



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:08 AM UTC

PDB ID : 2X36 / pdb_00002x36
Title : Structure of the proteolytic domain of the Human Mitochondrial Lon protease
Authors : Garcia, J.; Ondrovicova, G.; Blagova, E.; Levnikov, V.M.; Bauer, J.A.; Kutejova, E.; Wilkinson, A.J.; Wilson, K.S.
Deposited on : 2010-01-21
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

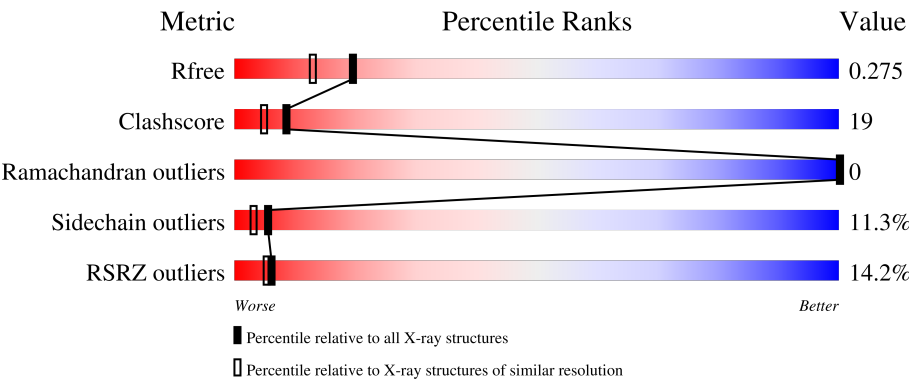
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	207	9% 47%38%6%8%
1	B	207	22% 52%25%8%13%
1	C	207	9% 52%37%7%
1	D	207	12% 51%29%6%14%
1	E	207	11% 51%29%8%13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	207	13% 52% 29% 5% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8705 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 LON PROTEASE HOMOLOG, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1440	918	243	270	9			
1	B	180	Total	C	N	O	S	21	1	0
			1365	876	229	251	9			
1	C	192	Total	C	N	O	S	0	2	0
			1475	939	253	274	9			
1	D	178	Total	C	N	O	S	0	2	0
			1358	868	231	251	8			
1	E	181	Total	C	N	O	S	0	1	0
			1374	878	235	253	8			
1	F	179	Total	C	N	O	S	2	2	0
			1363	873	233	249	8			

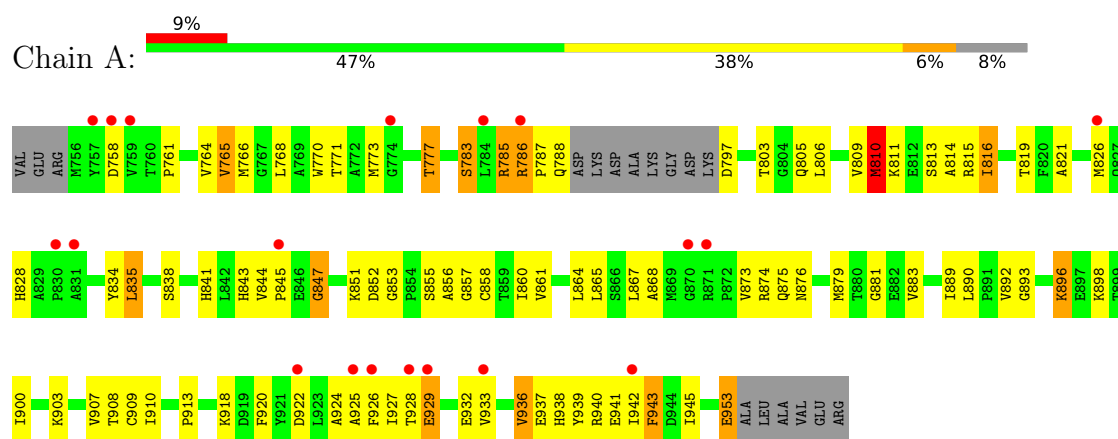
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	74	Total	O	0	0
			74	74		
2	B	42	Total	O	0	0
			42	42		
2	C	63	Total	O	1	2
			65	65		
2	D	42	Total	O	0	0
			42	42		
2	E	59	Total	O	0	0
			59	59		
2	F	48	Total	O	0	0
			48	48		

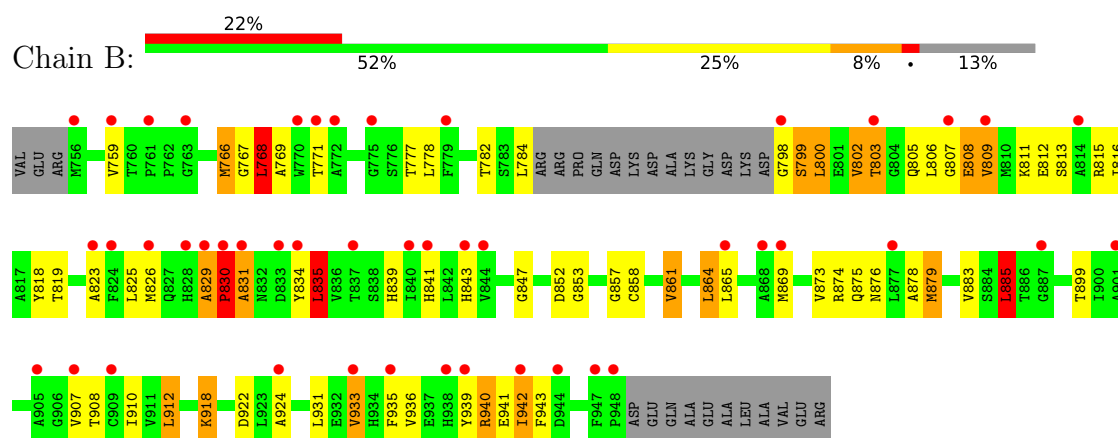
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

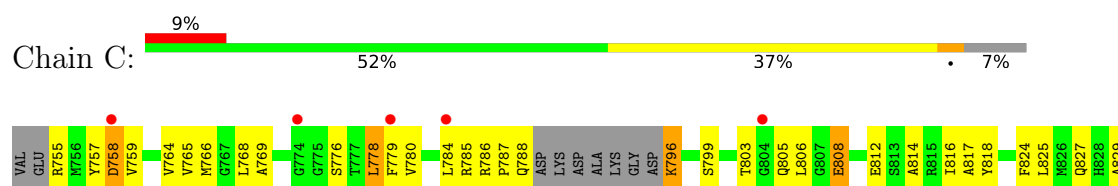
• Molecule 1: LON PROTEASE HOMOLOG, MITOCHONDRIAL



