Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:33 pm BST

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
https://www.wwpdb.org/validation/2017/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:

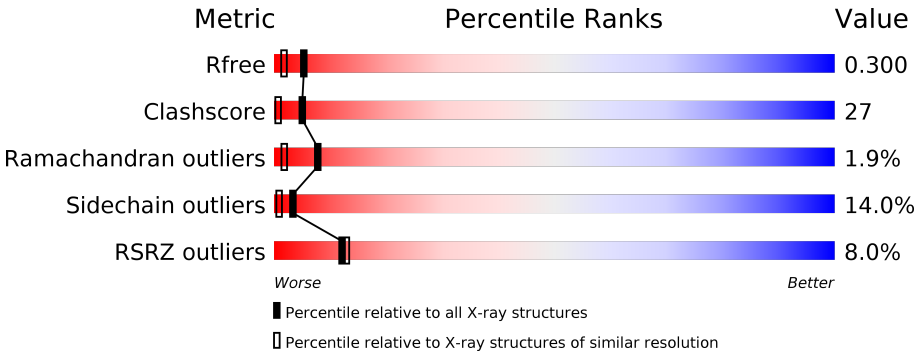
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.05 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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (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 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 <=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	4% 62% 24% 8% • 5%
1	B	205	15% 54% 33% 6% • 5%
1	C	205	5% 49% 32% 9% 5% 5%
1	D	205	3% 64% 21% 8% • 5%
1	E	205	12% 62% 26% 6% 5%
1	F	205	7% 58% 24% 8% 5% 5%

2 Entry composition (i)

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.

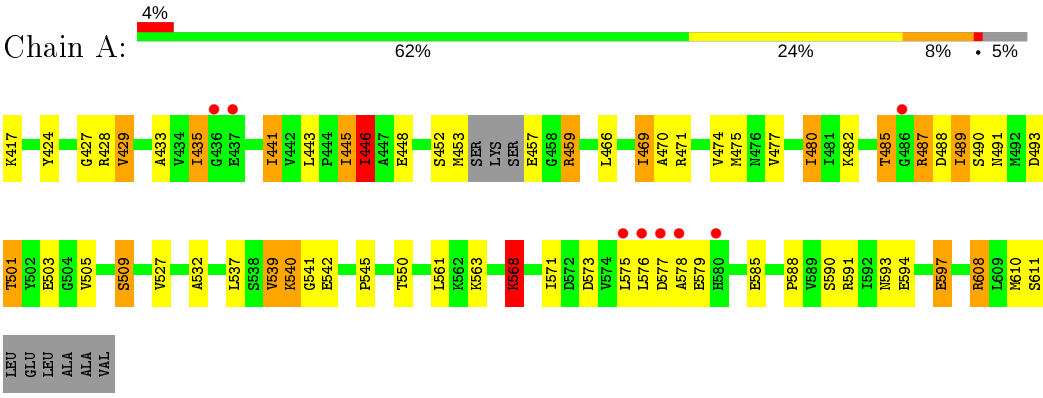
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	89	Total	O	0	0
			89	89		
2	B	65	Total	O	0	0
			65	65		
2	C	121	Total	O	0	0
			121	121		
2	D	106	Total	O	0	0
			106	106		
2	E	67	Total	O	0	0
			67	67		
2	F	104	Total	O	0	0
			104	104		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

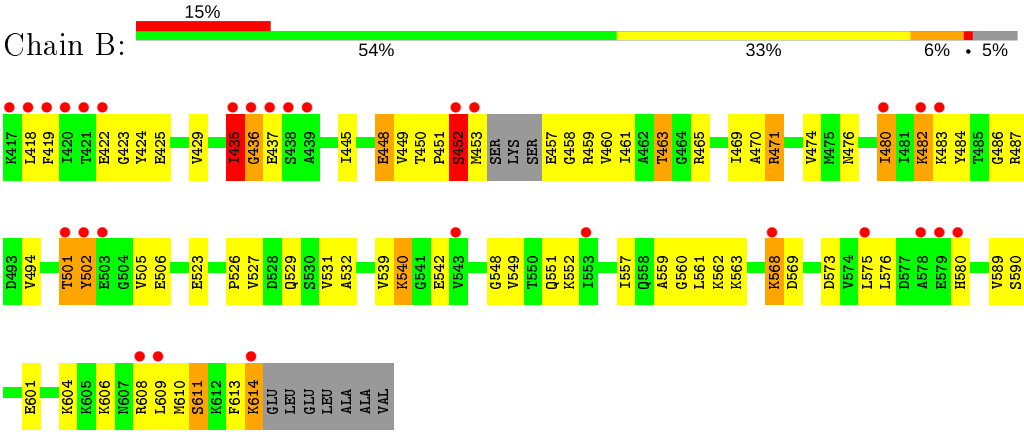
• Molecule 1: Putative protease La homolog type

