424:TYR:HB3	1:B:526:PRO:CB	2.49	0.43
1:F:477:VAL:N	2:F:647:HOH:O	2.52	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:537:LEU:HD23	2:F:647:HOH:O	2.19	0.42
1:F:532:ALA:HB2	1:F:561:LEU:HD13	2.01	0.42
1:C:463:THR:HG1	1:D:468:GLU:HG3	1.83	0.42
1:B:505:VAL:HB	2:B:671:HOH:O	2.18	0.42
1:A:482:LYS:CG	1:A:488:ASP:HA	2.49	0.42
1:E:418:LEU:HD23	1:F:544:LEU:HB3	2.01	0.42
1:B:576:LEU:HD22	1:B:580:HIS:HB2	2.01	0.42
1:F:604:LYS:NZ	1:F:604:LYS:HB2	2.34	0.42
1:B:502:TYR:HB2	1:B:505:VAL:HG21	2.02	0.42
1:B:460:VAL:HG21	1:B:474:VAL:HG11	2.00	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:D:428:ARG:NH2	2:D:713:HOH:O	2.51	0.42
1:C:534:THR:O	1:C:567:PRO:HD3	2.19	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
1:B:449:VAL:HG23	1:B:449:VAL:O	2.19	0.42
1:A:578:ALA:N	2:A:657:HOH:O	2.53	0.42
1:A:487:ARG:CD	2:A:710:HOH:O	2.58	0.42
1:C:465:ARG:HG3	1:C:503:GLU:HG2	2.01	0.42
1:C:463:THR:CG2	1:D:469:ILE:CD1	2.98	0.42
1:B:492:MET:HB2	1:B:492:MET:HE3	1.40	0.42
1:E:450:THR:CG2	1:E:493:ASP:HB2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG23	1:A:485:THR:O	2.19	0.41
1:A:594:GLU:HA	1:A:597:GLU:HG3	2.01	0.41
1:C:477:VAL:HG23	1:C:480:ILE:HG12	2.01	0.41
1:B:606:LYS:O	1:B:610:MET:HG2	2.19	0.41
1:E:606:LYS:O	1:E:610:MET:HG2	2.20	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:A:427:GLY:O	1:A:446:ILE:HA	2.21	0.41
1:F:446:ILE:HD12	1:F:497:GLN:HB2	2.00	0.41
1:B:562:LYS:HA	1:B:562:LYS:HE2	2.02	0.41
1:C:532:ALA:HB2	1:C:561:LEU:HD13	2.03	0.41
1:A:443:LEU:HD21	1:A:466:LEU:HD13	2.03	0.41
1:D:469:ILE:HA	1:D:469:ILE:HD12	1.90	0.41
1:E:554:GLU:HG2	1:E:580:HIS:CE1	2.56	0.41
1:D:611:SER:O	1:D:614:LYS:HD2	2.21	0.41
1:E:577:ASP:O	1:E:581:GLU:HB2	2.21	0.41
1:F:511:SER:HB3	1:F:514:ILE:HD12	2.03	0.41
1:C:612:LYS:NZ	2:C:729:HOH:O	2.53	0.41
1:B:424:TYR:HB3	1:B:526:PRO:HB2	2.03	0.40
1:B:448:GLU:CD	1:C:483:LYS:HE2	2.41	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:HD13	1:A:446:ILE:O	2.20	0.40
1:B:469:ILE:HG12	1:B:469:ILE:H	1.63	0.40
2:A:642:HOH:O	1:F:501:THR:HB	2.20	0.40
1:E:450:THR:HA	1:E:451:PRO:HD2	1.90	0.40
1:B:470:ALA:O	1:B:474:VAL:HG23	2.22	0.40
1:E:461:ILE:HD12	1:E:495:HIS:NE2	2.36	0.40
1:C:553:ILE:HG12	1:C:564:VAL:HG11	2.02	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	191/205 (93%)	183 (96%)	8 (4%)	0	100	100
1	B	191/205 (93%)	181 (95%)	5 (3%)	5 (3%)	7	1
1	C	190/205 (93%)	179 (94%)	5 (3%)	6 (3%)	5	0
1	D	191/205 (93%)	183 (96%)	6 (3%)	2 (1%)	19	8
1	E	191/205 (93%)	181 (95%)	9 (5%)	1 (0%)	34	22
1	F	191/205 (93%)	177 (93%)	6 (3%)	8 (4%)	3	0
All	All	1145/1230 (93%)	1084 (95%)	39 (3%)	22 (2%)	10	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
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

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Mol	Chain	Res	Type
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%)	142 (89%)	18 (11%)	7	2
1	B	160/168 (95%)	140 (88%)	20 (12%)	6	1
1	C	159/168 (95%)	131 (82%)	28 (18%)	2	0
1	D	160/168 (95%)	139 (87%)	21 (13%)	5	1
1	E	160/168 (95%)	138 (86%)	22 (14%)	4	1
1	F	160/168 (95%)	135 (84%)	25 (16%)	3	1
All	All	959/1008 (95%)	825 (86%)	134 (14%)	4	1

All (134) residues with a non-rotameric sidechain are listed below:

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

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Mol	Chain	Res	Type
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	568	LYS
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
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	483	LYS
1	C	484	TYR
1	C	490	SER