• Molecule 1: LON PROTEASE HOMOLOG, MITOCHONDRIAL



• Molecule 1: LON PROTEASE HOMOLOG, MITOCHONDRIAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.80Å 83.75Å 105.49Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	34.00 – 2.00 34.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (34.00-2.00) 97.0 (34.00-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.194 , 0.232 0.238 , 0.275	Depositor DCC
R_{free} test set	4328 reflections (5.41%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
Reported twinning fraction	0.321 for H, K, L 0.679 for -h,-k,l	Depositor
Outliers	0 of 80072 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8705	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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	1.82	31/1470 (2.1%)	1.42	15/1995 (0.8%)
1	B	1.51	12/1394 (0.9%)	1.40	17/1892 (0.9%)
1	C	1.87	30/1506 (2.0%)	1.42	13/2041 (0.6%)
1	D	1.40	9/1386 (0.6%)	1.27	5/1880 (0.3%)
1	E	1.70	22/1403 (1.6%)	1.44	19/1904 (1.0%)
1	F	1.51	8/1395 (0.6%)	1.23	7/1893 (0.4%)
All	All	1.65	112/8554 (1.3%)	1.37	76/11605 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (112) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	861	VAL	N-CA	-8.86	1.35	1.46
1	C	812	GLU	N-CA	-8.84	1.35	1.46
1	D	889	ILE	N-CA	-8.38	1.35	1.46
1	D	936	VAL	CA-CB	8.34	1.65	1.54
1	C	817	ALA	CA-CB	-8.27	1.40	1.53
1	A	853	GLY	C-O	-7.89	1.16	1.24
1	C	780	VAL	N-CA	-7.76	1.37	1.46
1	C	939	TYR	C-O	-7.70	1.14	1.24
1	A	815	ARG	C-O	-7.62	1.15	1.24
1	E	903	LYS	C-O	-7.45	1.14	1.24
1	A	764	VAL	C-O	-7.36	1.16	1.24
1	A	893	GLY	N-CA	7.34	1.51	1.44
1	D	780	VAL	CA-CB	7.33	1.63	1.54
1	A	856	ALA	CA-CB	-7.29	1.41	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	883	VAL	C-O	-6.96	1.16	1.24
1	C	829	ALA	CA-CB	-6.90	1.44	1.53
1	C	834	TYR	C-O	-6.83	1.16	1.24
1	F	857	GLY	C-O	-6.83	1.15	1.23
1	F	884	SER	N-CA	6.80	1.54	1.45
1	F	829	ALA	CA-CB	-6.76	1.44	1.53
1	E	877	LEU	C-O	-6.73	1.16	1.23
1	C	824	PHE	N-CA	6.69	1.54	1.46
1	C	860	ILE	C-O	-6.59	1.16	1.24
1	C	865	LEU	C-O	6.57	1.31	1.24
1	B	852	ASP	C-N	-6.43	1.30	1.34
1	C	859	THR	C-O	-6.37	1.16	1.24
1	F	760	THR	CA-CB	6.26	1.60	1.53
1	D	817	ALA	N-CA	6.26	1.54	1.46
1	C	835	LEU	C-O	-6.24	1.16	1.24
1	A	809	VAL	C-O	-6.23	1.16	1.24
1	F	859	THR	C-O	-6.22	1.16	1.24
1	E	856	ALA	CA-CB	6.17	1.64	1.53
1	E	840	ILE	CA-CB	6.14	1.62	1.54
1	A	844	VAL	C-O	-6.08	1.17	1.24
1	A	761	PRO	C-O	-6.07	1.17	1.24
1	A	814	ALA	CA-CB	-6.05	1.43	1.53
1	C	825	LEU	N-CA	6.05	1.53	1.46
1	A	821	ALA	C-O	-6.00	1.17	1.24
1	A	937	GLU	C-O	-5.99	1.15	1.23
1	E	815	ARG	C-O	-5.93	1.17	1.24
1	E	892	VAL	CA-C	-5.93	1.45	1.52
1	B	924	ALA	CA-C	5.92	1.60	1.52
1	C	817	ALA	C-O	-5.88	1.17	1.24
1	B	768	LEU	CA-C	-5.87	1.45	1.52
1	A	913	PRO	N-CA	-5.86	1.40	1.47
1	E	933	VAL	CA-CB	5.85	1.62	1.54
1	D	844	VAL	CA-CB	5.85	1.59	1.53
1	D	859	THR	CA-CB	5.83	1.62	1.53
1	A	816	ILE	C-O	-5.81	1.17	1.24
1	C	854	PRO	N-CA	-5.81	1.39	1.47
1	C	883	VAL	CA-CB	5.81	1.62	1.54
1	E	818	TYR	C-O	-5.80	1.17	1.24
1	E	863	ALA	N-CA	5.79	1.53	1.46
1	A	856	ALA	C-O	-5.79	1.16	1.24
1	C	814	ALA	CA-CB	-5.78	1.44	1.53
1	A	765	VAL	C-O	-5.73	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	843	HIS	C-O	-5.71	1.17	1.24
1	C	940	ARG	C-O	-5.71	1.17	1.24
1	A	943	PHE	N-CA	5.69	1.53	1.46
1	E	883	VAL	C-O	-5.66	1.17	1.24
1	A	858	CYS	C-O	5.65	1.31	1.24
1	B	885	LEU	N-CA	5.65	1.53	1.46
1	D	915	GLU	C-O	5.65	1.31	1.24
1	A	852	ASP	C-N	-5.63	1.30	1.34
1	C	764	VAL	N-CA	-5.62	1.39	1.46
1	A	896	LYS	C-O	-5.57	1.17	1.24
1	F	917	LYS	C-O	-5.56	1.17	1.24
1	E	857	GLY	N-CA	-5.56	1.39	1.45
1	C	827	GLN	C-O	-5.56	1.16	1.23
1	B	869	MET	CA-C	5.55	1.60	1.52
1	C	799	SER	CA-C	-5.52	1.45	1.52
1	F	907	VAL	CA-CB	-5.52	1.47	1.54
1	E	836	VAL	CA-CB	-5.47	1.47	1.54
1	B	829	ALA	CA-CB	-5.47	1.46	1.53
1	E	936	VAL	CA-C	-5.47	1.46	1.52
1	E	880	THR	C-O	-5.45	1.17	1.23
1	A	852	ASP	N-CA	-5.45	1.38	1.46
1	D	852	ASP	N-CA	5.39	1.53	1.46
1	A	783	SER	N-CA	5.39	1.52	1.46
1	C	818	TYR	C-O	-5.38	1.18	1.24
1	A	881	GLY	C-O	-5.37	1.16	1.23
1	C	912	LEU	CA-C	-5.34	1.46	1.52
1	E	942	ILE	CB-CG2	5.33	1.70	1.52
1	E	814	ALA	CA-CB	5.32	1.61	1.53
1	E	884	SER	C-O	5.28	1.30	1.23
1	C	766	MET	C-O	-5.27	1.17	1.24
1	A	813	SER	C-O	-5.24	1.18	1.24
1	A	879	MET	N-CA	-5.24	1.39	1.45
1	F	882	GLU	C-O	-5.23	1.17	1.23
1	A	844	VAL	CA-C	-5.22	1.48	1.53
1	A	860	ILE	C-O	5.22	1.30	1.24
1	C	844	VAL	CA-C	-5.18	1.47	1.52
1	B	858	CYS	CA-C	5.17	1.59	1.52
1	C	847	GLY	C-O	-5.17	1.17	1.23
1	C	943	PHE	CA-C	5.17	1.59	1.52
1	B	835	LEU	N-CA	5.17	1.52	1.46
1	C	916	ASN	CA-C	5.16	1.59	1.52
1	B	819	THR	CA-CB	5.12	1.61	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	884	SER	N-CA	5.11	1.52	1.45
1	E	911	VAL	CA-CB	-5.11	1.48	1.54
1	E	858	CYS	C-O	5.10	1.30	1.24
1	B	823	ALA	CA-C	-5.09	1.45	1.52
1	B	798	GLY	N-CA	5.08	1.53	1.45
1	C	870	GLY	C-O	-5.08	1.18	1.24
1	C	829	ALA	C-O	-5.07	1.18	1.24
1	D	819	THR	CA-C	-5.06	1.46	1.52
1	A	810	MET	C-O	-5.06	1.18	1.24
1	A	847	GLY	C-O	-5.04	1.17	1.23
1	B	879	MET	CG-SD	-5.04	1.68	1.80
1	A	936	VAL	C-O	-5.03	1.18	1.24
1	E	820	PHE	N-CA	5.01	1.52	1.46
1	A	940	ARG	C-O	-5.00	1.17	1.24