Chain A:



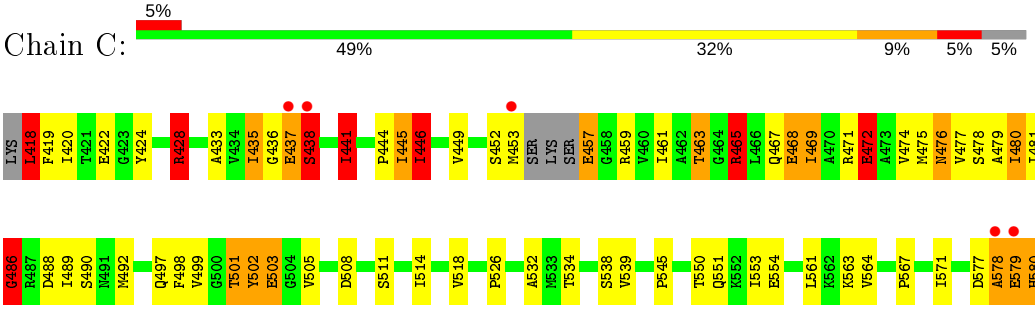
• Molecule 1: Putative protease La homolog type

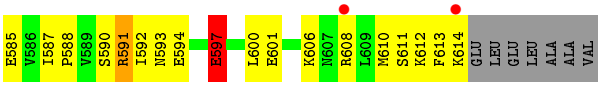
Chain B:



• Molecule 1: Putative protease La homolog type

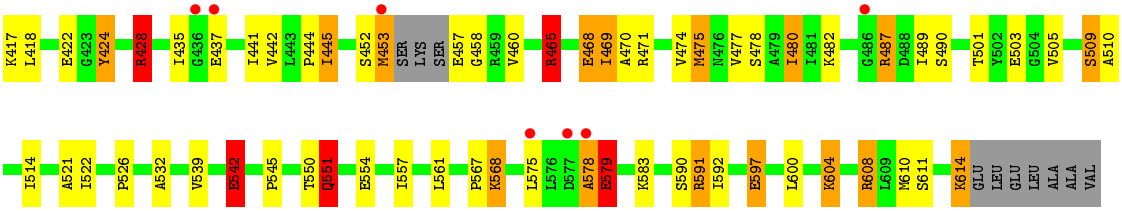
Chain C:





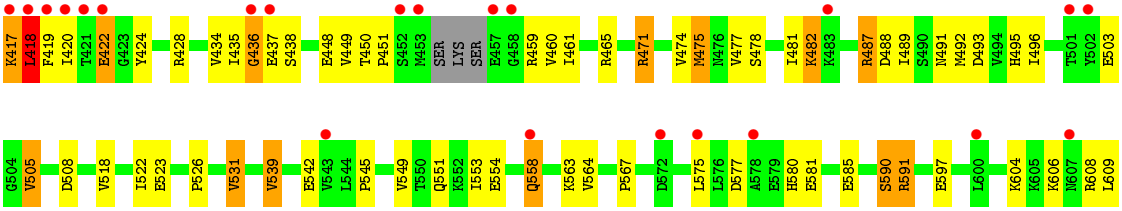
• Molecule 1: Putative protease La homolog type

Chain D:



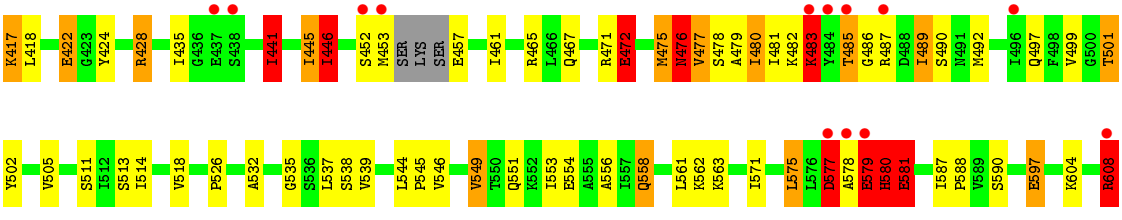
• Molecule 1: Putative protease La homolog type

