Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 12:47 pm BST

PDB ID	:	4D80
Title	:	Metallosphera sedula Vps4 crystal structure
Authors	:	Caillat, C.; Macheboeuf, P.; Wu, Y.; McCarthy, A.A.; Boeri-Erba, E.; Effantin, G.; Gottlinger, H.G.; Weissenhorn, W.; Renesto, P.
Deposited on	:	2014-12-02
Resolution	:	3.60 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:

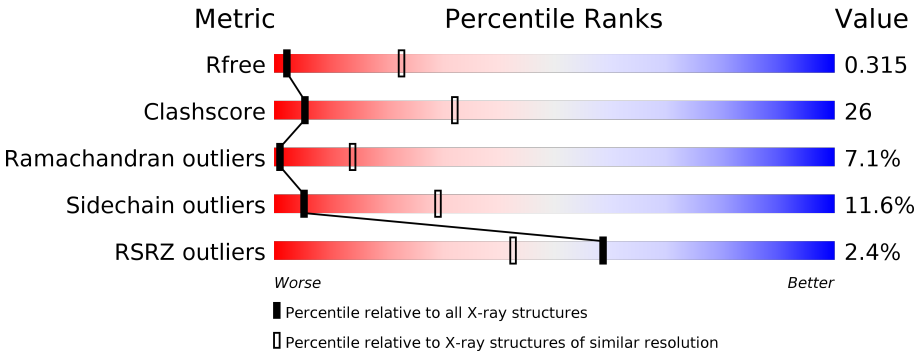
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	316	3% 43% 32% 8% • 15%
1	B	316	3% 46% 24% 10% • 19%
1	C	316	2% 47% 30% 9% • 14%
1	D	316	% 45% 32% 8% • 14%
1	E	316	2% 45% 27% 10% • 17%
1	F	316	% 43% 34% 9% • 13%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12875 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 AAA ATPASE, CENTRAL DOMAIN PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2152	1376	371	397	8			
1	B	257	Total	C	N	O	S	0	0	0
			2060	1319	356	377	8			
1	C	272	Total	C	N	O	S	0	0	0
			2177	1394	373	402	8			
1	D	273	Total	C	N	O	S	0	0	0
			2187	1400	376	403	8			
1	E	262	Total	C	N	O	S	0	0	0
			2106	1347	364	387	8			
1	F	274	Total	C	N	O	S	0	0	0
			2193	1405	378	402	8			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	MET	-	expression tag	UNP A4YHC5
A	55	SER	-	expression tag	UNP A4YHC5
A	56	TYR	-	expression tag	UNP A4YHC5
A	57	TYR	-	expression tag	UNP A4YHC5
A	58	HIS	-	expression tag	UNP A4YHC5
A	59	HIS	-	expression tag	UNP A4YHC5
A	60	HIS	-	expression tag	UNP A4YHC5
A	61	HIS	-	expression tag	UNP A4YHC5
A	62	HIS	-	expression tag	UNP A4YHC5
A	63	HIS	-	expression tag	UNP A4YHC5
A	64	LEU	-	expression tag	UNP A4YHC5
A	65	GLU	-	expression tag	UNP A4YHC5
A	66	SER	-	expression tag	UNP A4YHC5
A	67	THR	-	expression tag	UNP A4YHC5
A	68	SER	-	expression tag	UNP A4YHC5
A	69	LEU	-	expression tag	UNP A4YHC5
A	70	TYR	-	expression tag	UNP A4YHC5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	71	LYS	-	expression tag	UNP A4YHC5
A	72	LYS	-	expression tag	UNP A4YHC5
A	73	ALA	-	expression tag	UNP A4YHC5
A	74	GLY	-	expression tag	UNP A4YHC5
B	54	MET	-	expression tag	UNP A4YHC5
B	55	SER	-	expression tag	UNP A4YHC5
B	56	TYR	-	expression tag	UNP A4YHC5
B	57	TYR	-	expression tag	UNP A4YHC5
B	58	HIS	-	expression tag	UNP A4YHC5
B	59	HIS	-	expression tag	UNP A4YHC5
B	60	HIS	-	expression tag	UNP A4YHC5
B	61	HIS	-	expression tag	UNP A4YHC5
B	62	HIS	-	expression tag	UNP A4YHC5
B	63	HIS	-	expression tag	UNP A4YHC5
B	64	LEU	-	expression tag	UNP A4YHC5
B	65	GLU	-	expression tag	UNP A4YHC5
B	66	SER	-	expression tag	UNP A4YHC5
B	67	THR	-	expression tag	UNP A4YHC5
B	68	SER	-	expression tag	UNP A4YHC5
B	69	LEU	-	expression tag	UNP A4YHC5
B	70	TYR	-	expression tag	UNP A4YHC5
B	71	LYS	-	expression tag	UNP A4YHC5
B	72	LYS	-	expression tag	UNP A4YHC5
B	73	ALA	-	expression tag	UNP A4YHC5
B	74	GLY	-	expression tag	UNP A4YHC5
C	54	MET	-	expression tag	UNP A4YHC5
C	55	SER	-	expression tag	UNP A4YHC5
C	56	TYR	-	expression tag	UNP A4YHC5
C	57	TYR	-	expression tag	UNP A4YHC5
C	58	HIS	-	expression tag	UNP A4YHC5
C	59	HIS	-	expression tag	UNP A4YHC5
C	60	HIS	-	expression tag	UNP A4YHC5
C	61	HIS	-	expression tag	UNP A4YHC5
C	62	HIS	-	expression tag	UNP A4YHC5
C	63	HIS	-	expression tag	UNP A4YHC5
C	64	LEU	-	expression tag	UNP A4YHC5
C	65	GLU	-	expression tag	UNP A4YHC5
C	66	SER	-	expression tag	UNP A4YHC5
C	67	THR	-	expression tag	UNP A4YHC5
C	68	SER	-	expression tag	UNP A4YHC5
C	69	LEU	-	expression tag	UNP A4YHC5
C	70	TYR	-	expression tag	UNP A4YHC5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	71	LYS	-	expression tag	UNP A4YHC5
C	72	LYS	-	expression tag	UNP A4YHC5
C	73	ALA	-	expression tag	UNP A4YHC5
C	74	GLY	-	expression tag	UNP A4YHC5
D	54	MET	-	expression tag	UNP A4YHC5
D	55	SER	-	expression tag	UNP A4YHC5
D	56	TYR	-	expression tag	UNP A4YHC5
D	57	TYR	-	expression tag	UNP A4YHC5
D	58	HIS	-	expression tag	UNP A4YHC5
D	59	HIS	-	expression tag	UNP A4YHC5
D	60	HIS	-	expression tag	UNP A4YHC5
D	61	HIS	-	expression tag	UNP A4YHC5
D	62	HIS	-	expression tag	UNP A4YHC5
D	63	HIS	-	expression tag	UNP A4YHC5
D	64	LEU	-	expression tag	UNP A4YHC5
D	65	GLU	-	expression tag	UNP A4YHC5
D	66	SER	-	expression tag	UNP A4YHC5
D	67	THR	-	expression tag	UNP A4YHC5
D	68	SER	-	expression tag	UNP A4YHC5
D	69	LEU	-	expression tag	UNP A4YHC5
D	70	TYR	-	expression tag	UNP A4YHC5
D	71	LYS	-	expression tag	UNP A4YHC5
D	72	LYS	-	expression tag	UNP A4YHC5
D	73	ALA	-	expression tag	UNP A4YHC5
D	74	GLY	-	expression tag	UNP A4YHC5
E	54	MET	-	expression tag	UNP A4YHC5
E	55	SER	-	expression tag	UNP A4YHC5
E	56	TYR	-	expression tag	UNP A4YHC5
E	57	TYR	-	expression tag	UNP A4YHC5
E	58	HIS	-	expression tag	UNP A4YHC5
E	59	HIS	-	expression tag	UNP A4YHC5
E	60	HIS	-	expression tag	UNP A4YHC5
E	61	HIS	-	expression tag	UNP A4YHC5
E	62	HIS	-	expression tag	UNP A4YHC5
E	63	HIS	-	expression tag	UNP A4YHC5
E	64	LEU	-	expression tag	UNP A4YHC5
E	65	GLU	-	expression tag	UNP A4YHC5
E	66	SER	-	expression tag	UNP A4YHC5
E	67	THR	-	expression tag	UNP A4YHC5
E	68	SER	-	expression tag	UNP A4YHC5
E	69	LEU	-	expression tag	UNP A4YHC5
E	70	TYR	-	expression tag	UNP A4YHC5