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	805	GLN	N-CA-C	9.79	124.90	111.39
1	C	860	ILE	N-CA-C	8.64	118.72	110.42
1	B	802	VAL	N-CA-C	8.36	120.16	108.12
1	A	811	LYS	N-CA-C	-8.32	102.21	111.28
1	F	890	LEU	CA-C-N	7.70	128.30	120.14
1	F	890	LEU	C-N-CA	7.70	128.30	120.14
1	A	864	LEU	N-CA-C	7.26	119.19	111.28
1	F	799	SER	N-CA-C	7.26	119.90	108.79
1	B	813	SER	N-CA-C	-7.03	103.62	111.28
1	D	834	TYR	N-CA-C	7.03	118.59	111.07
1	A	838	SER	N-CA-C	6.91	119.87	110.55
1	B	899	THR	N-CA-C	-6.75	103.73	112.23
1	A	860	ILE	CA-C-N	6.71	129.01	120.56
1	A	860	ILE	C-N-CA	6.71	129.01	120.56
1	A	844	VAL	CB-CA-C	-6.68	103.50	111.18
1	B	864	LEU	N-CA-C	-6.55	104.06	111.07
1	E	861	VAL	N-CA-C	-6.47	104.19	110.72
1	B	809	VAL	CB-CA-C	-6.42	103.75	111.97
1	E	861	VAL	O-C-N	6.42	128.44	121.83
1	D	899	THR	N-CA-C	-6.38	104.25	111.14
1	A	861	VAL	N-CA-CB	6.29	117.91	110.55
1	E	890	LEU	CA-C-N	6.22	126.19	119.78
1	E	890	LEU	C-N-CA	6.22	126.19	119.78
1	E	817	ALA	N-CA-C	6.21	118.13	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	918	LYS	N-CA-C	6.17	120.54	112.89
1	C	890	LEU	CA-C-N	6.16	126.11	119.76
1	C	890	LEU	C-N-CA	6.16	126.11	119.76
1	C	780	VAL	N-CA-C	-6.14	101.07	109.55
1	E	889	ILE	N-CA-C	6.14	117.63	108.54
1	D	910	ILE	N-CA-C	6.12	117.83	108.71
1	A	864	LEU	CA-C-N	6.09	128.94	120.29
1	A	864	LEU	C-N-CA	6.09	128.94	120.29
1	E	930	GLY	N-CA-C	6.05	123.10	115.42
1	C	829	ALA	CA-C-N	6.03	125.92	119.28
1	C	829	ALA	C-N-CA	6.03	125.92	119.28
1	B	940	ARG	CA-C-N	5.95	128.18	120.44
1	B	940	ARG	C-N-CA	5.95	128.18	120.44
1	E	818	TYR	N-CA-C	5.92	117.73	111.28
1	A	857	GLY	N-CA-C	5.89	119.34	112.50
1	E	933	VAL	CB-CA-C	-5.80	101.86	110.33
1	E	805	GLN	N-CA-C	5.77	118.37	110.24
1	E	840	ILE	N-CA-C	5.75	116.76	108.48
1	F	857	GLY	N-CA-C	5.72	119.14	112.50
1	C	824	PHE	N-CA-C	-5.72	104.96	111.14
1	B	831	ALA	N-CA-C	5.65	117.44	111.28
1	F	829	ALA	CA-C-N	5.62	125.29	119.05
1	F	829	ALA	C-N-CA	5.62	125.29	119.05
1	E	844	VAL	CA-C-N	5.61	125.62	119.90
1	E	844	VAL	C-N-CA	5.61	125.62	119.90
1	B	830	PRO	N-CA-C	-5.59	105.70	113.81
1	D	873	VAL	CB-CA-C	-5.55	103.98	111.63
1	B	883	VAL	CA-C-N	5.44	131.37	122.07
1	B	883	VAL	C-N-CA	5.44	131.37	122.07
1	A	786	ARG	N-CA-C	-5.40	100.12	108.55
1	A	758	ASP	N-CA-C	-5.37	106.41	113.12
1	C	838	SER	CA-CB-OG	-5.36	100.37	111.10
1	C	838	SER	N-CA-C	5.36	118.41	110.48
1	C	846	GLU	N-CA-C	-5.34	103.34	110.55
1	E	862	THR	N-CA-C	-5.32	105.64	111.82
1	E	774	GLY	CA-C-N	5.32	126.21	122.33
1	E	774	GLY	C-N-CA	5.32	126.21	122.33
1	B	808	GLU	N-CA-C	-5.30	105.45	112.34
1	B	853	GLY	O-C-N	5.28	122.97	121.07
1	C	816	ILE	CB-CA-C	-5.23	105.27	111.97
1	F	802	VAL	N-CA-C	5.20	115.39	108.11
1	A	861	VAL	O-C-N	5.20	127.01	121.91

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	776	SER	N-CA-C	5.12	117.04	108.99
1	A	865	LEU	N-CA-C	-5.12	105.78	111.36
1	E	871	ARG	CA-C-N	-5.12	114.68	119.85
1	E	871	ARG	C-N-CA	-5.12	114.68	119.85
1	B	799	SER	N-CA-C	5.07	116.89	109.24
1	E	853	GLY	N-CA-C	5.05	121.64	115.22
1	A	777	THR	N-CA-C	-5.04	101.10	109.46
1	B	813	SER	CB-CA-C	5.03	119.15	110.79
1	B	865	LEU	N-CA-C	-5.02	105.72	111.14
1	D	883	VAL	N-CA-C	5.01	115.19	108.17

