Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:26 AM GMT

PDB ID	:	2X36
Title	:	STRUCTURE OF THE PROTEOLYTIC DOMAIN OF THE HUMAN MITOCHONDRIAL LON PROTEASE
Authors	:	Garcia, J.; Ondrovicova, G.; Blagova, E.; Levdikov, 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

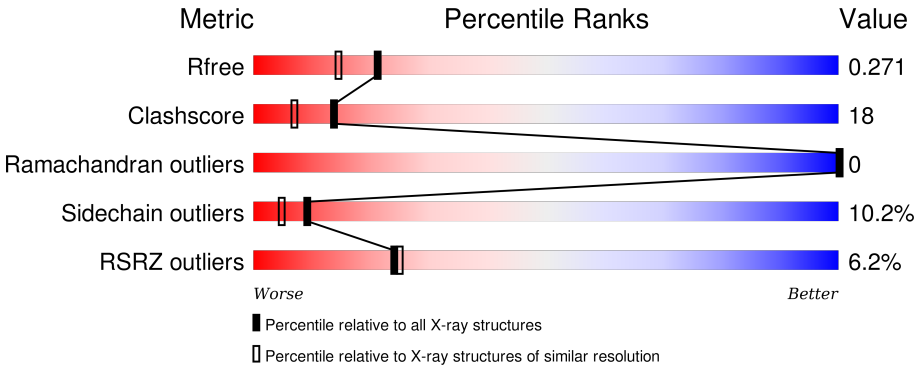
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 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 <=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	6% 58% 28% 5% 8%
1	B	207	7% 56% 25% 6% 13%
1	C	207	5% 64% 27% • 7%
1	D	207	4% 52% 30% • 14%
1	E	207	5% 61% 23% • 13%

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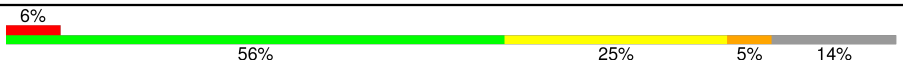
Mol	Chain	Length	Quality of chain
1	F	207	

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.

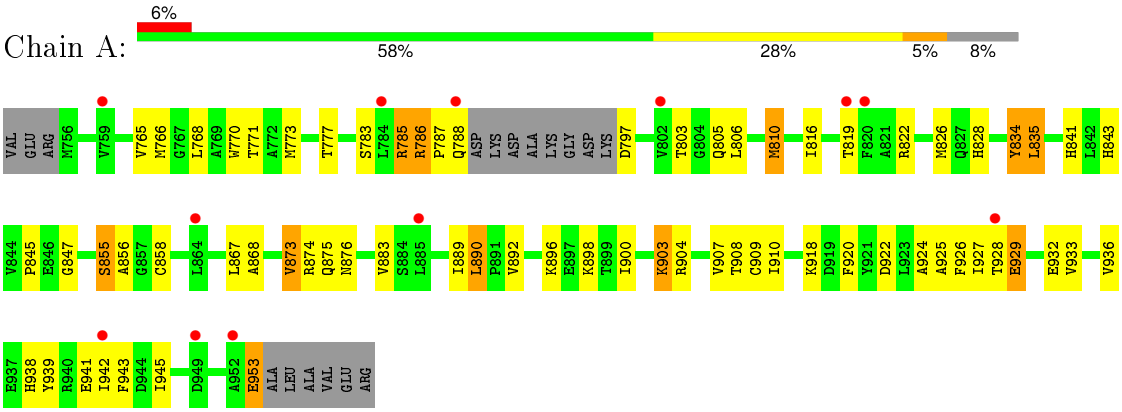
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	74	Total	O	0	0
			74	74		
2	B	42	Total	O	0	0
			42	42		
2	C	63	Total	O	1	2
			65	65		
2	D	42	Total	O	0	0
			42	42		
2	E	59	Total	O	0	0
			59	59		
2	F	48	Total	O	0	0
			48	48		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