Chain E:



• Molecule 1: Putative protease La homolog type

Chain F:



4 Data and refinement statistics (i)

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 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
$< I/\sigma(I) >$ [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)	0.35 , 54.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.35	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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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: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: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: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: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:D:597:GLU:HG2	1:D:610:MET:CE	2.03	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:B:463:THR:HG23	2:C:657:HOH:O	1.74	0.87
1:D:597:GLU:HG2	1:D:610:MET:HE1	1.54	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: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:A:608:ARG:HH11	1:A:608:ARG:HG3	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

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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: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:CG	1:A:608:ARG:HH11	2.02	0.73
1:D:583:LYS:HE2	2:D:630:HOH:O	1.88	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:A:501:THR:HG22	2:B:641:HOH:O	1.89	0.72
1:C:477:VAL:HG22	1:C:477:VAL:O	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: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:C:437:GLU:HA	1:C:437:GLU:OE1	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: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

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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: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: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: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: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: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:479:ALA:HB1	1:C:483:LYS:HG2	1.81	0.61
1:C:465:ARG:HD2	1:C:503:GLU:CD	2.20	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: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: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:D:579:GLU:OE1	2:D:711:HOH:O	2.16	0.59
1:F:608:ARG:HE	1:F:612:LYS:HZ1	1.47	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:F:578:ALA:O	1:F:579:GLU:HB2	2.03	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: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: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:B:492:MET:HE2	1:B:492:MET:CA	2.34	0.56
1:C:480:ILE:HG21	2:C:732:HOH:O	1.98	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: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: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: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: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:417:LYS:N	1:B:569:ASP:O	2.41	0.53
1:A:487:ARG:CG	1:A:487:ARG:NH1	2.55	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:C:459:ARG:HH22	1:D:475:MET:HE1	1.72	0.53
1:D:578:ALA:O	1:D:579:GLU:HB3	2.09	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: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:F:597:GLU:CG	1:F:610:MET:CE	2.86	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:C:479:ALA:HB3	2:C:720:HOH:O	2.11	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
2:A:648:HOH:O	1:F:418:LEU:HD22	2.08	0.49
1:F:578:ALA:C	1:F:579:GLU:O	2.50	0.49
1:C:597:GLU:CG	1:C:610:MET:CE	2.90	0.49
1:B:460:VAL:CG2	1:B:474:VAL:HG11	2.42	0.49
1:E:435:ILE:O	1:E:436:GLY:C	2.51	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:F:477:VAL:HG13	1:F:481:ILE:HD12	1.94	0.49
1:B:452:SER:C	2:B:666:HOH:O	2.50	0.48
1:B:482:LYS:HG2	1:B:487:ARG:O	2.13	0.48
1:D:487:ARG:NH1	1:D:487:ARG:CG	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:C:472:GLU:CD	2:C:640:HOH:O	2.52	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: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:F:514:ILE:O	1:F:518:VAL:HG23	2.12	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:B:489:ILE:HG23	2:B:681:HOH:O	2.13	0.47
1:B:422:GLU:O	1:B:529:GLN:HB2	2.14	0.47
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:A:452:SER:O	1:A:453:MET:HB2	2.13	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
2:A:637:HOH:O	1:F:501:THR:CG2	2.57	0.47
1:B:480:ILE:HD12	1:B:484:TYR:HD2	1.80	0.47
1:F:480:ILE:CD1	1:F:537:LEU:HD21	2.45	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: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: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: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: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:B:551:GLN:H	1:B:551:GLN:CD	2.19	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: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: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:E:475:MET:HE2	1:E:475:MET:HB2	1.71	0.45
1:B:488:ASP:OD2	1:B:490:SER:HB2	2.17	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: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:B:562:LYS:CA	1:B:562:LYS:HE2	2.47	0.44
1:C:597:GLU:HG2	1:C:610:MET:HE1	1.99	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:D:551:GLN:CD	1:D:551:GLN:H	2.20	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: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:D:480:ILE:CD1	1:D:592:ILE:CG2	2.86	0.44
1:D:509:SER:O	1:D:510:ALA:C	2.56	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:B:576:LEU:HD13	1:B:580:HIS:O	2.18	0.44
1:B:557:ILE:HD13	1:B:580:HIS:HB3	1.99	0.44
1:A:509:SER:HB3	1:F:497:GLN:OE1	2.17	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:H	1:C:446:ILE:HD13	1.83	0.43
1:C:591:ARG:HG2	2:C:660:HOH:O	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:597:GLU:CG	1:C:610:MET:HE2	2.48	0.43
1:F:477:VAL:CG2	1:F:477:VAL:O	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:C:463:THR:HG1	1:D:468:GLU:HG3	1.83	0.42
1:E:418:LEU:HD23	1:F:544:LEU:HB3	2.01	0.42
1:F:604:LYS:NZ	1:F:604:LYS:HB2	2.34	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:E:448:GLU:HB3	1:F:539:VAL:HG23	2.02	0.42
1:E:564:VAL:HG13	1:E:564:VAL:O	2.19	0.42
1:A:573:ASP:OD2	1:F:417:LYS:N	2.52	0.42
1:A:578:ALA:N	2:A:657:HOH:O	2.53	0.42
1:B:449:VAL:HG23	1:B:449:VAL:O	2.19	0.42
1:A:487:ARG:CD	2:A:710:HOH:O	2.58	0.42
1:B:492:MET:HB2	1:B:492:MET:HE3	1.40	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: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: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: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: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
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
2:A:642:HOH:O	1:F:501:THR:HB	2.20	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%)	5 1
1	C	190/205 (93%)	179 (94%)	5 (3%)	6 (3%)	4 0
1	D	191/205 (93%)	183 (96%)	6 (3%)	2 (1%)	15 6
1	E	191/205 (93%)	181 (95%)	9 (5%)	1 (0%)	29 18
1	F	191/205 (93%)	177 (93%)	6 (3%)	8 (4%)	3 0
All	All	1145/1230 (93%)	1084 (95%)	39 (3%)	22 (2%)	8 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 (i)