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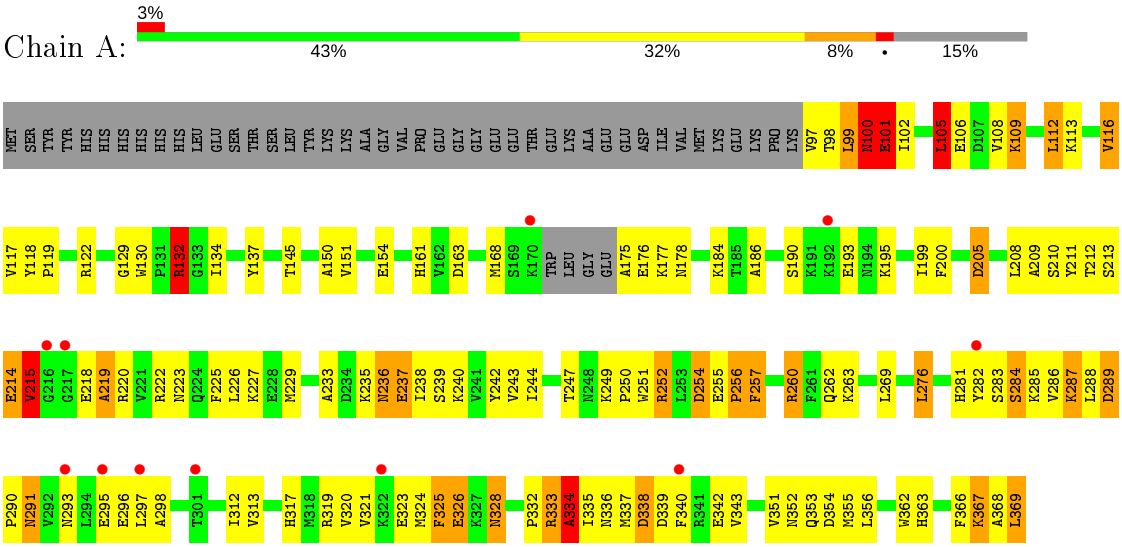
Chain	Residue	Modelled	Actual	Comment	Reference
E	71	LYS	-	expression tag	UNP A4YHC5
E	72	LYS	-	expression tag	UNP A4YHC5
E	73	ALA	-	expression tag	UNP A4YHC5
E	74	GLY	-	expression tag	UNP A4YHC5
F	54	MET	-	expression tag	UNP A4YHC5
F	55	SER	-	expression tag	UNP A4YHC5
F	56	TYR	-	expression tag	UNP A4YHC5
F	57	TYR	-	expression tag	UNP A4YHC5
F	58	HIS	-	expression tag	UNP A4YHC5
F	59	HIS	-	expression tag	UNP A4YHC5
F	60	HIS	-	expression tag	UNP A4YHC5
F	61	HIS	-	expression tag	UNP A4YHC5
F	62	HIS	-	expression tag	UNP A4YHC5
F	63	HIS	-	expression tag	UNP A4YHC5
F	64	LEU	-	expression tag	UNP A4YHC5
F	65	GLU	-	expression tag	UNP A4YHC5
F	66	SER	-	expression tag	UNP A4YHC5
F	67	THR	-	expression tag	UNP A4YHC5
F	68	SER	-	expression tag	UNP A4YHC5
F	69	LEU	-	expression tag	UNP A4YHC5
F	70	TYR	-	expression tag	UNP A4YHC5
F	71	LYS	-	expression tag	UNP A4YHC5
F	72	LYS	-	expression tag	UNP A4YHC5
F	73	ALA	-	expression tag	UNP A4YHC5
F	74	GLY	-	expression tag	UNP A4YHC5

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.

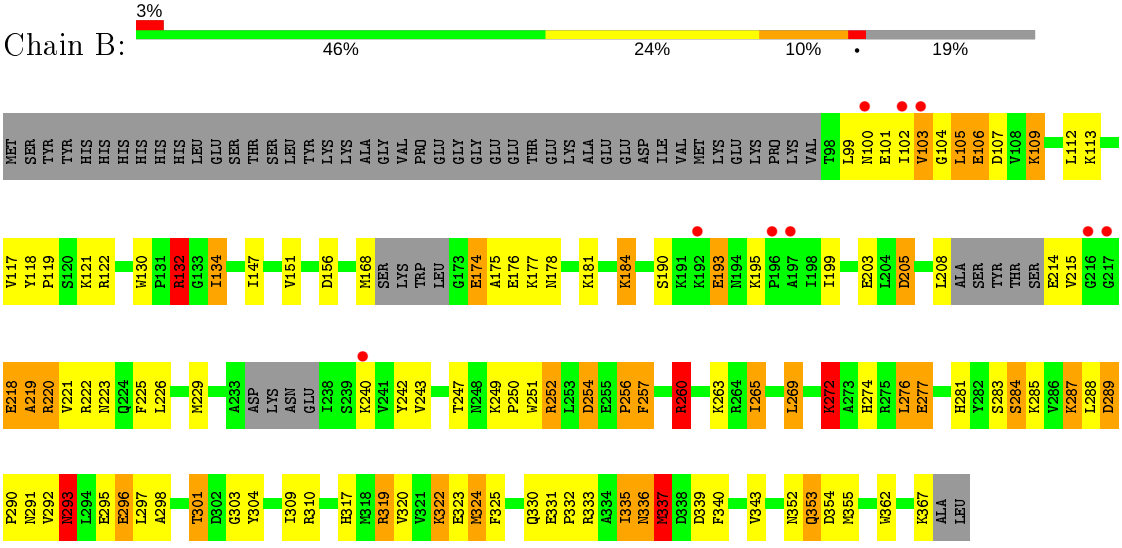
- Molecule 1: AAA ATPASE, CENTRAL DOMAIN PROTEIN

Chain A:



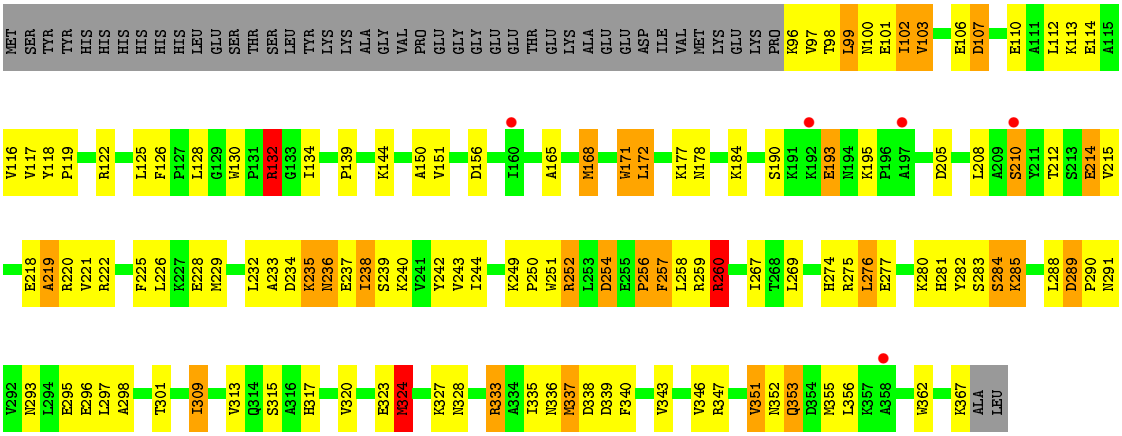
- Molecule 1: AAA ATPASE, CENTRAL DOMAIN PROTEIN

Chain B:



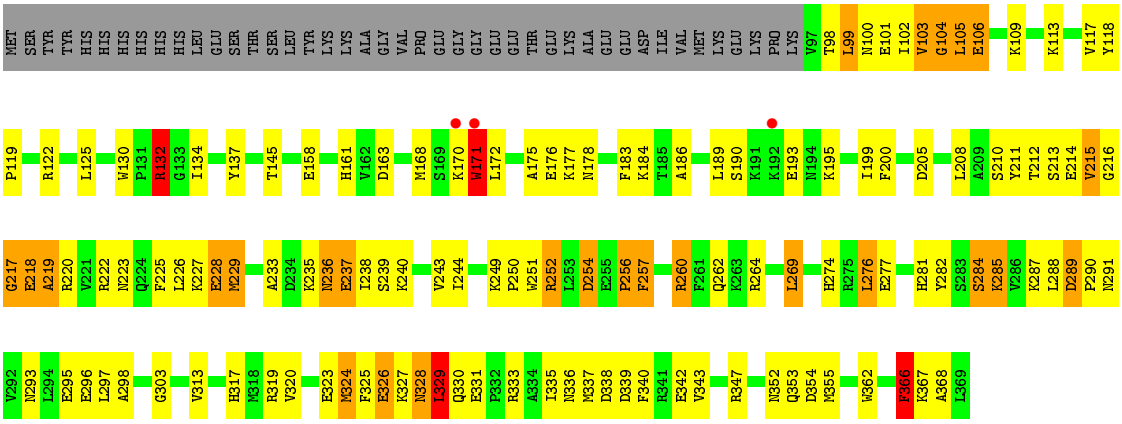
- Molecule 1: AAA ATPASE, CENTRAL DOMAIN PROTEIN

Chain C:



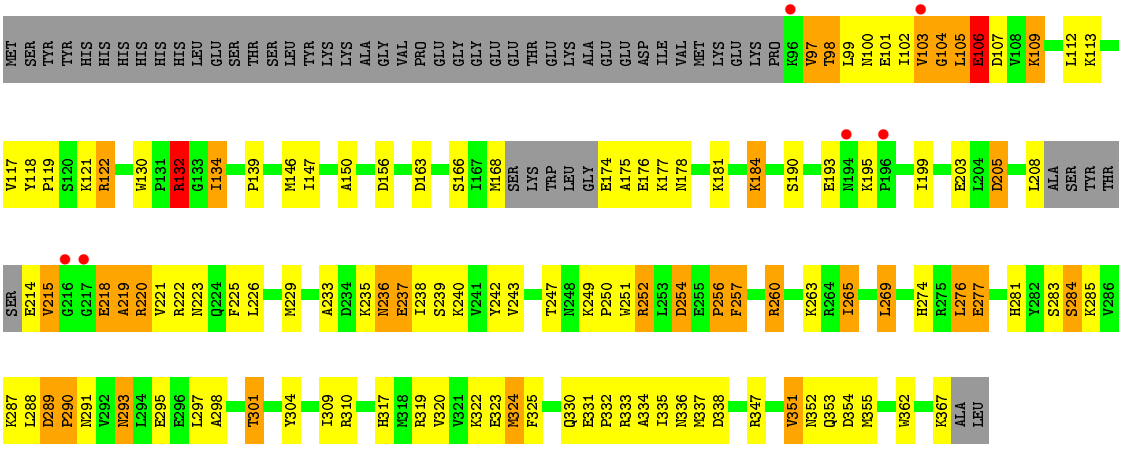
• Molecule 1: AAA ATPASE, CENTRAL DOMAIN PROTEIN

Chain D:



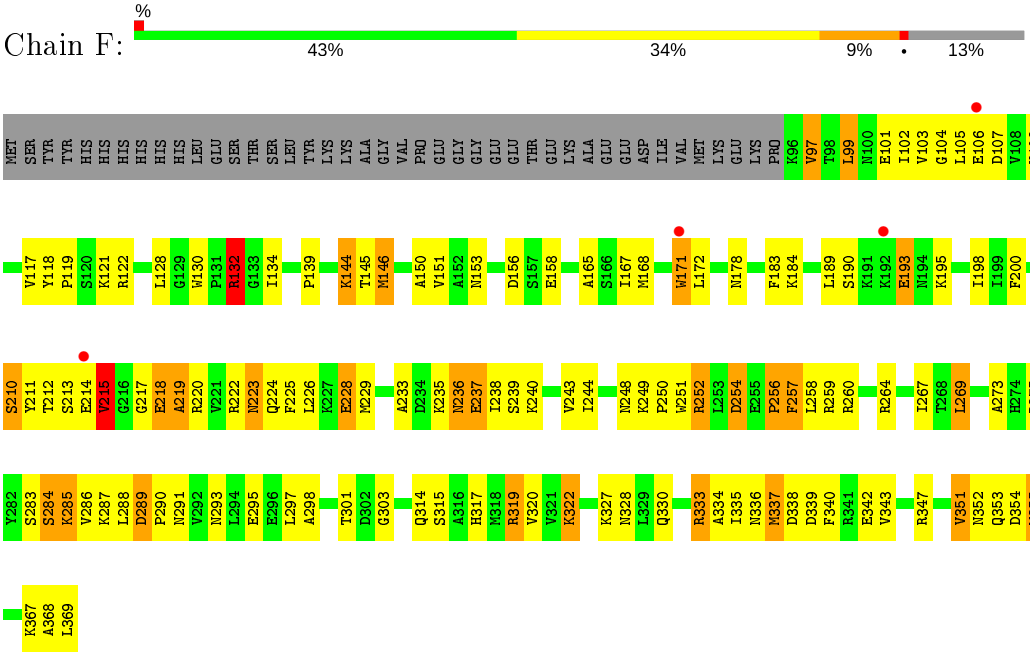
• Molecule 1: AAA ATPASE, CENTRAL DOMAIN PROTEIN

Chain E:



• Molecule 1: AAA ATPASE, CENTRAL DOMAIN PROTEIN

Chain F:


%
43%
34%
9%
13%
MET SER TYR TYR HIS HIS HIS HIS HIS HIS LEU GLU SER THR SER LEU TYR LYS LYS ALA GLY VAL PRO GLU GLY GLY GLU GLU GLU THR GLU LYS ALA GLU GLU ASP ILE VAL MET LYS GLU LYS PRO K96 V97 T98 L99 N100 E101 I102 V103 G104 L105 E106 D107 V108 K109 E110 A111 L112 K113
V117 Y118 P119 S120 K121 R122 L128 G129 W130 P131 R132 G133 I134 P139 K144 T145 M146 A150 V151 A162 N153 D156 S157 E158 A165 S166 I167 M168 W171 L172 N178 F183 K184 L189 S190 K191 K192 E193 N194 K195 I198 I199 F200 D205 L208 A209
S210 Y211 T212 S213 E214 V215 G216 G217 E218 A219 R220 V221 R222 N223 Q224 F225 L226 K227 E228 M229 A233 D234 K235 N236 E237 I238 S239 K240 V243 I244 N248 K249 P250 W251 R252 L253 D254 E255 P256 F257 L258 R259 R260 R264 I267 T268 L269 A273 H274 R275 L276 E277 H281
Y282 S283 S284 K285 V286 K287 L288 D289 P290 N291 V292 N293 L294 E295 E296 L297 A298 T301 D302 G303 Q314 S315 A316 H317 M318 R319 V320 V321 K322 K327 N328 L329 Q330 R333 A334 I335 N336 M337 D338 D339 F340 R341 E342 V343 R347 V351 N352 Q353 D354 M355 W362 H363 E364
K367 A368 L369

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	99.70Å 127.39Å 191.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	106.02 – 3.60 39.26 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (106.02-3.60) 99.8 (39.26-3.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0071	Depositor
R, R_{free}	0.264 , 0.318 0.263 , 0.315	Depositor DCC
R_{free} test set	1464 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	110.9	Xtriage
Anisotropy	0.574	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 79.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12875	wwPDB-VP
Average B, all atoms (Å^2)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1588e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.52	0/2191	0.89	5/2952 (0.2%)
1	B	0.51	0/2097	0.89	7/2823 (0.2%)
1	C	0.53	0/2220	0.88	5/2995 (0.2%)
1	D	0.51	0/2230	0.89	4/3009 (0.1%)
1	E	0.52	0/2144	0.83	4/2887 (0.1%)
1	F	0.52	0/2236	0.92	9/3016 (0.3%)
All	All	0.52	0/13118	0.88	34/17682 (0.2%)

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	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	366	PHE	CB-CG-CD1	12.31	129.42	120.80
1	D	366	PHE	CB-CG-CD2	-10.34	113.56	120.80
1	F	99	LEU	CA-CB-CG	8.48	134.80	115.30
1	A	132	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	D	132	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	C	333	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	C	333	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	C	132	ARG	NE-CZ-NH1	7.71	124.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	132	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	E	132	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	F	333	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	F	333	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	B	337	MET	CG-SD-CE	7.32	111.91	100.20
1	B	132	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	C	260	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	F	208	LEU	CB-CG-CD1	-6.69	99.63	111.00
1	A	105	LEU	CB-CG-CD2	-6.65	99.69	111.00
1	B	260	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	B	337	MET	CB-CG-SD	6.30	131.29	112.40
1	E	104	GLY	N-CA-C	-6.23	97.53	113.10
1	F	347	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	B	319	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	105	LEU	CB-CG-CD1	5.82	120.90	111.00
1	F	355	MET	CG-SD-CE	5.76	109.42	100.20
1	E	134	ILE	CB-CA-C	-5.57	100.47	111.60
1	E	319	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	134	ILE	CB-CA-C	-5.41	100.78	111.60
1	F	355	MET	CB-CA-C	5.36	121.12	110.40
1	A	100	ASN	C-N-CA	5.33	135.03	121.70
1	A	338	ASP	N-CA-CB	5.15	119.87	110.60
1	B	272	LYS	CB-CG-CD	-5.09	98.36	111.60
1	C	324	MET	CG-SD-CE	5.06	108.29	100.20
1	F	319	ARG	NE-CZ-NH1	-5.03	117.79	120.30
1	D	229	MET	CG-SD-CE	-5.02	92.17	100.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	334	ALA	Peptide
1	B	335	ILE	Peptide
1	C	107	ASP	Peptide
1	D	170	LYS	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	2152	0	2201	144	0
1	B	2060	0	2106	110	0
1	C	2177	0	2219	111	1
1	D	2187	0	2233	120	0
1	E	2106	0	2155	101	0
1	F	2193	0	2244	127	1
All	All	12875	0	13158	678	1

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 26.