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Mol	Chain	Res	Type
1	C	501	THR
1	C	508	ASP
1	C	538	SER
1	C	580	HIS
1	C	581	GLU
1	C	591	ARG
1	C	597	GLU
1	C	608	ARG
1	D	417	LYS
1	D	418	LEU
1	D	428	ARG
1	D	445	ILE
1	D	453	MET
1	D	465	ARG
1	D	469	ILE
1	D	475	MET
1	D	477	VAL
1	D	480	ILE
1	D	482	LYS
1	D	487	ARG
1	D	509	SER
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
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	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

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Mol	Chain	Res	Type
1	E	503	GLU
1	E	505	VAL
1	E	539	VAL
1	E	558	GLN
1	E	575	LEU
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	441	ILE
1	F	445	ILE
1	F	446	ILE
1	F	472	GLU
1	F	475	MET
1	F	480	ILE
1	F	485	THR
1	F	487	ARG
1	F	489	ILE
1	F	490	SER
1	F	501	THR
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	580	HIS
1	F	581	GLU
1	F	608	ARG
1	F	611	SER
1	F	614	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	491	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	195/205 (95%)	0.35	8 (4%) 41 47	26, 33, 52, 60	0
1	B	195/205 (95%)	0.98	32 (16%) 2 2	29, 39, 60, 78	0
1	C	194/205 (94%)	0.23	10 (5%) 31 36	23, 30, 54, 65	0
1	D	195/205 (95%)	0.16	9 (4%) 36 41	24, 31, 48, 60	0
1	E	195/205 (95%)	0.95	28 (14%) 3 3	30, 38, 57, 77	0
1	F	195/205 (95%)	0.39	14 (7%) 18 22	26, 33, 56, 60	0
All	All	1169/1230 (95%)	0.51	101 (8%) 13 14	23, 35, 56, 78	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	419	PHE	9.1
1	E	418	LEU	8.5
1	E	502	TYR	7.6
1	E	501	THR	7.3
1	E	578	ALA	6.9
1	C	578	ALA	6.6
1	B	420	ILE	6.5
1	B	418	LEU	6.5
1	B	501	THR	6.3
1	E	436	GLY	6.3
1	C	484	TYR	6.3
1	B	419	PHE	6.1
1	B	438	SER	6.1
1	D	453	MET	5.6
1	C	483	LYS	5.6
1	B	421	THR	5.5
1	F	453	MET	5.5
1	B	453	MET	5.4
1	C	453	MET	5.4

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Mol	Chain	Res	Type	RSRZ
1	E	437	GLU	5.2
1	B	437	GLU	4.7
1	A	577	ASP	4.6
1	D	437	GLU	4.6
1	B	614	LYS	4.6
1	B	502	TYR	4.5
1	A	578	ALA	4.4
1	A	486	GLY	4.4
1	B	436	GLY	4.3
1	C	485	THR	4.2
1	B	575	LEU	4.2
1	E	417	LYS	4.2
1	E	575	LEU	4.2
1	B	422	GLU	4.0
1	F	578	ALA	3.9
1	F	614	LYS	3.8
1	A	437	GLU	3.7
1	E	457	GLU	3.5
1	B	491	ASN	3.5
1	B	483	LYS	3.4
1	B	482	LYS	3.4
1	F	438	SER	3.4
1	E	421	THR	3.4
1	B	452	SER	3.4
1	F	484	TYR	3.4
1	E	614	LYS	3.3
1	C	614	LYS	3.3
1	B	578	ALA	3.3
1	B	543	VAL	3.1
1	F	485	THR	3.0
1	A	436	GLY	2.9
1	B	591	ARG	2.9
1	F	577	ASP	2.9
1	F	437	GLU	2.9
1	D	436	GLY	2.9
1	E	452	SER	2.8
1	A	575	LEU	2.8
1	E	558	GLN	2.8
1	C	579	GLU	2.8
1	F	452	SER	2.8
1	C	437	GLU	2.8
1	F	496	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	580	HIS	2.7
1	D	575	LEU	2.6
1	E	600	LEU	2.6
1	C	438	SER	2.6
1	E	611	SER	2.6
1	E	572	ASP	2.6
1	B	503	GLU	2.6
1	F	483	LYS	2.6
1	F	579	GLU	2.6
1	E	458	GLY	2.6
1	E	483	LYS	2.6
1	E	420	ILE	2.6
1	E	543	VAL	2.6
1	F	487	ARG	2.5
1	B	439	ALA	2.5
1	E	422	GLU	2.5
1	B	579	GLU	2.4
1	B	580	HIS	2.4
1	B	480	ILE	2.4
1	C	608	ARG	2.4
1	D	578	ALA	2.3
1	B	608	ARG	2.3
1	F	608	ARG	2.3
1	D	486	GLY	2.2
1	D	577	ASP	2.2
1	A	576	LEU	2.2
1	B	609	LEU	2.2
1	B	417	LYS	2.2
1	B	553	ILE	2.2
1	E	465	ARG	2.1
1	B	568	LYS	2.1
1	B	435	ILE	2.1
1	D	435	ILE	2.1
1	E	607	ASN	2.1
1	E	453	MET	2.1
1	E	609	LEU	2.0
1	E	496	ILE	2.0
1	E	579	GLU	2.0
1	D	608	ARG	2.0
1	B	572	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.