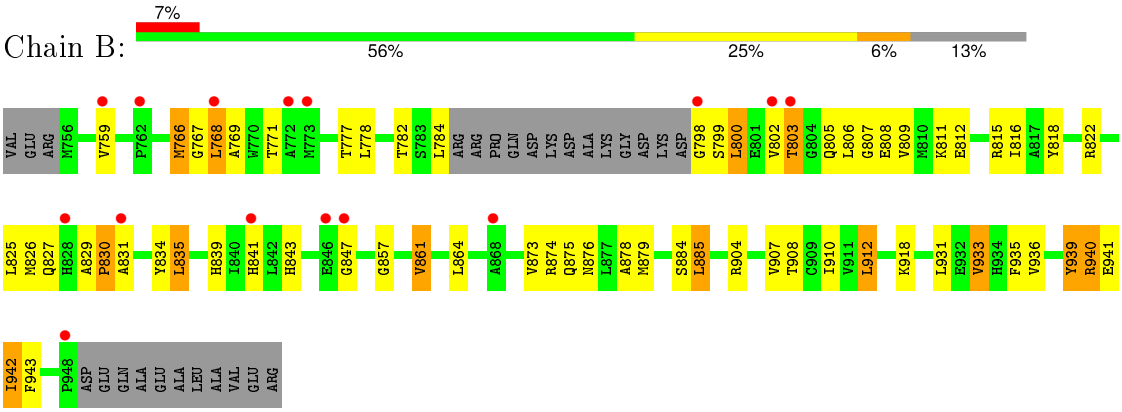
• Molecule 1: LON PROTEASE HOMOLOG, MITOCHONDRIAL

Chain A:



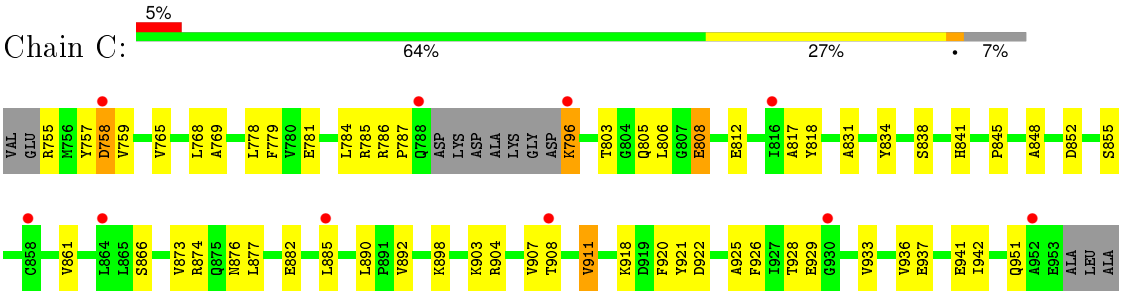
• Molecule 1: LON PROTEASE HOMOLOG, MITOCHONDRIAL

Chain B:



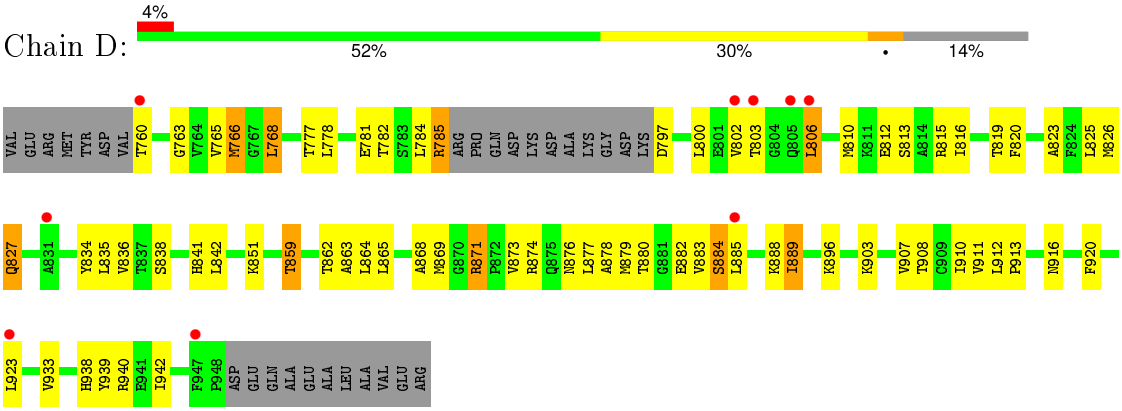
• Molecule 1: LON PROTEASE HOMOLOG, MITOCHONDRIAL

Chain C:



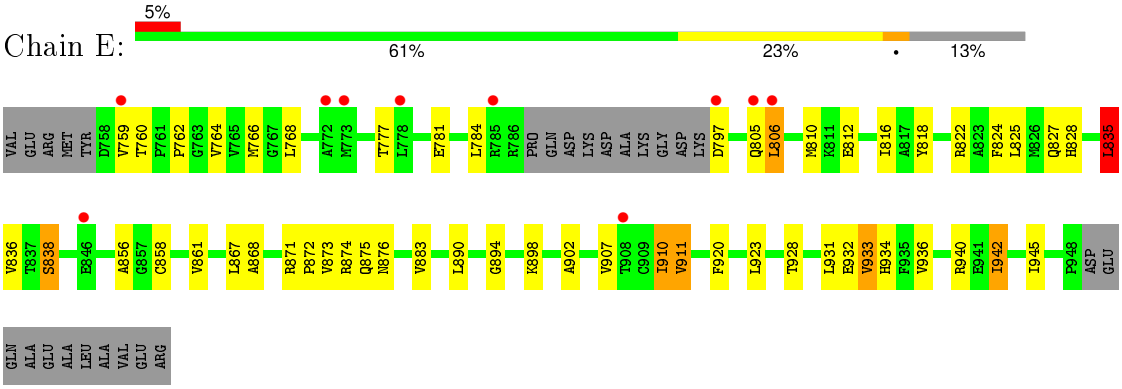
• Molecule 1: LON PROTEASE HOMOLOG, MITOCHONDRIAL

Chain D:



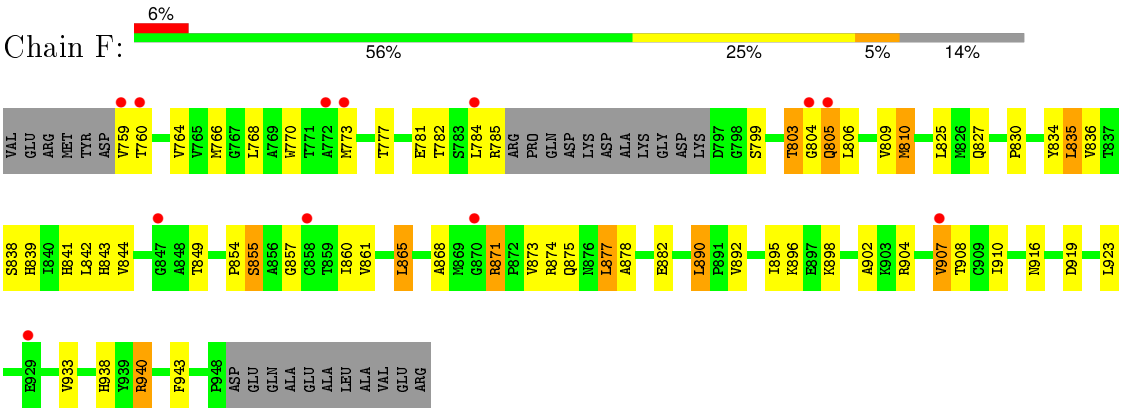
• Molecule 1: LON PROTEASE HOMOLOG, MITOCHONDRIAL

Chain E:



• Molecule 1: LON PROTEASE HOMOLOG, MITOCHONDRIAL

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	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) 96.8 (34.00-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.194 , 0.232 0.238 , 0.271	Depositor DCC
R_{free} test set	4328 reflections (5.41%)	DCC
Wilson B-factor (Å^2)	43.8	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.6	EDS
Estimated twinning fraction	0.321 for H, K, L 0.679 for -H, -K, L 0.039 for h,-k,-l	Xtriage
Reported twinning fraction	0.321 for H, K, L 0.679 for -H, -K, L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.39$	Xtriage
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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.40	6/1470 (0.4%)	1.07	4/1995 (0.2%)
1	B	1.17	4/1394 (0.3%)	1.01	2/1892 (0.1%)
1	C	1.47	11/1506 (0.7%)	1.08	1/2041 (0.0%)
1	D	1.10	2/1386 (0.1%)	1.01	6/1880 (0.3%)
1	E	1.28	6/1403 (0.4%)	1.05	2/1904 (0.1%)
1	F	1.15	1/1395 (0.1%)	0.96	2/1893 (0.1%)
All	All	1.27	30/8554 (0.4%)	1.03	17/11605 (0.1%)