All (678) 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:A:287:LYS:O	1:A:335:ILE:CG2	1.68	1.38
1:A:210:SER:HB3	1:A:211:TYR:N	1.54	1.19
1:B:288:LEU:O	1:B:335:ILE:O	1.66	1.11
1:A:287:LYS:O	1:A:335:ILE:HG21	0.96	1.10
1:A:112:LEU:HD22	1:A:151:VAL:HG11	1.35	1.08
1:E:100:ASN:HB2	1:E:101:GLU:HA	1.39	1.04
1:B:292:VAL:HA	1:B:337:MET:HG3	1.40	1.01
1:B:100:ASN:HB2	1:B:101:GLU:HA	1.40	1.00
1:A:324:MET:O	1:A:325:PHE:HB2	1.64	0.97
1:F:273:ALA:O	1:F:277:GLU:OE1	1.85	0.94
1:D:328:ASN:O	1:D:329:LEU:HB2	1.68	0.94
1:D:336:ASN:OD1	1:D:337:MET:N	2.02	0.93
1:E:336:ASN:OD1	1:E:337:MET:N	2.02	0.92
1:C:144:LYS:HG2	1:C:267:ILE:HD11	1.50	0.92
1:D:215:VAL:HG13	1:D:216:GLY:H	1.36	0.91
1:A:210:SER:CB	1:A:211:TYR:N	2.34	0.90
1:B:287:LYS:HE2	1:B:332:PRO:HG2	1.54	0.89
1:A:210:SER:HB3	1:A:211:TYR:CA	2.02	0.89
1:A:289:ASP:HB3	1:A:335:ILE:O	1.73	0.89
1:D:329:LEU:HD12	1:D:331:GLU:O	1.72	0.88
1:B:103:VAL:HG13	1:B:277:GLU:HB2	1.54	0.87
1:B:99:LEU:HA	1:B:101:GLU:HB2	1.58	0.86
1:C:234:ASP:O	1:C:236:ASN:N	2.08	0.86
1:B:292:VAL:HA	1:B:337:MET:CG	2.05	0.86
1:E:103:VAL:HG13	1:E:277:GLU:HB2	1.56	0.86
1:F:144:LYS:NZ	1:F:248:ASN:OD1	2.09	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:ASN:O	1:D:101:GLU:HG2	1.77	0.85
1:A:215:VAL:HG21	1:F:211:TYR:CZ	2.12	0.84
1:A:112:LEU:CD2	1:A:151:VAL:HG11	2.05	0.84
1:A:289:ASP:OD1	1:A:290:PRO:O	1.94	0.84
1:A:99:LEU:HG	1:A:109:LYS:CE	2.06	0.84
1:B:289:ASP:OD1	1:B:290:PRO:O	1.96	0.84
1:C:289:ASP:OD1	1:C:290:PRO:O	1.95	0.84
1:F:289:ASP:OD1	1:F:290:PRO:O	1.95	0.84
1:E:289:ASP:OD1	1:E:290:PRO:O	1.97	0.83
1:B:134:ILE:HD13	1:B:263:LYS:HB3	1.59	0.83
1:E:134:ILE:HD13	1:E:263:LYS:HB3	1.59	0.82
1:A:99:LEU:HD11	1:A:154:GLU:HB2	1.59	0.82
1:E:229:MET:HE2	1:E:243:VAL:HG11	1.61	0.82
1:D:289:ASP:OD1	1:D:290:PRO:O	1.97	0.82
1:E:214:GLU:OE1	1:E:214:GLU:N	2.13	0.82
1:A:99:LEU:CD1	1:A:154:GLU:HB2	2.09	0.82
1:C:336:ASN:OD1	1:C:339:ASP:CG	2.18	0.82
1:D:175:ALA:O	1:D:178:ASN:OD1	1.96	0.81
1:A:175:ALA:O	1:A:178:ASN:OD1	1.97	0.81
1:D:362:TRP:CH2	1:D:367:LYS:HE3	2.15	0.81
1:F:336:ASN:OD1	1:F:339:ASP:CG	2.19	0.81
1:B:293:ASN:O	1:B:293:ASN:ND2	2.12	0.81
1:E:99:LEU:HA	1:E:101:GLU:HB2	1.63	0.81
1:B:214:GLU:N	1:B:214:GLU:OE1	2.14	0.80
1:D:339:ASP:O	1:D:343:VAL:HG13	1.81	0.80
1:A:333:ARG:N	1:A:334:ALA:HB2	1.98	0.78
1:A:324:MET:SD	1:A:332:PRO:CA	2.72	0.77
1:E:199:ILE:CG2	1:E:243:VAL:HG22	2.15	0.77
1:B:199:ILE:CG2	1:B:243:VAL:HG22	2.15	0.77
1:D:328:ASN:O	1:D:329:LEU:CB	2.34	0.76
1:A:215:VAL:HG21	1:F:211:TYR:CE1	2.22	0.75
1:A:287:LYS:HG2	1:A:287:LYS:O	1.85	0.74
1:D:211:TYR:HB3	1:D:217:GLY:HA3	1.70	0.74
1:D:229:MET:HE2	1:D:243:VAL:HG11	1.68	0.74
1:A:229:MET:HE2	1:A:243:VAL:HG11	1.69	0.74
1:A:215:VAL:HG11	1:F:211:TYR:CD2	2.23	0.73
1:F:99:LEU:O	1:F:99:LEU:HD13	1.88	0.73
1:B:287:LYS:CE	1:B:332:PRO:HG2	2.17	0.73
1:A:333:ARG:HB3	1:A:334:ALA:HA	1.71	0.73
1:B:229:MET:HE2	1:B:243:VAL:HG11	1.71	0.73
1:F:214:GLU:O	1:F:215:VAL:HB	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:HD22	1:A:151:VAL:CG1	2.18	0.72
1:A:105:LEU:O	1:A:105:LEU:HD22	1.90	0.72
1:E:100:ASN:CB	1:E:101:GLU:HA	2.17	0.72
1:A:214:GLU:O	1:A:215:VAL:HB	1.88	0.72
1:D:215:VAL:HG13	1:D:216:GLY:N	2.05	0.71
1:F:183:PHE:CD2	1:F:228:GLU:HG2	2.24	0.71
1:D:183:PHE:CD2	1:D:228:GLU:HG2	2.25	0.71
1:C:260:ARG:HH11	1:C:260:ARG:HG3	1.55	0.71
1:F:229:MET:HE2	1:F:243:VAL:HG11	1.72	0.70
1:C:229:MET:HE2	1:C:243:VAL:HG11	1.73	0.70
1:A:320:VAL:HB	1:A:334:ALA:HB1	1.73	0.70
1:A:324:MET:CG	1:A:332:PRO:HA	2.21	0.70
1:D:362:TRP:CZ2	1:D:367:LYS:HE3	2.27	0.70
1:A:324:MET:SD	1:A:332:PRO:HA	2.31	0.70
1:B:291:ASN:OD1	1:B:336:ASN:O	2.10	0.70
1:B:260:ARG:HG3	1:B:260:ARG:HH11	1.57	0.69
1:A:105:LEU:CD2	1:A:108:VAL:HB	2.21	0.69
1:C:235:LYS:HB2	1:C:237:GLU:OE1	1.92	0.69
1:D:330:GLN:O	1:E:122:ARG:NH2	2.24	0.69
1:D:362:TRP:CH2	1:D:367:LYS:CE	2.75	0.69
1:B:102:ILE:O	1:B:103:VAL:HG23	1.93	0.69
1:C:102:ILE:O	1:C:103:VAL:HG23	1.93	0.69
1:B:99:LEU:HD13	1:B:109:LYS:CE	2.24	0.68
1:C:297:LEU:HD11	1:C:337:MET:HE1	1.75	0.68
1:E:102:ILE:O	1:E:103:VAL:HG23	1.92	0.68
1:E:287:LYS:O	1:E:335:ILE:HG22	1.94	0.68
1:F:297:LEU:HD11	1:F:337:MET:HE1	1.76	0.68
1:F:223:ASN:OD1	1:F:224:GLN:N	2.27	0.68
1:D:186:ALA:HB2	1:D:199:ILE:HD11	1.76	0.67
1:A:186:ALA:HB2	1:A:199:ILE:HD11	1.77	0.67
1:D:132:ARG:HH11	1:D:132:ARG:HG2	1.59	0.67
1:E:163:ASP:OD1	1:E:166:SER:OG	2.12	0.67
1:F:287:LYS:O	1:F:335:ILE:HG22	1.94	0.67
1:B:293:ASN:ND2	1:B:296:GLU:OE1	2.27	0.67
1:B:102:ILE:O	1:B:103:VAL:CB	2.42	0.67
1:B:102:ILE:O	1:B:103:VAL:HB	1.95	0.66
1:D:287:LYS:O	1:D:335:ILE:HG22	1.94	0.66
1:A:132:ARG:HG2	1:A:132:ARG:HH11	1.59	0.66
1:C:132:ARG:HG2	1:C:132:ARG:HH11	1.59	0.66
1:A:319:ARG:HH11	1:A:339:ASP:HA	1.61	0.66
1:B:323:GLU:OE1	1:B:333:ARG:NE	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:ILE:HG21	1:B:243:VAL:HG22	1.77	0.66
1:B:310:ARG:NH2	1:C:128:LEU:O	2.29	0.66
1:F:132:ARG:HG2	1:F:132:ARG:HH11	1.59	0.66
1:A:324:MET:O	1:A:325:PHE:CB	2.41	0.65