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	803	THR	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	1440	0	1441	52	0
1	B	1365	0	1379	67	0
1	C	1475	0	1475	39	0
1	D	1358	0	1370	76	0
1	E	1374	0	1385	46	0
1	F	1363	0	1381	53	0
2	A	74	0	0	3	0
2	B	42	0	0	3	0
2	C	65	0	0	3	0
2	D	42	0	0	0	0
2	E	59	0	0	4	0
2	F	48	0	0	5	0
All	All	8705	0	8431	317	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (317) 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:766:MET:CE	1:D:878:ALA:HB2	1.73	1.18
1:D:825:LEU:HD23	1:D:835:LEU:HD13	1.24	1.17
1:D:766:MET:HE3	1:D:878:ALA:CB	1.80	1.11
1:B:784:LEU:HD11	1:B:834:TYR:OH	1.55	1.07
1:F:877:LEU:HD12	1:F:878:ALA:N	1.70	1.06
1:D:765:VAL:HG22	1:D:873:VAL:HG21	1.41	1.03
1:D:825:LEU:CD2	1:D:835:LEU:HD13	1.93	0.99
1:B:768:LEU:HD21	1:B:878:ALA:HB1	1.46	0.95
1:D:815[B]:ARG:HH21	1:D:815[B]:ARG:HG3	1.33	0.91
1:C:796:LYS:N	1:C:796:LYS:HE3	1.85	0.91
1:D:835:LEU:HD11	1:D:868:ALA:CB	2.02	0.90
1:F:766:MET:HE2	1:F:777:THR:CG2	2.03	0.89
1:B:940:ARG:HG2	1:B:941:GLU:N	1.85	0.88
1:C:920:PHE:CZ	1:C:933:VAL:HG21	2.09	0.87
1:B:808:GLU:HA	1:B:811:LYS:HD3	1.59	0.85
1:D:825:LEU:CD2	1:D:835:LEU:CD1	2.56	0.84
1:B:876:ASN:HD21	1:B:908:THR:HB	1.40	0.84
1:D:766:MET:HE1	1:D:907:VAL:HG21	1.59	0.84
1:F:766:MET:HE2	1:F:777:THR:HG21	1.59	0.83
1:D:815[B]:ARG:HH21	1:D:815[B]:ARG:CG	1.92	0.83
1:D:815[B]:ARG:HG3	1:D:815[B]:ARG:NH2	1.89	0.83
1:D:876:ASN:HD21	1:D:908:THR:HG23	1.42	0.83
1:F:877:LEU:HD12	1:F:877:LEU:C	2.05	0.80
1:B:825:LEU:HD22	1:B:835:LEU:HD22	1.63	0.80
1:A:925:ALA:O	1:A:929:GLU:HB2	1.82	0.79
1:F:896:LYS:HB2	1:F:923:LEU:HD21	1.65	0.78
1:D:876:ASN:HD21	1:D:908:THR:CG2	1.95	0.78
1:A:924:ALA:HA	1:F:827:GLN:HE21	1.49	0.76
1:D:835:LEU:HD11	1:D:868:ALA:HB2	1.68	0.76
1:B:766:MET:HE1	1:B:907:VAL:HG22	1.68	0.76
1:A:803:THR:OG1	1:A:841:HIS:HE1	1.70	0.75
1:A:903:LYS:NZ	1:A:929:GLU:O	2.20	0.73
1:B:936:VAL:HG21	1:B:942:ILE:HG22	1.69	0.72
1:F:843:HIS:CE1	2:F:2012:HOH:O	2.42	0.71
1:D:766:MET:HE3	1:D:878:ALA:HB2	0.85	0.71
1:C:785:ARG:HB3	1:D:819:THR:HG23	1.71	0.71
1:D:765:VAL:CG2	1:D:873:VAL:HG21	2.19	0.71
1:A:786:ARG:N	1:B:826:MET:HE1	2.06	0.70
1:D:806:LEU:HD22	1:D:810:MET:HG2	1.73	0.70
1:F:938:HIS:HD2	1:F:940:ARG:H	1.40	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:784:LEU:CD1	1:B:834:TYR:OH	2.37	0.69
1:D:835:LEU:HD11	1:D:868:ALA:HB1	1.73	0.69
1:B:778:LEU:HD12	1:B:778:LEU:O	1.92	0.69
1:A:785:ARG:C	1:B:826:MET:HE1	2.17	0.69
1:B:803:THR:OG1	1:B:841:HIS:NE2	2.22	0.69
1:B:815[A]:ARG:NH1	2:B:2011:HOH:O	2.26	0.69
1:D:806:LEU:HB2	1:D:810:MET:HB3	1.75	0.69
1:D:880:THR:O	1:D:913:PRO:HD3	1.94	0.68
1:A:766:MET:HE3	1:A:777:THR:HB	1.76	0.68
1:B:876:ASN:OD1	1:B:907:VAL:HA	1.93	0.68
1:D:766:MET:HE1	1:D:907:VAL:CG2	2.24	0.68
1:B:769:ALA:HB2	1:B:778:LEU:CD2	2.23	0.68
1:A:816:ILE:HG12	1:E:816:ILE:HD11	1.75	0.67
1:D:835:LEU:N	1:D:835:LEU:HD12	2.10	0.67
1:C:755:ARG:HD3	1:C:779:PHE:HZ	1.57	0.67
1:D:803:THR:OG1	1:D:841:HIS:NE2	2.25	0.67
1:C:920:PHE:CE2	1:C:933:VAL:HG21	2.28	0.67
1:B:874:ARG:NH1	2:B:2020:HOH:O	2.28	0.66
1:F:896:LYS:HB2	1:F:923:LEU:CD2	2.26	0.66
1:F:766:MET:HE2	1:F:777:THR:HG22	1.75	0.66
1:A:903:LYS:NZ	1:A:927:ILE:O	2.28	0.65
1:F:877:LEU:HD12	1:F:878:ALA:H	1.58	0.65
1:C:808[A]:GLU:H	1:C:808[A]:GLU:CD	2.02	0.65
1:B:808:GLU:OE1	1:B:811:LYS:NZ	2.30	0.65
1:C:758:ASP:OD2	1:C:758:ASP:N	2.30	0.64
1:D:883:VAL:HG22	1:D:884:SER:O	1.98	0.64
1:E:806:LEU:HB3	1:E:810:MET:HB3	1.79	0.64
1:D:835:LEU:HD12	1:D:835:LEU:H	1.63	0.64
1:B:807:GLY:O	1:B:809:VAL:N	2.32	0.62
1:D:889:ILE:HD11	1:D:939:TYR:HA	1.80	0.62
1:C:911:VAL:HG11	1:C:942:ILE:HG12	1.82	0.61
1:F:830:PRO:HD2	2:F:2019:HOH:O	2.01	0.61
1:F:902:ALA:O	1:F:907:VAL:CG1	2.48	0.61
1:E:835:LEU:HD13	1:E:868:ALA:HB2	1.83	0.61
1:A:924:ALA:HA	1:F:827:GLN:NE2	2.16	0.60
1:A:765:VAL:HG22	1:A:873:VAL:HG21	1.82	0.60
1:F:855:SER:HB3	1:F:892:VAL:HG11	1.83	0.60
1:B:835:LEU:HD11	1:B:864:LEU:HB3	1.84	0.60
1:F:902:ALA:O	1:F:907:VAL:HG13	2.02	0.60
1:C:848:ALA:HB1	1:C:852:ASP:HB3	1.83	0.59
1:A:936:VAL:HG21	1:A:942:ILE:HD11	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:827:GLN:HA	1:D:827:GLN:HE21	1.67	0.59
1:A:920:PHE:CZ	1:A:928:THR:HG23	2.38	0.58
1:B:910:ILE:CG2	1:B:933:VAL:HG13	2.34	0.58
1:D:939:TYR:HD1	1:D:942:ILE:HD12	1.68	0.58
1:B:940:ARG:HG2	1:B:941:GLU:H	1.67	0.58
1:A:953:GLU:HA	2:A:2074:HOH:O	2.02	0.58
1:F:855:SER:HB3	1:F:892:VAL:CG1	2.33	0.58
1:D:823:ALA:HA	1:D:826:MET:HE2	1.85	0.58
1:E:902:ALA:O	1:E:907:VAL:HG23	2.04	0.57
1:C:855:SER:HB2	1:C:892:VAL:HG11	1.86	0.57
1:A:936:VAL:HA	1:A:941:GLU:OE2	2.04	0.57
1:C:784:LEU:HD22	1:C:786:ARG:O	2.04	0.57
1:E:932:GLU:OE2	1:E:934:HIS:NE2	2.35	0.57
1:F:784:LEU:HD13	1:F:838:SER:HB3	1.87	0.57
1:D:896:LYS:HB2	1:D:923:LEU:HD21	1.87	0.57
1:D:782:THR:HG23	1:D:863:ALA:HB1	1.84	0.57
1:F:803:THR:C	2:F:2012:HOH:O	2.47	0.57