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 (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	937	GLU	CD-OE1	5.90	1.32	1.25
1	D	820	PHE	CD1-CE1	5.79	1.50	1.39
1	C	834	TYR	CD2-CE2	-5.74	1.30	1.39
1	C	817	ALA	CA-CB	-5.74	1.40	1.52
1	A	873	VAL	CB-CG1	-5.68	1.41	1.52
1	A	858	CYS	CB-SG	-5.67	1.72	1.81
1	B	939	TYR	CD1-CE1	5.61	1.47	1.39
1	E	911	VAL	CB-CG2	5.60	1.64	1.52
1	E	942	ILE	CB-CG2	5.58	1.70	1.52
1	A	834	TYR	CD1-CE1	-5.55	1.31	1.39
1	C	818	TYR	CD1-CE1	-5.53	1.31	1.39
1	E	856	ALA	CA-CB	5.47	1.64	1.52
1	A	856	ALA	CA-CB	-5.46	1.41	1.52
1	E	936	VAL	CB-CG2	5.46	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	812	GLU	N-CA	-5.43	1.35	1.46
1	A	883	VAL	CB-CG2	-5.40	1.41	1.52
1	C	882	GLU	CD-OE2	-5.38	1.19	1.25
1	B	884	SER	CB-OG	5.34	1.49	1.42
1	E	883	VAL	CB-CG2	-5.33	1.41	1.52
1	E	861	VAL	N-CA	-5.33	1.35	1.46
1	C	898	LYS	CE-NZ	-5.33	1.35	1.49
1	C	882	GLU	CD-OE1	-5.29	1.19	1.25
1	B	822	ARG	CG-CD	-5.23	1.38	1.51
1	D	889	ILE	N-CA	-5.18	1.35	1.46
1	A	855	SER	CB-OG	-5.17	1.35	1.42
1	B	798	GLY	N-CA	5.09	1.53	1.46
1	F	857	GLY	C-O	-5.07	1.15	1.23
1	C	911	VAL	CB-CG2	-5.05	1.42	1.52
1	C	781	GLU	CB-CG	-5.04	1.42	1.52
1	C	861	VAL	CB-CG1	-5.00	1.42	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	786	ARG	NE-CZ-NH1	-5.97	117.32	120.30
1	D	871	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	E	835	LEU	CB-CG-CD1	5.90	121.03	111.00
1	C	904	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	B	904	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	F	871	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	D	912	LEU	CB-CG-CD2	5.46	120.29	111.00
1	D	879	MET	CG-SD-CE	5.44	108.90	100.20
1	A	890	LEU	CB-CG-CD1	5.34	120.07	111.00
1	A	904	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	D	766	MET	CG-SD-CE	5.32	108.71	100.20
1	D	903	LYS	CD-CE-NZ	-5.27	99.58	111.70
1	D	912	LEU	CA-CB-CG	5.25	127.39	115.30
1	F	865	LEU	CB-CG-CD1	-5.21	102.15	111.00
1	B	805	GLN	N-CA-C	5.15	124.90	111.00
1	A	822	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	E	933	VAL	CB-CA-C	-5.02	101.86	111.40

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	51	0
1	B	1365	0	1379	63	0
1	C	1475	0	1475	38	0
1	D	1358	0	1370	78	0
1	E	1374	0	1385	44	0
1	F	1363	0	1381	52	0
2	A	74	0	0	3	0
2	B	42	0	0	2	0
2	C	65	0	0	3	0
2	D	42	0	0	1	0
2	E	59	0	0	4	0
2	F	48	0	0	5	0
All	All	8705	0	8431	310	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 18.