1:E:199:ILE:HG21	1:E:243:VAL:HG22	1.78	0.65
1:F:218:GLU:HA	1:F:222:ARG:NE	2.12	0.65
1:B:132:ARG:HH11	1:B:132:ARG:HG2	1.59	0.65
1:D:319:ARG:HH11	1:D:339:ASP:HA	1.62	0.65
1:F:249:LYS:HE3	1:F:252:ARG:NH1	2.11	0.65
1:F:319:ARG:HH12	1:F:342:GLU:HB2	1.61	0.65
1:A:289:ASP:CB	1:A:335:ILE:O	2.45	0.65
1:B:287:LYS:O	1:B:335:ILE:HG22	1.96	0.64
1:D:216:GLY:C	1:D:218:GLU:H	1.99	0.64
1:E:132:ARG:HH11	1:E:132:ARG:HG2	1.59	0.64
1:A:333:ARG:HB3	1:A:334:ALA:CA	2.26	0.64
1:E:199:ILE:HG22	1:E:242:TYR:O	1.97	0.64
1:F:150:ALA:O	1:F:153:ASN:OD1	2.16	0.64
1:B:100:ASN:CB	1:B:101:GLU:HA	2.18	0.64
1:C:118:TYR:HB2	1:C:119:PRO:HD3	1.80	0.64
1:F:118:TYR:HB2	1:F:119:PRO:HD3	1.80	0.64
1:F:226:LEU:HD21	1:F:260:ARG:NH1	2.12	0.64
1:A:363:HIS:O	1:A:367:LYS:HD3	1.98	0.64
1:F:146:MET:SD	1:F:146:MET:C	2.77	0.64
1:A:333:ARG:CB	1:A:334:ALA:HA	2.28	0.63
1:D:103:VAL:CG1	1:D:277:GLU:HB3	2.28	0.63
1:A:105:LEU:C	1:A:105:LEU:HD22	2.19	0.63
1:E:323:GLU:OE1	1:E:333:ARG:NE	2.30	0.63
1:F:319:ARG:HH11	1:F:339:ASP:HA	1.64	0.63
1:A:226:LEU:HG	1:A:260:ARG:HD3	1.80	0.63
1:F:144:LYS:CE	1:F:248:ASN:OD1	2.46	0.63
1:D:226:LEU:HG	1:D:260:ARG:HD3	1.80	0.63
1:B:199:ILE:HG22	1:B:242:TYR:O	1.98	0.63
1:A:99:LEU:HD12	1:A:150:ALA:O	1.98	0.63
1:F:336:ASN:OD1	1:F:339:ASP:OD2	2.15	0.63
1:D:262:GLN:OE1	1:D:262:GLN:N	2.32	0.62
1:F:319:ARG:NH1	1:F:339:ASP:HA	2.14	0.62
1:B:134:ILE:CD1	1:B:263:LYS:HB3	2.28	0.62
1:D:118:TYR:HB2	1:D:119:PRO:HD3	1.82	0.62
1:B:269:LEU:HD21	1:B:303:GLY:HA2	1.81	0.62
1:E:134:ILE:CD1	1:E:263:LYS:HB3	2.28	0.62
1:D:102:ILE:O	1:D:103:VAL:HG22	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:LYS:O	1:B:287:LYS:HG2	1.97	0.62
1:F:237:GLU:O	1:F:239:SER:N	2.33	0.62
1:F:269:LEU:HD21	1:F:303:GLY:HA2	1.81	0.62
1:C:336:ASN:OD1	1:C:339:ASP:OD2	2.16	0.62
1:A:118:TYR:HB2	1:A:119:PRO:HD3	1.82	0.62
1:C:277:GLU:HA	1:C:280:LYS:HE2	1.81	0.62
1:E:226:LEU:HG	1:E:260:ARG:HD3	1.81	0.62
1:C:102:ILE:O	1:C:103:VAL:CB	2.47	0.62
1:D:323:GLU:OE1	1:D:333:ARG:NE	2.31	0.62
1:E:118:TYR:HB2	1:E:119:PRO:HD3	1.82	0.61
1:A:319:ARG:NH1	1:A:339:ASP:HA	2.15	0.61
1:E:293:ASN:O	1:E:293:ASN:OD1	2.19	0.61
1:B:118:TYR:HB2	1:B:119:PRO:HD3	1.82	0.61
1:F:167:ILE:HD11	1:F:178:ASN:HB3	1.82	0.61
1:D:325:PHE:O	1:D:326:GLU:HG2	2.01	0.61
1:A:262:GLN:N	1:A:262:GLN:OE1	2.33	0.61
1:C:226:LEU:HG	1:C:260:ARG:HD3	1.82	0.61
1:A:237:GLU:O	1:A:239:SER:N	2.34	0.61
1:B:102:ILE:O	1:B:103:VAL:CG2	2.49	0.61
1:C:212:THR:HA	1:D:215:VAL:HG11	1.83	0.61
1:D:237:GLU:O	1:D:239:SER:N	2.34	0.61
1:D:340:PHE:HA	1:D:343:VAL:HG22	1.83	0.61
1:A:211:TYR:CE1	1:A:218:GLU:OE2	2.53	0.61
1:A:333:ARG:CA	1:A:334:ALA:HB2	2.31	0.61
1:B:317:HIS:NE2	1:C:125:LEU:O	2.28	0.61
1:E:102:ILE:O	1:E:103:VAL:CB	2.47	0.60
1:D:269:LEU:HD21	1:D:303:GLY:HA2	1.82	0.60
1:F:226:LEU:HG	1:F:260:ARG:HD3	1.83	0.60
1:C:260:ARG:HH11	1:C:260:ARG:CG	2.14	0.60
1:D:186:ALA:CB	1:D:199:ILE:HD11	2.32	0.60
1:D:319:ARG:NH1	1:D:339:ASP:HA	2.16	0.60
1:E:237:GLU:O	1:E:239:SER:N	2.35	0.60
1:A:220:ARG:HE	1:F:212:THR:CG2	2.13	0.60
1:F:354:ASP:OD1	1:F:355:MET:N	2.35	0.60
1:E:301:THR:HG21	1:E:309:ILE:CD1	2.32	0.60
1:A:210:SER:C	1:A:211:TYR:N	2.55	0.60
1:C:346:VAL:HG22	1:D:368:ALA:O	2.03	0.59
1:C:229:MET:CE	1:C:243:VAL:HG11	2.33	0.59
1:A:186:ALA:CB	1:A:199:ILE:HD11	2.32	0.59
1:A:320:VAL:CG1	1:A:334:ALA:HB1	2.32	0.59
1:B:301:THR:HG21	1:B:309:ILE:CD1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:LEU:HD11	1:C:356:LEU:HD21	1.85	0.59
1:F:229:MET:CE	1:F:243:VAL:HG11	2.33	0.59
1:C:102:ILE:O	1:C:103:VAL:HB	2.02	0.59
1:E:102:ILE:O	1:E:103:VAL:CG2	2.51	0.58
1:C:193:GLU:CG	1:C:193:GLU:O	2.51	0.58
1:E:229:MET:CE	1:E:243:VAL:HG11	2.33	0.58
1:C:315:SER:OG	1:C:343:VAL:HG21	2.03	0.58
1:C:102:ILE:O	1:C:103:VAL:CG2	2.51	0.58
1:E:226:LEU:HD11	1:E:257:PHE:HA	1.86	0.58
1:E:99:LEU:HD13	1:E:109:LYS:HE3	1.86	0.58
1:C:238:ILE:HG22	1:C:239:SER:O	2.02	0.58
1:E:102:ILE:O	1:E:103:VAL:HB	2.04	0.58
1:A:333:ARG:H	1:A:334:ALA:HB2	1.68	0.58
1:C:193:GLU:HG2	1:C:193:GLU:O	2.04	0.58
1:F:193:GLU:CG	1:F:193:GLU:O	2.52	0.58
1:F:193:GLU:HG2	1:F:193:GLU:O	2.04	0.58
1:F:144:LYS:HB3	1:F:267:ILE:HD11	1.86	0.58
1:B:226:LEU:HD11	1:B:257:PHE:HA	1.86	0.58
1:D:229:MET:CE	1:D:243:VAL:HG11	2.33	0.58
1:F:97:VAL:O	1:F:153:ASN:ND2	2.37	0.58
1:B:287:LYS:NZ	1:B:332:PRO:HG2	2.18	0.57
1:B:193:GLU:O	1:B:193:GLU:CG	2.52	0.57
1:B:229:MET:CE	1:B:243:VAL:HG11	2.33	0.57
1:F:118:TYR:HB2	1:F:119:PRO:CD	2.34	0.57
1:C:118:TYR:HB2	1:C:119:PRO:CD	2.34	0.57
1:A:229:MET:CE	1:A:243:VAL:HG11	2.33	0.57
1:A:354:ASP:OD1	1:A:355:MET:N	2.37	0.57
1:B:193:GLU:O	1:B:193:GLU:HG2	2.04	0.57
1:B:99:LEU:HD13	1:B:109:LYS:HE3	1.84	0.57
1:E:98:THR:O	1:E:101:GLU:OE1	2.22	0.57
1:C:208:LEU:HD21	1:C:254:ASP:HB3	1.87	0.57
1:C:347:ARG:HA	1:D:368:ALA:HB1	1.85	0.57
1:F:315:SER:OG	1:F:343:VAL:HG21	2.05	0.57
1:A:324:MET:SD	1:A:332:PRO:HB3	2.44	0.57
1:B:317:HIS:HA	1:B:335:ILE:HD12	1.85	0.57
1:F:144:LYS:HB3	1:F:267:ILE:CD1	2.35	0.57