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

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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, 95^{th} 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%)	0.29	8 (4%) 37 40	26, 33, 52, 60	0
1	B	195/205 (95%)	0.91	31 (15%) 1 1	29, 39, 60, 78	0
1	C	194/205 (94%)	0.18	10 (5%) 27 29	23, 30, 54, 65	0
1	D	195/205 (95%)	0.10	7 (3%) 42 46	24, 31, 48, 60	0
1	E	195/205 (95%)	0.88	24 (12%) 4 3	30, 38, 57, 77	0
1	F	195/205 (95%)	0.33	14 (7%) 15 17	26, 33, 56, 60	0
All	All	1169/1230 (95%)	0.45	94 (8%) 12 13	23, 35, 56, 78	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	419	PHE	8.7
1	E	418	LEU	8.3
1	E	502	TYR	7.5
1	E	501	THR	7.1
1	E	578	ALA	6.8
1	C	578	ALA	6.4
1	B	420	ILE	6.3
1	B	418	LEU	6.3
1	B	501	THR	6.1
1	C	484	TYR	6.1
1	E	436	GLY	6.1
1	B	438	SER	5.9
1	B	419	PHE	5.9
1	C	483	LYS	5.5
1	D	453	MET	5.5
1	B	421	THR	5.4
1	B	453	MET	5.4
1	F	453	MET	5.3
1	C	453	MET	5.2

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Mol	Chain	Res	Type	RSRZ
1	E	437	GLU	5.1
1	B	437	GLU	4.6
1	D	437	GLU	4.5
1	A	577	ASP	4.5
1	B	614	LYS	4.4
1	B	502	TYR	4.4
1	B	436	GLY	4.3
1	A	486	GLY	4.2
1	A	578	ALA	4.1
1	E	417	LYS	4.0
1	C	485	THR	4.0
1	B	575	LEU	4.0
1	B	422	GLU	3.9
1	E	575	LEU	3.9
1	F	578	ALA	3.8
1	F	614	LYS	3.7
1	A	437	GLU	3.6
1	E	457	GLU	3.4
1	B	491	ASN	3.4
1	B	482	LYS	3.3
1	B	452	SER	3.3
1	F	438	SER	3.3
1	E	421	THR	3.2
1	F	484	TYR	3.2
1	B	483	LYS	3.2
1	B	578	ALA	3.2
1	E	614	LYS	3.1
1	C	614	LYS	3.1
1	F	485	THR	2.9
1	B	543	VAL	2.9
1	B	591	ARG	2.8
1	A	436	GLY	2.8
1	F	437	GLU	2.8
1	F	577	ASP	2.7
1	E	452	SER	2.7
1	A	575	LEU	2.7
1	D	436	GLY	2.7
1	C	437	GLU	2.7
1	E	558	GLN	2.7
1	C	579	GLU	2.7
1	F	452	SER	2.7
1	A	580	HIS	2.6

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.