All (310) 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:HB2	1.29	1.13
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:HG3	1:D:815[B]:ARG:HH21	1.33	0.91
1:C:796:LYS:HE3	1:C:796:LYS:N	1.85	0.91
1:D:835:LEU:HD11	1:D:868:ALA:CB	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:940:ARG:HG2	1:B:941:GLU:N	1.85	0.88
1:D:766:MET:HE2	1:D:878:ALA:HB2	1.54	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:815[B]:ARG:CG	1:D:815[B]:ARG:HH21	1.92	0.83
1:D:815[B]:ARG:NH2	1:D:815[B]:ARG:HG3	1.89	0.83
1:D:876:ASN:HD21	1:D:908:THR:HG23	1.42	0.83
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:F:877:LEU:HD12	1:F:877:LEU:C	2.05	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: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: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
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:O	1:B:778:LEU:HD12	1.92	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:B:876:ASN:OD1	1:B:907:VAL:HA	1.93	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:A:810:MET:HE2	2:A:2034:HOH:O	1.96	0.66
1:F:896:LYS:HB2	1:F:923:LEU:CD2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:784:LEU:HD11	1:B:834:TYR:HH	1.62	0.65
1:B:808:GLU:OE1	1:B:811:LYS:NZ	2.30	0.65
1:C:758:ASP:N	1:C:758:ASP:OD2	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:A:785:ARG:C	1:B:826:MET:HE1	2.20	0.62
1:B:807:GLY:O	1:B:809:VAL:N	2.32	0.62
1:D:823:ALA:HA	1:D:826:MET:HE2	1.80	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:C:808[A]:GLU:CD	1:C:808[A]:GLU:H	2.02	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:D:827:GLN:HA	1:D:827:GLN:HE21	1.67	0.59
1:A:936:VAL:HG21	1:A:942:ILE:HD11	1.84	0.59
1:B:910:ILE:CG2	1:B:933:VAL:HG13	2.34	0.58
1:A:920:PHE:CZ	1:A:928:THR:HG23	2.38	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: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:F:784:LEU:HD13	1:F:838:SER:HB3	1.87	0.57
1:E:932:GLU:OE2	1:E:934:HIS:NE2	2.35	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:768:LEU:CD1	1:A:910:ILE:HD11	2.34	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:A:819:THR:OG1	1:E:812:GLU:HG3	2.05	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: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:F:836:VAL:O	1:F:836:VAL:HG12	2.06	0.55
1:C:951:GLN:HB2	2:C:2062:HOH:O	2.06	0.55
1:A:855:SER:HB2	1:A:892:VAL:HG11	1.89	0.54
1:D:834:TYR:O	1:D:838:SER:OG	2.24	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:E:806:LEU:CD2	1:E:810:MET:CB	2.86	0.53
1:D:763:GLY:O	1:D:781:GLU:HA	2.08	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:E:762:PRO:HD3	1:E:872:PRO:HB3	1.91	0.53
1:A:766:MET:HE3	1:A:777:THR:HB	1.90	0.53
1:C:784:LEU:HD21	1:C:838:SER:HB3	1.90	0.53
1:B:812:GLU:O	1:B:816:ILE:HD12	2.09	0.53
1:F:809:VAL:CG1	1:F:854:PRO:HG3	2.38	0.53
1:F:803:THR:C	2:F:2012:HOH:O	2.47	0.52
1:A:835:LEU:HD13	1:A:868:ALA:HB2	1.92	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: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:D:802:VAL:HG11	1:D:806:LEU:HD11	1.93	0.51
1:B:799:SER:HG	1:B:839:HIS:HD1	1.59	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:B:766:MET:HE1	1:B:907:VAL:HG22	1.93	0.51
1:A:889:ILE:CD1	1:A:938:HIS:C	2.79	0.51
1:F:766:MET:HE1	1:F:777:THR:HG21	1.93	0.50