1:A:269:LEU:HD11	1:A:356:LEU:HD21	1.87	0.57
1:D:354:ASP:OD1	1:D:355:MET:N	2.38	0.57
1:E:203:GLU:OE2	1:F:259:ARG:NH2	2.38	0.57
1:D:118:TYR:HB2	1:D:119:PRO:CD	2.35	0.56
1:F:317:HIS:HA	1:F:335:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ARG:HH12	1:A:342:GLU:HB2	1.69	0.56
1:A:99:LEU:HG	1:A:109:LYS:HE2	1.87	0.56
1:E:118:TYR:HB2	1:E:119:PRO:CD	2.36	0.56
1:A:321:VAL:O	1:A:324:MET:O	2.24	0.56
1:B:118:TYR:HB2	1:B:119:PRO:CD	2.36	0.56
1:B:99:LEU:HD13	1:B:109:LYS:HE2	1.88	0.56
1:D:249:LYS:HG2	1:D:252:ARG:HD2	1.87	0.56
1:A:99:LEU:CD2	1:A:109:LYS:HE3	2.36	0.56
1:A:249:LYS:HG2	1:A:252:ARG:HD2	1.88	0.56
1:B:249:LYS:HG2	1:B:252:ARG:HD2	1.87	0.56
1:C:226:LEU:HD11	1:C:257:PHE:HA	1.87	0.56
1:A:118:TYR:HB2	1:A:119:PRO:CD	2.35	0.56
1:A:226:LEU:HD11	1:A:257:PHE:HA	1.87	0.56
1:A:320:VAL:CB	1:A:334:ALA:HB1	2.35	0.56
1:F:256:PRO:C	1:F:260:ARG:NH1	2.59	0.56
1:B:336:ASN:O	1:B:337:MET:HB2	2.04	0.56
1:D:319:ARG:HH12	1:D:342:GLU:HB2	1.70	0.56
1:A:333:ARG:CB	1:A:334:ALA:CA	2.82	0.56
1:B:324:MET:HE2	1:B:332:PRO:CA	2.36	0.56
1:D:176:GLU:OE1	1:D:220:ARG:NH1	2.39	0.56
1:A:176:GLU:OE1	1:A:220:ARG:NH1	2.39	0.55
1:D:226:LEU:HD11	1:D:257:PHE:HA	1.87	0.55
1:C:249:LYS:HG2	1:C:252:ARG:HD2	1.88	0.55
1:A:333:ARG:HB3	1:A:334:ALA:CB	2.36	0.55
1:B:102:ILE:HD12	1:B:147:ILE:HG13	1.88	0.55
1:D:103:VAL:HG12	1:D:277:GLU:HB3	1.87	0.55
1:F:218:GLU:HA	1:F:222:ARG:HE	1.71	0.55
1:A:208:LEU:HD21	1:A:254:ASP:HB3	1.88	0.55
1:F:226:LEU:HD11	1:F:257:PHE:HA	1.88	0.55
1:D:264:ARG:HD3	1:D:367:LYS:HD3	1.88	0.55
1:D:264:ARG:NH1	1:D:367:LYS:HE2	2.22	0.55
1:F:319:ARG:NH1	1:F:342:GLU:HB2	2.21	0.55
1:D:208:LEU:HD21	1:D:254:ASP:HB3	1.88	0.55
1:A:99:LEU:HG	1:A:109:LYS:NZ	2.22	0.55
1:A:209:ALA:O	1:A:210:SER:HB2	2.07	0.54
1:A:324:MET:SD	1:A:332:PRO:N	2.79	0.54
1:F:102:ILE:HD13	1:F:277:GLU:HB3	1.89	0.54
1:E:269:LEU:HD11	1:E:351:VAL:HG21	1.89	0.54
1:B:132:ARG:HH11	1:B:132:ARG:CG	2.20	0.54
1:E:317:HIS:HA	1:E:335:ILE:HD12	1.88	0.54
1:F:103:VAL:O	1:F:105:LEU:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:LYS:HG2	1:F:252:ARG:HD2	1.88	0.54
1:E:222:ARG:NH2	1:E:254:ASP:OD2	2.40	0.54
1:C:320:VAL:HG22	1:C:333:ARG:HB3	1.88	0.54
1:B:291:ASN:O	1:B:337:MET:HG3	2.08	0.54
1:B:203:GLU:OE2	1:C:259:ARG:NH2	2.41	0.54
1:B:272:LYS:NZ	1:B:272:LYS:HB3	2.23	0.54
1:C:132:ARG:CG	1:C:132:ARG:HH11	2.21	0.54
1:F:291:ASN:OD1	1:F:291:ASN:C	2.47	0.54
1:D:317:HIS:O	1:D:320:VAL:HG22	2.08	0.53
1:A:132:ARG:CG	1:A:132:ARG:HH11	2.21	0.53
1:A:324:MET:SD	1:A:332:PRO:CB	2.96	0.53
1:B:319:ARG:O	1:B:322:LYS:HB2	2.08	0.53
1:E:324:MET:HE2	1:E:332:PRO:CA	2.38	0.53
1:F:132:ARG:HH11	1:F:132:ARG:CG	2.21	0.53
1:D:132:ARG:HH11	1:D:132:ARG:CG	2.21	0.53
1:A:317:HIS:O	1:A:320:VAL:HG22	2.09	0.53
1:D:250:PRO:HB2	1:D:362:TRP:CZ2	2.43	0.53
1:A:100:ASN:OD1	1:A:102:ILE:N	2.42	0.53
1:E:132:ARG:HH11	1:E:132:ARG:CG	2.21	0.53
1:B:222:ARG:NH2	1:B:254:ASP:OD2	2.41	0.53
1:C:291:ASN:C	1:C:291:ASN:OD1	2.47	0.53
1:D:222:ARG:NH2	1:D:254:ASP:OD2	2.41	0.53
1:E:320:VAL:HG22	1:E:333:ARG:HB3	1.90	0.53
1:B:208:LEU:HD21	1:B:254:ASP:HB3	1.89	0.53
1:C:234:ASP:C	1:C:236:ASN:N	2.62	0.53
1:F:112:LEU:HD12	1:F:134:ILE:HD11	1.90	0.53
1:B:320:VAL:HG22	1:B:333:ARG:HB3	1.91	0.52
1:C:97:VAL:O	1:C:98:THR:OG1	2.23	0.52
1:E:156:ASP:O	1:E:195:LYS:HD3	2.09	0.52
1:F:320:VAL:HG22	1:F:333:ARG:HB3	1.90	0.52
1:D:317:HIS:HA	1:D:335:ILE:HD12	1.91	0.52
1:E:208:LEU:HD21	1:E:254:ASP:HB3	1.89	0.52
1:B:284:SER:OG	1:B:285:LYS:N	2.42	0.52
1:F:319:ARG:O	1:F:322:LYS:HG2	2.09	0.52
1:C:336:ASN:OD1	1:C:339:ASP:OD1	2.28	0.52
1:D:324:MET:HE2	1:D:331:GLU:C	2.30	0.52
1:E:291:ASN:OD1	1:E:291:ASN:C	2.47	0.52
1:A:205:ASP:OD1	1:A:247:THR:OG1	2.25	0.52
1:B:112:LEU:HD13	1:B:265:ILE:CD1	2.39	0.52
1:C:269:LEU:HD21	1:C:351:VAL:HG21	1.92	0.52
1:F:144:LYS:HD3	1:F:267:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:HIS:HA	1:C:335:ILE:CD1	2.39	0.52
1:E:284:SER:OG	1:E:285:LYS:N	2.43	0.51
1:F:284:SER:OG	1:F:285:LYS:N	2.42	0.51
1:A:227:LYS:HE2	1:F:165:ALA:HB3	1.92	0.51
1:F:336:ASN:OD1	1:F:339:ASP:OD1	2.29	0.51
1:A:284:SER:OG	1:A:285:LYS:N	2.43	0.51
1:F:101:GLU:HB3	1:F:109:LYS:HD3	1.91	0.51
1:A:99:LEU:HD23	1:A:109:LYS:HE3	1.93	0.51
1:E:112:LEU:HD13	1:E:265:ILE:CD1	2.40	0.51
1:A:100:ASN:OD1	1:A:101:GLU:N	2.43	0.51
1:E:301:THR:HG21	1:E:309:ILE:HD13	1.92	0.51
1:A:116:VAL:HG23	1:A:242:TYR:CD2	2.46	0.51
1:A:269:LEU:HD21	1:A:351:VAL:HG11	1.91	0.51
1:C:171:TRP:O	1:C:172:LEU:C	2.47	0.51
1:C:210:SER:CB	1:D:219:ALA:HB1	2.41	0.51
1:B:291:ASN:OD1	1:B:291:ASN:C	2.49	0.51
1:F:139:PRO:CB	1:F:351:VAL:HG11	2.40	0.51
1:B:225:PHE:CZ	1:B:229:MET:HE3	2.46	0.51
1:C:323:GLU:HG2	1:C:327:LYS:CG	2.41	0.50
1:D:291:ASN:OD1	1:D:291:ASN:C	2.48	0.50
1:F:364:GLU:HA	1:F:367:LYS:HD3	1.94	0.50
1:D:284:SER:OG	1:D:285:LYS:N	2.44	0.50
1:E:301:THR:HG21	1:E:309:ILE:HD11	1.93	0.50
1:F:144:LYS:CD	1:F:267:ILE:HD11	2.42	0.50
1:C:171:TRP:O	1:C:172:LEU:O	2.29	0.50
1:E:99:LEU:CA	1:E:101:GLU:HB2	2.38	0.50