1:D:806:LEU:HD22	1:D:810:MET:CG	2.33	0.57
1:B:771:THR:HG22	1:B:847:GLY:O	2.05	0.56
1:E:872:PRO:HA	2:E:2029:HOH:O	2.05	0.56
1:B:829:ALA:O	1:B:831:ALA:N	2.37	0.56
1:F:810:MET:HE1	1:F:844:VAL:HG11	1.87	0.56
1:A:768:LEU:CD1	1:A:910:ILE:HD11	2.34	0.56
1:A:819:THR:OG1	1:E:812:GLU:HG3	2.05	0.56
1:A:876:ASN:O	1:A:907:VAL:HG13	2.06	0.56
1:F:760:THR:HG23	1:F:875:GLN:HE22	1.69	0.56
1:B:777:THR:HG23	1:B:777:THR:O	2.06	0.56
1:A:889:ILE:HD12	1:A:938:HIS:CA	2.36	0.55
1:A:889:ILE:CD1	1:A:938:HIS:C	2.79	0.55
1:A:876:ASN:HB2	1:A:908:THR:HG22	1.88	0.55
1:C:936:VAL:HA	1:C:941:GLU:OE2	2.07	0.55
1:C:951:GLN:HB2	2:C:2062:HOH:O	2.06	0.55
1:F:836:VAL:HG12	1:F:836:VAL:O	2.06	0.55
1:B:939:TYR:O	1:B:940:ARG:C	2.49	0.54
1:A:855:SER:HB2	1:A:892:VAL:HG11	1.89	0.54
1:B:829:ALA:O	1:B:830:PRO:C	2.49	0.54
1:A:939:TYR:C	1:A:939:TYR:CD2	2.85	0.54
1:C:918:LYS:HB2	1:C:918:LYS:HZ3	1.73	0.54
1:A:768:LEU:CD2	1:A:777:THR:HG22	2.37	0.54
1:D:812[B]:GLU:HG2	1:D:816:ILE:HD12	1.89	0.54
1:D:763:GLY:O	1:D:781:GLU:HA	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:806:LEU:CD2	1:E:810:MET:CB	2.86	0.53
1:F:810:MET:CE	1:F:844:VAL:HG11	2.37	0.53
1:C:918:LYS:HB2	1:C:918:LYS:NZ	2.24	0.53
1:C:903:LYS:NZ	1:C:929:GLU:O	2.39	0.53
1:E:762:PRO:HD3	1:E:872:PRO:HB3	1.91	0.53
1:B:767:GLY:C	1:B:768:LEU:HD22	2.32	0.53
1:B:829:ALA:C	1:B:831:ALA:N	2.61	0.53
1:A:889:ILE:HD12	1:A:938:HIS:C	2.34	0.53
1:B:812:GLU:O	1:B:816:ILE:HD12	2.09	0.53
1:C:784:LEU:HD21	1:C:838:SER:HB3	1.90	0.53
1:F:809:VAL:CG1	1:F:854:PRO:HG3	2.38	0.53
1:A:835:LEU:HD13	1:A:868:ALA:HB2	1.92	0.52
1:B:766:MET:HE1	1:B:907:VAL:CG2	2.38	0.52
1:C:936:VAL:HG21	1:C:942:ILE:HD11	1.91	0.52
1:A:834:TYR:CD2	1:A:868:ALA:HA	2.45	0.52
1:D:862:THR:O	1:D:863:ALA:C	2.52	0.51
1:A:876:ASN:CB	1:A:908:THR:HG22	2.41	0.51
1:F:825:LEU:HD22	1:F:835:LEU:HD22	1.92	0.51
1:B:799:SER:HG	1:B:839:HIS:HD1	1.59	0.51
1:D:802:VAL:HG11	1:D:806:LEU:HD11	1.93	0.51
1:B:910:ILE:HG23	1:B:933:VAL:HG13	1.92	0.51
1:B:784:LEU:HD21	1:B:834:TYR:CZ	2.46	0.51
1:E:797:ASP:CG	1:E:797:ASP:O	2.53	0.50
1:D:825:LEU:CD2	1:D:835:LEU:HD11	2.38	0.50
1:F:809:VAL:HG11	1:F:854:PRO:HG3	1.92	0.50
1:B:777:THR:O	1:B:777:THR:CG2	2.59	0.50
1:B:807:GLY:O	1:B:808:GLU:C	2.54	0.50
1:C:755:ARG:HD2	1:C:757:TYR:O	2.11	0.50
1:E:797:ASP:O	1:E:797:ASP:OD2	2.29	0.50
1:F:843:HIS:ND1	2:F:2012:HOH:O	2.35	0.50
1:B:876:ASN:O	1:B:876:ASN:CG	2.55	0.50
1:D:889:ILE:HD12	1:D:938:HIS:C	2.36	0.50
1:D:825:LEU:HD22	1:D:835:LEU:CD1	2.40	0.50
1:D:939:TYR:CD1	1:D:942:ILE:HD12	2.46	0.50
1:A:786:ARG:CA	1:B:826:MET:HE1	2.41	0.49
1:D:768:LEU:HD13	1:D:878:ALA:HB1	1.94	0.49
1:F:940:ARG:HH11	1:F:940:ARG:HB2	1.76	0.49
1:B:939:TYR:CE1	1:B:942:ILE:HG12	2.47	0.49
1:D:876:ASN:ND2	1:D:908:THR:CG2	2.71	0.49
1:F:865:LEU:HD13	1:F:943:PHE:CE2	2.46	0.49
1:C:803:THR:OG1	1:C:841:HIS:HE1	1.96	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:860:ILE:O	1:F:861:VAL:C	2.55	0.49
1:E:806:LEU:HD22	1:E:810:MET:CB	2.43	0.49
1:F:835:LEU:HD13	1:F:868:ALA:HB2	1.93	0.49
1:C:876:ASN:CB	1:C:908:THR:HG22	2.42	0.49
1:D:785:ARG:HB3	1:D:841:HIS:HB2	1.94	0.49
1:A:920:PHE:CZ	1:A:933:VAL:HG21	2.48	0.49
1:B:759:VAL:O	1:B:759:VAL:HG13	2.12	0.49
1:D:765:VAL:HG22	1:D:873:VAL:CG2	2.26	0.49
1:D:782:THR:HG21	1:D:864:LEU:HD23	1.94	0.49
1:E:824:PHE:CE2	1:E:828[A]:HIS:CE1	3.01	0.49
1:B:876:ASN:ND2	1:B:908:THR:HB	2.20	0.49
1:C:873:VAL:HG12	1:C:874:ARG:N	2.28	0.49
1:D:835:LEU:CD1	1:D:868:ALA:HB1	2.42	0.49
1:E:910:ILE:HG23	1:E:931:LEU:HD22	1.94	0.49
1:E:934:HIS:CG	1:E:945:ILE:HD13	2.47	0.49
1:D:913:PRO:HB2	1:D:916:ASN:OD1	2.13	0.48
1:D:835:LEU:CD1	1:D:835:LEU:H	2.25	0.48
1:B:769:ALA:HB2	1:B:778:LEU:HD23	1.96	0.48
1:C:885:LEU:HD12	1:F:854:PRO:HB3	1.95	0.48
1:E:920:PHE:O	1:E:923:LEU:HG	2.13	0.48
1:D:835:LEU:CD1	1:D:868:ALA:CB	2.85	0.48
1:D:802:VAL:CG1	1:D:806:LEU:HD21	2.43	0.48
1:A:810:MET:HE2	2:A:2034:HOH:O	2.12	0.48
1:E:876:ASN:CG	1:E:876:ASN:O	2.52	0.48
1:E:806:LEU:CB	1:E:810:MET:HG2	2.44	0.47
1:B:943:PHE:CD1	1:B:943:PHE:C	2.92	0.47
1:E:759:VAL:HG23	1:E:875:GLN:NE2	2.30	0.47
1:F:834:TYR:CD2	1:F:868:ALA:HA	2.49	0.47
1:C:925:ALA:HB3	1:E:827:GLN:O	2.14	0.47
1:D:880:THR:O	1:D:880:THR:HG23	2.15	0.47
1:B:800:LEU:HB2	1:B:818:TYR:CE1	2.50	0.47
1:C:755:ARG:N	2:C:2001:HOH:O	2.46	0.47
1:E:806:LEU:HB2	1:E:810:MET:HG2	1.97	0.47
1:D:938:HIS:HD2	1:D:940:ARG:H	1.62	0.47
1:E:894:GLY:O	1:E:898:LYS:HG3	2.14	0.47
1:E:873:VAL:N	2:E:2029:HOH:O	2.27	0.47
1:A:936:VAL:HG21	1:A:942:ILE:CG1	2.43	0.47
1:B:918:LYS:NZ	2:B:2033:HOH:O	2.30	0.47
1:D:800:LEU:HD11	1:D:842:LEU:HB2	1.96	0.47
1:E:766:MET:HG3	1:E:777:THR:HG23	1.98	0.46
1:E:858:CYS:O	1:E:862:THR:OG1	2.33	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:936:VAL:HG21	1:B:942:ILE:CG2	2.44	0.46
1:E:760:THR:H	1:E:875:GLN:HE22	1.62	0.46
1:E:799:SER:OG	1:E:839:HIS:ND1	2.33	0.46