1:D:766:MET:HE2	1:D:878:ALA:CB	2.34	0.50
1:D:766:MET:CE	1:D:907:VAL:HG21	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:768:LEU:HD13	1:D:878:ALA:HB1	1.94	0.49
1:B:939:TYR:O	1:B:940:ARG:C	2.49	0.49
1:F:940:ARG:HB2	1:F:940:ARG:HH11	1.76	0.49
1:F:766:MET:HE2	1:F:777:THR:HG22	1.94	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:B:829:ALA:O	1:B:830:PRO:C	2.49	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
1:E:806:LEU:HD22	1:E:810:MET:CB	2.43	0.49
1:A:939:TYR:C	1:A:939:TYR:CD2	2.85	0.49
1:F:835:LEU:HD13	1:F:868:ALA:HB2	1.93	0.49
1:B:767:GLY:C	1:B:768:LEU:HD22	2.32	0.49
1:D:785:ARG:HB3	1:D:841:HIS:HB2	1.94	0.49
1:C:876:ASN:CB	1:C:908:THR:HG22	2.42	0.49
1:D:765:VAL:HG22	1:D:873:VAL:CG2	2.26	0.49
1:A:920:PHE:CZ	1:A:933:VAL:HG21	2.48	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:759:VAL:O	1:B:759:VAL:HG13	2.12	0.49
1:B:876:ASN:ND2	1:B:908:THR:HB	2.20	0.49
1:D:835:LEU:CD1	1:D:868:ALA:HB1	2.42	0.49
1:E:934:HIS:CG	1:E:945:ILE:HD13	2.47	0.49
1:C:873:VAL:HG12	1:C:874:ARG:N	2.28	0.49
1:E:910:ILE:HG23	1:E:931:LEU:HD22	1.94	0.49
1:D:913:PRO:HB2	1:D:916:ASN:OD1	2.13	0.48
1:B:766:MET:HE3	1:B:878:ALA:HB2	1.95	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:A:889:ILE:HD12	1:A:938:HIS:C	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:802:VAL:CG1	1:D:806:LEU:HD21	2.43	0.48
1:B:807:GLY:C	1:B:809:VAL:N	2.67	0.47
1:A:786:ARG:N	1:B:826:MET:HE1	2.28	0.47
1:E:806:LEU:CB	1:E:810:MET:HG2	2.44	0.47
1:A:766:MET:HE2	1:A:907:VAL:HG21	1.96	0.47
1:F:834:TYR:CD2	1:F:868:ALA:HA	2.49	0.47
1:E:759:VAL:HG23	1:E:875:GLN:NE2	2.30	0.47
1:D:766:MET:HE3	1:D:878:ALA:CB	2.20	0.47
1:D:880:THR:O	1:D:880:THR:HG23	2.15	0.47
1:C:925:ALA:HB3	1:E:827:GLN:O	2.14	0.47
1:C:755:ARG:N	2:C:2001:HOH:O	2.46	0.47
1:B:829:ALA:C	1:B:831:ALA:N	2.61	0.47
1:B:800:LEU:HB2	1:B:818:TYR:CE1	2.50	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:D:862:THR:O	1:D:863:ALA:C	2.52	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: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: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: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:C:903:LYS:NZ	1:C:929:GLU:O	2.39	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:A:889:ILE:HD11	1:A:939:TYR:HA	1.97	0.46
1:F:766:MET:CE	1:F:777:THR:HG21	2.46	0.46
1:F:799:SER:OG	1:F:839:HIS:ND1	2.34	0.46
1:E:797:ASP:CG	1:E:797:ASP:O	2.53	0.46
1:F:896:LYS:CB	1:F:923:LEU:HD21	2.39	0.46
1:C:876:ASN:HB3	1:C:908:THR:HG22	1.97	0.46
1:B:768:LEU:N	1:B:768:LEU:HD22	2.31	0.45
1:B:807:GLY:O	1:B:808:GLU:C	2.54	0.45
1:F:766:MET:CE	1:F:777:THR:CG2	2.94	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:B:876:ASN:O	1:B:876:ASN:CG	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:841:HIS:CE1	1:B:843:HIS:HB2	2.52	0.45
1:E:876:ASN:O	1:E:876:ASN:CG	2.52	0.45
1:F:873:VAL:HG12	1:F:874:ARG:N	2.32	0.45
1:F:860:ILE:O	1:F:861:VAL:C	2.55	0.45
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:B:939:TYR:CE1	1:B:942:ILE:CG1	3.00	0.44
1:B:769:ALA:HB2	1:B:778:LEU:HD21	1.95	0.44
1:D:889:ILE:HD12	1:D:938:HIS:C	2.36	0.44
1:B:800:LEU:HD23	1:B:800:LEU:HA	1.82	0.44
1:A:945:ILE:O	1:A:945:ILE:HG22	2.17	0.44
1:A:924:ALA:CA	1:F:827:GLN:HE21	2.23	0.44
1:D:851:LYS:NZ	2:D:2020:HOH:O	2.51	0.44
1:B:759:VAL:HG23	1:B:875:GLN:HE21	1.82	0.44