1:F:102:ILE:CD1	1:F:277:GLU:HB3	2.42	0.50
1:A:250:PRO:HB2	1:A:362:TRP:CZ2	2.46	0.50
1:A:130:TRP:HA	1:F:314:GLN:NE2	2.26	0.50
1:C:225:PHE:CZ	1:C:229:MET:HE3	2.46	0.50
1:B:301:THR:HG21	1:B:309:ILE:HD13	1.93	0.50
1:B:322:LYS:HE3	1:C:114:GLU:HB2	1.94	0.50
1:C:139:PRO:CB	1:C:351:VAL:HG11	2.41	0.49
1:C:284:SER:OG	1:C:285:LYS:N	2.44	0.49
1:C:113:LYS:CA	1:C:117:VAL:HG12	2.42	0.49
1:D:211:TYR:O	1:D:212:THR:OG1	2.28	0.49
1:F:113:LYS:CA	1:F:117:VAL:HG12	2.42	0.49
1:F:99:LEU:O	1:F:99:LEU:CD1	2.59	0.49
1:D:101:GLU:CD	1:D:104:GLY:HA2	2.33	0.49
1:E:105:LEU:HG	1:E:274:HIS:HD2	1.78	0.49
1:E:336:ASN:OD1	1:E:338:ASP:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:VAL:HG11	1:C:274:HIS:N	2.28	0.49
1:B:301:THR:HG21	1:B:309:ILE:HD11	1.93	0.49
1:D:327:LYS:O	1:D:328:ASN:HB2	2.12	0.49
1:F:151:VAL:HG23	1:F:198:ILE:HD13	1.95	0.49
1:F:211:TYR:CG	1:F:217:GLY:HA3	2.48	0.49
1:B:113:LYS:HA	1:B:117:VAL:HG13	1.95	0.49
1:B:301:THR:HG22	1:B:304:TYR:HB2	1.95	0.49
1:F:226:LEU:CD2	1:F:260:ARG:NH1	2.76	0.49
1:F:225:PHE:CZ	1:F:229:MET:HE3	2.48	0.49
1:E:249:LYS:HG3	1:E:251:TRP:HE3	1.78	0.49
1:B:105:LEU:HG	1:B:274:HIS:HD2	1.78	0.48
1:E:113:LYS:HA	1:E:117:VAL:HG13	1.95	0.48
1:C:96:LYS:N	1:C:150:ALA:O	2.46	0.48
1:C:276:LEU:HD11	1:C:295:GLU:HG2	1.95	0.48
1:A:212:THR:HG22	1:B:218:GLU:CD	2.33	0.48
1:D:113:LYS:CA	1:D:117:VAL:HG12	2.44	0.48
1:C:165:ALA:HB3	1:D:227:LYS:HE2	1.94	0.48
1:C:301:THR:HG21	1:C:309:ILE:HD11	1.95	0.48
1:F:276:LEU:HD11	1:F:295:GLU:HG2	1.95	0.48
1:A:99:LEU:H	1:A:99:LEU:HD13	1.78	0.48
1:C:116:VAL:HG21	1:C:151:VAL:HG11	1.96	0.48
1:D:105:LEU:HG	1:D:274:HIS:HD2	1.77	0.48
1:A:113:LYS:CA	1:A:117:VAL:HG12	2.43	0.48
1:D:130:TRP:CH2	1:D:132:ARG:CZ	2.97	0.48
1:B:113:LYS:HB3	1:B:118:TYR:HE1	1.78	0.48
1:B:249:LYS:HG3	1:B:251:TRP:HE3	1.79	0.48
1:C:234:ASP:C	1:C:236:ASN:H	2.17	0.48
1:D:216:GLY:C	1:D:218:GLU:N	2.66	0.48
1:F:256:PRO:CB	1:F:260:ARG:HH12	2.26	0.48
1:C:112:LEU:O	1:C:116:VAL:HG22	2.14	0.47
1:C:144:LYS:CG	1:C:267:ILE:HD11	2.33	0.47
1:F:113:LYS:HB3	1:F:118:TYR:HE1	1.79	0.47
1:B:156:ASP:O	1:B:195:LYS:HD3	2.14	0.47
1:E:113:LYS:HB3	1:E:118:TYR:HE1	1.79	0.47
1:F:256:PRO:HB3	1:F:260:ARG:HH12	1.80	0.47
1:A:249:LYS:HG3	1:A:251:TRP:HE3	1.80	0.47
1:B:112:LEU:HD13	1:B:265:ILE:HD11	1.97	0.47
1:A:323:GLU:HA	1:A:326:GLU:HG2	1.97	0.47
1:A:333:ARG:CG	1:A:334:ALA:HA	2.45	0.47
1:C:113:LYS:HB3	1:C:118:TYR:HE1	1.79	0.47
1:C:229:MET:HA	1:C:232:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:264:ARG:HD2	1:F:368:ALA:HB3	1.97	0.47
1:A:129:GLY:C	1:F:314:GLN:HE21	2.17	0.47
1:A:263:LYS:NZ	1:A:369:LEU:HD23	2.30	0.47
1:D:336:ASN:OD1	1:D:338:ASP:N	2.47	0.47
1:E:139:PRO:CB	1:E:351:VAL:HG11	2.44	0.47
1:F:158:GLU:CG	1:F:189:LEU:HD21	2.45	0.47
1:C:234:ASP:O	1:C:235:LYS:C	2.54	0.47
1:C:99:LEU:HD12	1:C:150:ALA:HB1	1.97	0.47
1:E:301:THR:HG22	1:E:304:TYR:HB2	1.96	0.47
1:A:225:PHE:CZ	1:A:229:MET:HE3	2.50	0.46
1:B:352:ASN:HB3	1:B:355:MET:HG3	1.98	0.46
1:C:97:VAL:CG1	1:C:100:ASN:HD21	2.28	0.46
1:A:130:TRP:CH2	1:A:132:ARG:CZ	2.98	0.46
1:A:219:ALA:HB1	1:F:210:SER:HB3	1.97	0.46
1:A:99:LEU:HG	1:A:109:LYS:HE3	1.93	0.46
1:B:130:TRP:CH2	1:B:132:ARG:CZ	2.98	0.46
1:A:333:ARG:HB3	1:A:334:ALA:HB2	1.97	0.46
1:D:276:LEU:HD11	1:D:295:GLU:HG2	1.98	0.46
1:E:112:LEU:HD13	1:E:265:ILE:HD11	1.98	0.46
1:F:139:PRO:HB3	1:F:351:VAL:HG11	1.97	0.46
1:F:213:SER:O	1:F:214:GLU:C	2.54	0.46
1:A:276:LEU:HD11	1:A:295:GLU:HG2	1.98	0.46
1:B:225:PHE:CZ	1:B:229:MET:CE	2.98	0.46
1:E:287:LYS:HE2	1:E:334:ALA:HB2	1.98	0.46
1:D:214:GLU:CD	1:E:215:VAL:HG23	2.36	0.46
1:A:210:SER:CA	1:A:211:TYR:N	2.79	0.46
1:E:283:SER:O	1:E:285:LYS:N	2.49	0.46
1:F:352:ASN:OD1	1:F:353:GLN:N	2.49	0.46
1:C:113:LYS:HA	1:C:117:VAL:HG12	1.97	0.46
1:A:219:ALA:O	1:A:220:ARG:C	2.53	0.46
1:B:176:GLU:HG2	1:B:221:VAL:HG12	1.97	0.46
1:C:352:ASN:OD1	1:C:353:GLN:N	2.49	0.46
1:F:105:LEU:O	1:F:107:ASP:N	2.49	0.46
1:F:113:LYS:HA	1:F:117:VAL:HG12	1.97	0.46
1:F:158:GLU:HG3	1:F:189:LEU:HG	1.98	0.46
1:F:219:ALA:O	1:F:220:ARG:C	2.54	0.46
1:A:254:ASP:OD1	1:A:256:PRO:HD2	2.16	0.46
1:B:336:ASN:HD22	1:B:339:ASP:CG	2.18	0.46
1:C:323:GLU:HG2	1:C:327:LYS:HG3	1.98	0.46
1:E:176:GLU:HG2	1:E:221:VAL:HG12	1.97	0.46
1:A:105:LEU:HD21	1:A:108:VAL:CG1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:HD21	1:A:108:VAL:HB	1.97	0.45
1:D:352:ASN:OD1	1:D:353:GLN:N	2.49	0.45
1:E:225:PHE:CZ	1:E:229:MET:CE	2.99	0.45
1:E:97:VAL:HG21	1:E:146:MET:CE	2.46	0.45
1:D:215:VAL:HG22	1:D:216:GLY:N	2.30	0.45
1:E:104:GLY:O	1:E:105:LEU:HB2	2.16	0.45
1:E:97:VAL:HG13	1:E:97:VAL:O	2.16	0.45
1:A:352:ASN:OD1	1:A:353:GLN:N	2.49	0.45
1:C:250:PRO:O	1:C:362:TRP:CH2	2.70	0.45
1:D:158:GLU:CG	1:D:189:LEU:HD21	2.46	0.45
1:E:130:TRP:CH2	1:E:132:ARG:CZ	2.99	0.45
1:C:106:GLU:O	1:C:107:ASP:CB	2.64	0.45
1:E:288:LEU:HA	1:E:335:ILE:CG2	2.47	0.45
1:A:97:VAL:O	1:A:97:VAL:HG13	2.17	0.45
1:B:276:LEU:HD11	1:B:295:GLU:HG2	1.99	0.45
1:B:105:LEU:O	1:B:106:GLU:C	2.55	0.45