1:E:806:LEU:HD22	1:E:810:MET:CG	2.45	0.46
1:D:800:LEU:HD11	1:D:842:LEU:CB	2.45	0.46
1:A:889:ILE:HD11	1:A:939:TYR:HA	1.97	0.46
1:D:806:LEU:HB2	1:D:810:MET:CB	2.44	0.46
1:E:825:LEU:HD22	1:E:835:LEU:HD22	1.98	0.46
1:F:799:SER:OG	1:F:839:HIS:ND1	2.34	0.46
1:C:876:ASN:HB3	1:C:908:THR:HG22	1.97	0.46
1:F:896:LYS:CB	1:F:923:LEU:HD21	2.39	0.46
1:B:768:LEU:HD22	1:B:768:LEU:N	2.31	0.45
1:C:876:ASN:O	1:C:907:VAL:HG13	2.16	0.45
1:D:765:VAL:HG12	1:D:859:THR:CG2	2.46	0.45
1:A:785:ARG:NH2	1:B:815[A]:ARG:NH1	2.64	0.45
1:D:889:ILE:CD1	1:D:938:HIS:C	2.89	0.45
1:B:807:GLY:C	1:B:809:VAL:N	2.67	0.45
1:B:841:HIS:CE1	1:B:843:HIS:HB2	2.52	0.45
1:F:895:ILE:HD11	1:F:916:ASN:CG	2.42	0.45
1:F:873:VAL:HG12	1:F:874:ARG:N	2.32	0.45
1:B:808:GLU:CD	1:B:811:LYS:NZ	2.74	0.44
1:E:806:LEU:HD23	1:E:810:MET:CB	2.47	0.44
1:D:825:LEU:HD22	1:D:835:LEU:HD11	1.98	0.44
1:D:910:ILE:HG13	1:D:933:VAL:HG23	1.99	0.44
1:E:784:LEU:HD11	1:E:838:SER:HB3	2.00	0.44
1:A:945:ILE:O	1:A:945:ILE:HG22	2.17	0.44
1:B:769:ALA:HB2	1:B:778:LEU:HD21	1.95	0.44
1:B:800:LEU:HD23	1:B:800:LEU:HA	1.82	0.44
1:B:939:TYR:CE1	1:B:942:ILE:CG1	3.00	0.44
1:A:924:ALA:CA	1:F:827:GLN:HE21	2.23	0.44
1:B:759:VAL:HG23	1:B:875:GLN:HE21	1.82	0.44
1:A:766:MET:HE1	1:A:907:VAL:CG2	2.48	0.44
1:A:936:VAL:HG21	1:A:942:ILE:CD1	2.48	0.44
1:D:784:LEU:HD21	1:D:838:SER:HB3	2.00	0.44
1:F:805:GLN:HE21	1:F:805:GLN:HB2	1.71	0.44
1:F:760:THR:HG23	1:F:875:GLN:NE2	2.33	0.43
1:F:770:TRP:O	1:F:849:THR:HG23	2.18	0.43
1:A:787:PRO:O	1:A:787:PRO:CD	2.64	0.43
1:B:782:THR:HG21	1:B:864:LEU:HD23	2.01	0.43
1:D:765:VAL:HG12	1:D:859:THR:HG23	2.01	0.43
1:E:872:PRO:CA	2:E:2029:HOH:O	2.63	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:941:GLU:OE1	2:A:2067:HOH:O	2.21	0.43
1:B:912:LEU:O	1:B:935:PHE:HA	2.18	0.43
1:E:764:VAL:HG22	1:E:781:GLU:HG3	2.01	0.43
1:E:875:GLN:O	1:E:876:ASN:HB3	2.17	0.43
1:F:804:GLY:N	2:F:2012:HOH:O	2.51	0.43
1:A:806:LEU:HB3	1:A:810:MET:HB3	2.00	0.43
1:C:779:PHE:O	1:C:845:PRO:CG	2.66	0.43
1:C:786:ARG:HD3	1:D:797:ASP:OD2	2.19	0.43
1:E:875:GLN:HB2	2:E:2031:HOH:O	2.17	0.43
1:A:925:ALA:O	1:A:929:GLU:N	2.51	0.42
1:B:768:LEU:CD2	1:B:878:ALA:HB1	2.34	0.42
1:B:918:LYS:O	1:B:922:ASP:CG	2.62	0.42
1:F:849:THR:O	1:F:850:PRO:C	2.62	0.42
1:D:873:VAL:HG12	1:D:874:ARG:N	2.34	0.42
1:E:806:LEU:HD22	1:E:810:MET:HE2	2.02	0.42
1:A:909:CYS:HA	1:A:932:GLU:O	2.19	0.42
1:B:931:LEU:HD12	1:B:931:LEU:HA	1.93	0.42
1:D:910:ILE:HD11	1:D:920:PHE:CE1	2.55	0.42
1:C:831:ALA:HB3	2:C:2019:HOH:O	2.18	0.42
1:F:770:TRP:HB2	1:F:898:LYS:HE3	2.02	0.42
1:E:818:TYR:O	1:E:822:ARG:CD	2.68	0.42
1:F:910:ILE:HD13	1:F:910:ILE:HG21	1.64	0.42
1:A:803:THR:OG1	1:A:843:HIS:HD2	2.02	0.42
1:C:877:LEU:HD11	1:C:911:VAL:HG23	2.01	0.42
1:C:920:PHE:CZ	1:C:933:VAL:CG2	2.93	0.42
1:C:921:TYR:CD1	1:E:940:ARG:HG2	2.55	0.42
1:E:858:CYS:HB2	1:E:942:ILE:HD13	2.02	0.42
1:B:807:GLY:C	1:B:809:VAL:H	2.27	0.42
1:C:787:PRO:HD3	1:D:836:VAL:HG11	2.01	0.42
1:E:806:LEU:HD22	1:E:810:MET:HG2	2.02	0.42
1:D:876:ASN:HD21	1:D:908:THR:HG22	1.82	0.41
1:A:873:VAL:HG12	1:A:874:ARG:N	2.33	0.41
1:D:877:LEU:HD11	1:D:911:VAL:HG23	2.02	0.41
1:B:829:ALA:C	1:B:831:ALA:H	2.28	0.41
1:D:802:VAL:CG1	1:D:806:LEU:HD11	2.50	0.41
1:B:857:GLY:O	1:B:861:VAL:HG12	2.20	0.41
1:D:852:ASP:OD1	1:D:898:LYS:NZ	2.46	0.41
1:E:806:LEU:CD2	1:E:810:MET:HB2	2.51	0.41
1:E:911:VAL:HG11	1:E:942:ILE:HG12	2.03	0.41
1:F:803:THR:OG1	1:F:841:HIS:NE2	2.50	0.41
1:A:828:HIS:CE1	1:A:943:PHE:CZ	3.09	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:LYS:HG2	1:A:900:ILE:HD12	2.01	0.41
1:B:769:ALA:CB	1:B:778:LEU:HD23	2.50	0.41
1:B:825:LEU:HD22	1:B:835:LEU:CD2	2.42	0.41
1:C:769:ALA:HB2	1:C:778:LEU:HD22	2.02	0.41
1:F:895:ILE:HG13	1:F:919:ASP:CB	2.50	0.41
1:F:784:LEU:HD12	1:F:785:ARG:H	1.86	0.41
1:C:921:TYR:CE1	1:E:940:ARG:HG2	2.56	0.41
1:F:782:THR:HA	1:F:841:HIS:O	2.21	0.41
1:F:882:GLU:HB3	1:F:890:LEU:HB2	2.01	0.41
1:E:806:LEU:HD23	1:E:810:MET:HB3	2.03	0.41
1:A:771:THR:HG22	1:A:847:GLY:O	2.21	0.41
1:B:879:MET:SD	1:B:942:ILE:HD13	2.61	0.41
1:E:784:LEU:HD12	1:E:784:LEU:HA	1.88	0.41
1:A:924:ALA:HB1	1:A:926:PHE:CE1	2.56	0.41
1:B:816:ILE:HG23	1:B:885:LEU:HD23	2.02	0.41
1:D:810:MET:HE3	1:D:844:VAL:HG11	2.03	0.41
1:D:882:GLU:O	1:D:889:ILE:HA	2.21	0.41
1:D:889:ILE:HD11	1:D:939:TYR:CA	2.47	0.41
1:F:902:ALA:C	1:F:907:VAL:HG13	2.45	0.41
1:D:938:HIS:CD2	1:D:940:ARG:H	2.39	0.40
1:E:759:VAL:O	1:E:759:VAL:HG13	2.21	0.40
1:F:764:VAL:HG13	1:F:781:GLU:HG2	2.03	0.40
1:C:765:VAL:HG22	1:C:873:VAL:HG21	2.02	0.40
1:C:938[B]:HIS:O	1:C:939:TYR:C	2.63	0.40
1:A:766:MET:HE1	1:A:907:VAL:HG21	2.03	0.40
1:A:889:ILE:HD12	1:A:938:HIS:HA	2.03	0.40
1:D:827:GLN:HA	1:D:827:GLN:NE2	2.35	0.40
1:F:895:ILE:HD11	1:F:916:ASN:ND2	2.36	0.40
1:C:876:ASN:HB2	1:C:908:THR:HG22	2.03	0.40
1:A:770:TRP:HB2	1:A:898:LYS:HE3	2.03	0.40
1:D:865:LEU:O	1:D:869:MET:HG3	2.21	0.40