1:E:875:GLN:O	1:E:876:ASN:HB3	2.17	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:D:765:VAL:HG12	1:D:859:THR:HG23	2.01	0.43
1:B:782:THR:HG21	1:B:864:LEU:HD23	2.01	0.43
1:A:873:VAL:HG12	1:A:874:ARG:N	2.33	0.43
1:E:872:PRO:CA	2:E:2029:HOH:O	2.63	0.43
1:A:787:PRO:CD	1:A:787:PRO:O	2.64	0.43
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:F:804:GLY:N	2:F:2012:HOH:O	2.51	0.43
1:C:779:PHE:O	1:C:845:PRO:CG	2.66	0.43
1:A:806:LEU:HB3	1:A:810:MET:HB3	2.00	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:B:943:PHE:CD1	1:B:943:PHE:C	2.92	0.43
1:B:768:LEU:CD2	1:B:878:ALA:HB1	2.34	0.42
1:A:925:ALA:O	1:A:929:GLU:N	2.51	0.42
1:D:873:VAL:HG12	1:D:874:ARG:N	2.34	0.42
1:D:766:MET:HE3	1:D:907:VAL:HG21	2.00	0.42
1:A:909:CYS:HA	1:A:932:GLU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:910:ILE:HD11	1:D:920:PHE:CE1	2.55	0.42
1:B:931:LEU:HA	1:B:931:LEU:HD12	1.93	0.42
1:F:770:TRP:HB2	1:F:898:LYS:HE3	2.02	0.42
1:C:831:ALA:HB3	2:C:2019:HOH:O	2.18	0.42
1:F:910:ILE:HG21	1:F:910:ILE:HD13	1.64	0.42
1:E:818:TYR:O	1:E:822:ARG:CD	2.68	0.42
1:A:803:THR:OG1	1:A:843:HIS:HD2	2.02	0.42
1:C:920:PHE:CZ	1:C:933:VAL:CG2	2.93	0.42
1:C:877:LEU:HD11	1:C:911:VAL:HG23	2.01	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:E:806:LEU:HD22	1:E:810:MET:HG2	2.02	0.42
1:C:787:PRO:HD3	1:D:836:VAL:HG11	2.01	0.42
1:D:876:ASN:HD21	1:D:908:THR:HG22	1.82	0.41
1:E:836:VAL:O	1:E:836:VAL:CG1	2.68	0.41
1:D:877:LEU:HD11	1:D:911:VAL:HG23	2.02	0.41
1:D:802:VAL:CG1	1:D:806:LEU:HD11	2.50	0.41
1:F:803:THR:OG1	1:F:841:HIS:NE2	2.50	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:B:857:GLY:O	1:B:861:VAL:HG12	2.20	0.41
1:B:825:LEU:HD22	1:B:835:LEU:CD2	2.42	0.41
1:B:769:ALA:CB	1:B:778:LEU:HD23	2.50	0.41
1:A:828:HIS:CE1	1:A:943:PHE:CZ	3.09	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:A:896:LYS:HG2	1:A:900:ILE:HD12	2.01	0.41
1:F:784:LEU:HD12	1:F:785:ARG:H	1.86	0.41
1:F:810:MET:HE1	1:F:844:VAL:HG11	2.02	0.41
1:F:782:THR:HA	1:F:841:HIS:O	2.21	0.41
1:C:921:TYR:CE1	1:E:940:ARG:HG2	2.56	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: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:771:THR:HG22	1:A:847:GLY:O	2.21	0.41
1:A:924:ALA:HB1	1:A:926:PHE:CE1	2.56	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:B:816:ILE:HG23	1:B:885:LEU:HD23	2.02	0.41
1:E:759:VAL:HG13	1:E:759:VAL:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:889:ILE:CD1	1:D:938:HIS:C	2.89	0.40
1:D:938:HIS:CD2	1:D:940:ARG:H	2.39	0.40
1:F:764:VAL:HG13	1:F:781:GLU:HG2	2.03	0.40
1:A:786:ARG:HA	1:B:826:MET:HE2	2.03	0.40
1:C:765:VAL:HG22	1:C:873:VAL:HG21	2.02	0.40
1:D:827:GLN:HA	1:D:827:GLN:NE2	2.35	0.40
1:A:889:ILE:HD12	1:A:938:HIS:HA	2.03	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:F:895:ILE:HD11	1:F:916:ASN:CG	2.42	0.40
1:D:865:LEU:O	1:D:869:MET:HG3	2.21	0.40
1:A:770:TRP:HB2	1:A:898:LYS:HE3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 (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	152/165 (92%)	134 (88%)	18 (12%)	6 3
1	B	144/165 (87%)	128 (89%)	16 (11%)	8 4
1	C	155/165 (94%)	142 (92%)	13 (8%)	14 8
1	D	143/165 (87%)	130 (91%)	13 (9%)	12 6
1	E	145/165 (88%)	133 (92%)	12 (8%)	14 8
1	F	144/165 (87%)	126 (88%)	18 (12%)	6 3
All	All	883/990 (89%)	793 (90%)	90 (10%)	9 5

All (90) 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
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	867	LEU
1	A	875	GLN
1	A	890	LEU
1	A	903	LYS
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

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Mol	Chain	Res	Type
1	B	806	LEU
1	B	827	GLN
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	940	ARG
1	B	942	ILE
1	C	758	ASP
1	C	759	VAL
1	C	768	LEU
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	890	LEU
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	813	SER
1	D	827	GLN
1	D	859	THR
1	D	871	ARG
1	D	884	SER
1	D	885	LEU
1	D	888	LYS
1	E	768	LEU
1	E	805	GLN
1	E	806	LEU
1	E	835	LEU

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Mol	Chain	Res	Type
1	E	838	SER
1	E	867	LEU
1	E	871	ARG
1	E	874	ARG
1	E	890	LEU
1	E	910	ILE
1	E	928	THR
1	E	933	VAL
1	F	759	VAL
1	F	768	LEU
1	F	773	MET
1	F	803	THR
1	F	805	GLN
1	F	806	LEU
1	F	810	MET
1	F	835	LEU
1	F	842	LEU
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) 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	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

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Mol	Chain	Res	Type
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 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, 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	190/207 (91%)	0.52	12 (6%)	23	24	25, 44, 66, 75	0
1	B	177/207 (85%)	0.71	15 (8%)	13	14	34, 53, 74, 86	0
1	C	192/207 (92%)	0.53	10 (5%)	31	33	26, 43, 62, 77	0
1	D	178/207 (85%)	0.56	9 (5%)	32	33	33, 52, 68, 93	0
1	E	181/207 (87%)	0.53	10 (5%)	29	30	27, 47, 70, 84	0
1	F	179/207 (86%)	0.67	12 (6%)	21	22	33, 55, 71, 87	1 (0%)
All	All	1097/1242 (88%)	0.58	68 (6%)	24	25	25, 49, 70, 93	1 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	805	GLN	6.2
1	F	805	GLN	5.2
1	E	772	ALA	5.1
1	B	772	ALA	4.8
1	E	797	ASP	4.7
1	B	803	THR	4.5
1	D	806	LEU	4.3
1	B	798	GLY	4.1
1	F	858	CYS	4.1
1	F	759	VAL	4.0
1	F	804	GLY	4.0
1	E	805	GLN	3.8
1	F	772	ALA	3.8
1	B	847	GLY	3.6
1	F	847	GLY	3.5
1	C	930	GLY	3.4
1	C	796	LYS	3.3
1	B	773	MET	3.2
1	B	762	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	908	THR	2.8
1	A	885	LEU	2.8
1	D	760	THR	2.7
1	E	773	MET	2.7
1	C	952	ALA	2.7
1	A	942	ILE	2.6
1	E	759	VAL	2.6
1	E	806	LEU	2.6
1	B	828	HIS	2.6
1	B	831	ALA	2.6
1	E	846	GLU	2.5
1	D	802	VAL	2.5
1	E	785	ARG	2.5
1	B	868	ALA	2.5
1	D	923	LEU	2.5
1	B	841	HIS	2.5
1	C	858	CYS	2.5
1	C	788	GLN	2.4
1	A	819	THR	2.4
1	F	784	LEU	2.4
1	A	759	VAL	2.3
1	B	846	GLU	2.3
1	C	885	LEU	2.3
1	A	820	PHE	2.3
1	D	831	ALA	2.3
1	C	758	ASP	2.3
1	D	885	LEU	2.3
1	F	929	GLU	2.3
1	D	803	THR	2.2
1	C	864	LEU	2.2
1	E	778	LEU	2.2
1	D	947	PHE	2.2
1	A	952	ALA	2.2
1	A	949	ASP	2.2
1	A	928	THR	2.2
1	B	802	VAL	2.2
1	B	768	LEU	2.2
1	F	773	MET	2.2
1	A	788	GLN	2.2
1	A	802	VAL	2.2
1	B	759	VAL	2.1
1	B	948	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	908	THR	2.1
1	F	760	THR	2.1
1	F	870	GLY	2.1
1	A	864	LEU	2.1
1	F	907	VAL	2.1
1	A	784	LEU	2.1
1	C	816	ILE	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.