There are no symmetry-related clashes.

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	186/207 (90%)	181 (97%)	5 (3%)	0	100	100
1	B	177/207 (86%)	174 (98%)	3 (2%)	0	100	100
1	C	190/207 (92%)	185 (97%)	5 (3%)	0	100	100
1	D	176/207 (85%)	169 (96%)	7 (4%)	0	100	100
1	E	178/207 (86%)	172 (97%)	6 (3%)	0	100	100
1	F	177/207 (86%)	170 (96%)	7 (4%)	0	100	100
All	All	1084/1242 (87%)	1051 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	152/165 (92%)	134 (88%)	18 (12%)	5	3
1	B	144/165 (87%)	130 (90%)	14 (10%)	8	5
1	C	155/165 (94%)	138 (89%)	17 (11%)	6	3
1	D	143/165 (87%)	130 (91%)	13 (9%)	9	6
1	E	145/165 (88%)	127 (88%)	18 (12%)	4	2
1	F	144/165 (87%)	123 (85%)	21 (15%)	3	2
All	All	883/990 (89%)	782 (89%)	101 (11%)	5	3

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	773	MET
1	A	783	SER
1	A	785	ARG
1	A	788	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	797	ASP
1	A	805	GLN
1	A	810	MET
1	A	826	MET
1	A	835	LEU
1	A	845	PRO
1	A	851	LYS
1	A	867	LEU
1	A	875	GLN
1	A	890	LEU
1	A	918	LYS
1	A	922	ASP
1	A	929	GLU
1	A	953	GLU
1	B	766	MET
1	B	768	LEU
1	B	800	LEU
1	B	802	VAL
1	B	806	LEU
1	B	830	PRO
1	B	835	LEU
1	B	861	VAL
1	B	873	VAL
1	B	885	LEU
1	B	912	LEU
1	B	918	LYS
1	B	933	VAL
1	B	942	ILE
1	C	758	ASP
1	C	759	VAL
1	C	768	LEU
1	C	778	LEU
1	C	788	GLN
1	C	796	LYS
1	C	805	GLN
1	C	806	LEU
1	C	808[A]	GLU
1	C	808[B]	GLU
1	C	866	SER
1	C	875	GLN
1	C	890	LEU
1	C	918	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	922	ASP
1	C	926	PHE
1	C	928	THR
1	D	760	THR
1	D	768	LEU
1	D	777	THR
1	D	778	LEU
1	D	785	ARG
1	D	806	LEU
1	D	815[A]	ARG
1	D	815[B]	ARG
1	D	827	GLN
1	D	859	THR
1	D	885	LEU
1	D	888	LYS
1	D	903	LYS
1	E	768	LEU
1	E	777	THR
1	E	805	GLN
1	E	806	LEU
1	E	822	ARG
1	E	835	LEU
1	E	836	VAL
1	E	838	SER
1	E	846	GLU
1	E	851	LYS
1	E	867	LEU
1	E	871	ARG
1	E	874	ARG
1	E	883	VAL
1	E	890	LEU
1	E	910	ILE
1	E	928	THR
1	E	933	VAL
1	F	759	VAL
1	F	765	VAL
1	F	768	LEU
1	F	773	MET
1	F	801	GLU
1	F	803	THR
1	F	805	GLN
1	F	806	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	810	MET
1	F	835	LEU
1	F	842	LEU
1	F	851	LYS
1	F	855	SER
1	F	871	ARG
1	F	877	LEU
1	F	890	LEU
1	F	904	ARG
1	F	907	VAL
1	F	908	THR
1	F	933	VAL
1	F	940	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	828	HIS
1	A	841	HIS
1	A	843	HIS
1	A	938	HIS
1	B	828	HIS
1	B	875	GLN
1	C	828	HIS
1	C	841	HIS
1	C	843	HIS
1	C	934	HIS
1	D	805	GLN
1	D	827	GLN
1	D	876	ASN
1	D	934	HIS
1	D	938	HIS
1	E	827	GLN
1	E	843	HIS
1	E	875	GLN
1	F	805	GLN
1	F	827	GLN
1	F	875	GLN
1	F	938	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	190/207 (91%)	0.85	19 (10%)	12 11	25, 44, 66, 75	0
1	B	177/207 (85%)	1.46	46 (25%)	1 1	21, 53, 74, 86	1 (0%)
1	C	192/207 (92%)	0.84	18 (9%)	14 13	16, 43, 62, 77	2 (1%)
1	D	178/207 (85%)	1.26	24 (13%)	7 6	21, 52, 68, 93	2 (1%)
1	E	181/207 (87%)	0.98	22 (12%)	8 7	24, 47, 70, 84	1 (0%)
1	F	179/207 (86%)	1.18	27 (15%)	5 5	20, 55, 71, 87	3 (1%)
All	All	1097/1242 (88%)	1.09	156 (14%)	6 5	16, 49, 70, 93	9 (0%)

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	798	GLY	7.6
1	C	930	GLY	5.1
1	E	806	LEU	5.0
1	A	933	VAL	4.6
1	F	870	GLY	4.6
1	B	807	GLY	4.5
1	F	858	CYS	4.4
1	F	804	GLY	4.3
1	D	798	GLY	4.3
1	A	928	THR	4.3
1	B	803	THR	4.3
1	E	772	ALA	4.2
1	D	947	PHE	4.1
1	E	797	ASP	4.0
1	D	821	ALA	3.8
1	A	925	ALA	3.5
1	C	929	GLU	3.5
1	D	760	THR	3.5
1	F	806	LEU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	837	THR	3.5
1	D	923	LEU	3.4
1	A	870	GLY	3.2
1	B	841	HIS	3.2
1	F	850	PRO	3.2
1	B	868	ALA	3.2
1	F	798	GLY	3.2
1	E	778	LEU	3.1
1	D	812[A]	GLU	3.1
1	C	952	ALA	3.0
1	C	758	ASP	3.0
1	C	926	PHE	3.0
1	B	865	LEU	2.9
1	A	774	GLY	2.9
1	B	948	PRO	2.9
1	B	823	ALA	2.9
1	B	770	TRP	2.9
1	B	833	ASP	2.9
1	B	947	PHE	2.9
1	E	804	GLY	2.9
1	B	869	MET	2.8
1	B	759	VAL	2.8
1	B	834	TYR	2.8
1	B	772	ALA	2.8
1	A	784	LEU	2.8
1	F	841	HIS	2.8
1	B	831	ALA	2.8
1	F	933	VAL	2.7
1	B	938	HIS	2.7
1	C	938[A]	HIS	2.7
1	B	901	ALA	2.7
1	B	935	PHE	2.7
1	D	935	PHE	2.7
1	A	757	TYR	2.7
1	F	832	ASN	2.7
1	A	922	ASP	2.7
1	E	928	THR	2.6
1	F	773	MET	2.6
1	E	761	PRO	2.6
1	C	908	THR	2.6
1	D	871	ARG	2.6
1	F	807	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	908	THR	2.6
1	F	867	LEU	2.6
1	B	809	VAL	2.6
1	B	771	THR	2.6
1	B	924	ALA	2.6
1	F	772	ALA	2.6
1	B	830	PRO	2.6
1	E	759	VAL	2.5
1	C	804	GLY	2.5
1	E	773	MET	2.5
1	E	930	GLY	2.5
1	F	904	ARG	2.5
1	A	845	PRO	2.5
1	E	901	ALA	2.4
1	B	828	HIS	2.4
1	C	779	PHE	2.4
1	B	844	VAL	2.4
1	A	926	PHE	2.4
1	F	922	ASP	2.4
1	A	942	ILE	2.4
1	A	871	ARG	2.4
1	C	851	LYS	2.4
1	A	831	ALA	2.4
1	C	774	GLY	2.4
1	B	944	ASP	2.4
1	F	926	PHE	2.4
1	B	840	ILE	2.4
1	B	763	GLY	2.3
1	A	758	ASP	2.3
1	E	785	ARG	2.3
1	A	759	VAL	2.3
1	F	771	THR	2.3
1	F	928	THR	2.3
1	E	829	ALA	2.3
1	D	806	LEU	2.3
1	A	929	GLU	2.3
1	D	873	VAL	2.3
1	B	761	PRO	2.3
1	B	814	ALA	2.3
1	D	770	TRP	2.3
1	D	813	SER	2.3
1	B	775	GLY	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	930	GLY	2.3
1	B	939	TYR	2.3
1	E	770	TRP	2.3
1	F	943	PHE	2.2
1	D	761	PRO	2.2
1	F	871	ARG	2.2
1	B	826	MET	2.2
1	B	887	GLY	2.2
1	B	843	HIS	2.2
1	D	836	VAL	2.2
1	F	759	VAL	2.2
1	C	924	ALA	2.2
1	A	786	ARG	2.2
1	F	907	VAL	2.2
1	E	798	GLY	2.2
1	E	870	GLY	2.2
1	F	929	GLU	2.2
1	D	829	ALA	2.2
1	E	909	CYS	2.2
1	B	756	MET	2.2
1	B	824	PHE	2.1
1	C	927	ILE	2.1
1	B	907	VAL	2.1
1	D	933	VAL	2.1
1	F	843	HIS	2.1
1	C	867	LEU	2.1
1	D	825	LEU	2.1
1	D	869	MET	2.1
1	E	760	THR	2.1
1	B	779	PHE	2.1
1	B	877	LEU	2.1
1	A	830	PRO	2.1
1	B	933	VAL	2.1
1	B	905	ALA	2.1
1	A	826	MET	2.1
1	B	942	ILE	2.1
1	B	829	ALA	2.1
1	E	848	ALA	2.1
1	E	925	ALA	2.1
1	F	863	ALA	2.1
1	B	909	CYS	2.0
1	C	858	CYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	805	GLN	2.0
1	C	921	TYR	2.0
1	D	927	ILE	2.0
1	D	838	SER	2.0
1	C	925	ALA	2.0
1	D	924	ALA	2.0
1	C	784	LEU	2.0
1	E	841	HIS	2.0
1	F	777	THR	2.0
1	D	906	GLY	2.0
1	D	921	TYR	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 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.