1:D:250:PRO:HB2	1:D:362:TRP:CH2	2.51	0.45
1:C:139:PRO:HB3	1:C:351:VAL:HG11	1.99	0.45
1:A:109:LYS:HD3	1:A:109:LYS:HA	1.83	0.45
1:A:352:ASN:HB3	1:A:355:MET:HG3	1.98	0.45
1:B:283:SER:O	1:B:285:LYS:N	2.49	0.45
1:C:219:ALA:O	1:C:220:ARG:C	2.53	0.45
1:C:282:TYR:HB3	1:C:313:VAL:HG11	1.98	0.45
1:D:254:ASP:OD1	1:D:256:PRO:HD2	2.17	0.45
1:D:320:VAL:HG11	1:D:335:ILE:HA	1.98	0.45
1:F:283:SER:O	1:F:285:LYS:N	2.50	0.45
1:A:320:VAL:HG11	1:A:335:ILE:HA	1.99	0.45
1:B:254:ASP:OD1	1:B:256:PRO:HD2	2.17	0.45
1:B:352:ASN:OD1	1:B:353:GLN:N	2.50	0.45
1:C:228:GLU:O	1:C:232:LEU:HD13	2.16	0.45
1:C:254:ASP:OD1	1:C:256:PRO:HD2	2.17	0.45
1:C:352:ASN:HB3	1:C:355:MET:HG3	1.98	0.45
1:D:219:ALA:O	1:D:220:ARG:C	2.54	0.45
1:D:325:PHE:HE2	1:E:121:LYS:CD	2.30	0.45
1:E:310:ARG:NH2	1:F:128:LEU:O	2.50	0.45
1:F:258:LEU:HD11	1:F:362:TRP:HH2	1.82	0.45
1:F:97:VAL:O	1:F:97:VAL:HG13	2.16	0.45
1:A:116:VAL:HG23	1:A:242:TYR:CE2	2.51	0.45
1:A:281:HIS:O	1:A:284:SER:HB3	2.17	0.45
1:B:288:LEU:O	1:B:289:ASP:HB3	2.17	0.45
1:E:208:LEU:HD22	1:E:252:ARG:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:LYS:HG3	1:D:251:TRP:HE3	1.81	0.44
1:E:276:LEU:HD11	1:E:295:GLU:HG2	1.99	0.44
1:F:327:LYS:O	1:F:328:ASN:HB2	2.16	0.44
1:A:227:LYS:HE2	1:F:165:ALA:CB	2.47	0.44
1:A:225:PHE:CZ	1:A:229:MET:CE	3.00	0.44
1:A:134:ILE:HG23	1:A:244:ILE:HG12	1.99	0.44
1:B:99:LEU:CA	1:B:101:GLU:HB2	2.38	0.44
1:F:134:ILE:HG23	1:F:244:ILE:HG12	1.98	0.44
1:F:156:ASP:O	1:F:195:LYS:HD2	2.18	0.44
1:B:325:PHE:CG	1:C:118:TYR:CE2	3.06	0.44
1:B:330:GLN:O	1:B:331:GLU:HB2	2.17	0.44
1:D:137:TYR:CD2	1:D:362:TRP:HZ3	2.36	0.44
1:F:254:ASP:OD1	1:F:256:PRO:HD2	2.17	0.44
1:A:98:THR:OG1	1:A:99:LEU:N	2.50	0.44
1:D:225:PHE:CZ	1:D:229:MET:HE3	2.53	0.44
1:E:254:ASP:OD1	1:E:256:PRO:HD2	2.17	0.44
1:D:158:GLU:HG3	1:D:189:LEU:HG	1.98	0.44
1:B:99:LEU:CD1	1:B:109:LYS:HE2	2.48	0.44
1:C:156:ASP:O	1:C:195:LYS:HD2	2.18	0.44
1:C:327:LYS:O	1:C:328:ASN:HB2	2.16	0.44
1:D:171:TRP:CZ2	1:D:177:LYS:HD3	2.53	0.44
1:E:105:LEU:O	1:E:106:GLU:C	2.55	0.44
1:D:281:HIS:O	1:D:284:SER:HB3	2.18	0.44
1:E:288:LEU:O	1:E:289:ASP:HB3	2.17	0.44
1:B:219:ALA:O	1:B:220:ARG:C	2.56	0.44
1:C:134:ILE:HG23	1:C:244:ILE:HG12	1.98	0.44
1:D:134:ILE:HG23	1:D:244:ILE:HG12	1.99	0.44
1:E:99:LEU:HD23	1:E:150:ALA:HB1	2.00	0.44
1:E:269:LEU:CD1	1:E:351:VAL:HG21	2.47	0.44
1:A:113:LYS:HB3	1:A:118:TYR:HE1	1.83	0.44
1:A:213:SER:O	1:A:214:GLU:C	2.56	0.44
1:B:249:LYS:HE2	1:B:252:ARG:NH1	2.33	0.44
1:D:249:LYS:HE2	1:D:252:ARG:NH1	2.33	0.44
1:E:219:ALA:O	1:E:220:ARG:C	2.56	0.44
1:E:139:PRO:HB3	1:E:351:VAL:HG11	2.00	0.44
1:E:97:VAL:HG21	1:E:146:MET:HE1	2.00	0.44
1:A:161:HIS:HE1	1:A:163:ASP:OD1	2.01	0.43
1:B:287:LYS:HZ3	1:B:332:PRO:HG2	1.82	0.43
1:C:168:MET:HE1	1:C:221:VAL:HB	1.99	0.43
1:C:249:LYS:HE2	1:C:252:ARG:NH1	2.33	0.43
1:D:177:LYS:HG3	1:D:178:ASN:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:THR:OG1	1:D:99:LEU:N	2.50	0.43
1:E:330:GLN:O	1:E:331:GLU:HB2	2.17	0.43
1:F:275:ARG:HD3	1:F:301:THR:HG23	1.99	0.43
1:A:100:ASN:O	1:A:101:GLU:HB2	2.17	0.43
1:A:249:LYS:HE2	1:A:252:ARG:NH1	2.33	0.43
1:A:287:LYS:O	1:A:335:ILE:HG22	1.96	0.43
1:D:113:LYS:HB3	1:D:118:TYR:HE1	1.83	0.43
1:A:99:LEU:HB3	1:A:150:ALA:HB1	2.00	0.43
1:C:258:LEU:HD11	1:C:362:TRP:HH2	1.83	0.43
1:D:213:SER:O	1:D:214:GLU:C	2.57	0.43
1:E:352:ASN:HB3	1:E:355:MET:HG3	2.00	0.43
1:F:158:GLU:HG3	1:F:189:LEU:CD2	2.49	0.43
1:A:113:LYS:HA	1:A:117:VAL:HG12	1.99	0.43
1:D:105:LEU:O	1:D:106:GLU:C	2.56	0.43
1:D:113:LYS:HA	1:D:117:VAL:HG12	1.99	0.43
1:D:352:ASN:HB3	1:D:355:MET:HG3	1.99	0.43
1:D:340:PHE:HA	1:D:343:VAL:CG2	2.48	0.43
1:F:110:GLU:HA	1:F:113:LYS:HE3	2.01	0.43
1:F:158:GLU:HG3	1:F:189:LEU:HD21	2.00	0.43
1:F:288:LEU:HA	1:F:335:ILE:CG2	2.48	0.43
1:A:208:LEU:HD22	1:A:252:ARG:O	2.18	0.43
1:B:208:LEU:HD22	1:B:252:ARG:O	2.18	0.43
1:C:260:ARG:NH1	1:C:260:ARG:CG	2.80	0.43
1:C:275:ARG:HD3	1:C:301:THR:HG23	1.99	0.43
1:D:282:TYR:HB3	1:D:313:VAL:HG21	2.00	0.43
1:D:340:PHE:O	1:D:343:VAL:HG22	2.18	0.43
1:E:166:SER:HA	1:F:223:ASN:ND2	2.33	0.43
1:F:145:THR:HG23	1:F:200:PHE:CE2	2.53	0.43
1:F:102:ILE:HD11	1:F:277:GLU:HG2	2.00	0.43
1:A:210:SER:HB3	1:A:211:TYR:CB	2.48	0.43
1:B:174:GLU:O	1:B:175:ALA:HB3	2.19	0.43
1:C:96:LYS:HB2	1:C:150:ALA:HA	1.99	0.43
1:D:208:LEU:HD22	1:D:252:ARG:O	2.18	0.43
1:D:288:LEU:HA	1:D:335:ILE:CG2	2.49	0.43
1:D:324:MET:HE2	1:D:331:GLU:O	2.18	0.43
1:E:166:SER:HA	1:F:223:ASN:HD21	1.84	0.43
1:E:205:ASP:OD1	1:E:247:THR:OG1	2.25	0.43
1:E:325:PHE:CG	1:F:118:TYR:CE2	3.06	0.43
1:F:225:PHE:CZ	1:F:229:MET:CE	3.01	0.43
1:F:287:LYS:HE2	1:F:334:ALA:HB2	1.99	0.43
1:B:292:VAL:HA	1:B:337:MET:HG2	1.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:PRO:HB2	1:C:362:TRP:CE2	2.54	0.43
1:C:97:VAL:O	1:C:97:VAL:HG13	2.17	0.43
1:D:161:HIS:HE1	1:D:163:ASP:OD1	2.02	0.43
1:E:297:LEU:O	1:E:298:ALA:C	2.56	0.43
1:A:283:SER:O	1:A:285:LYS:N	2.52	0.43
1:B:99:LEU:CD1	1:B:109:LYS:CE	2.94	0.43
1:C:118:TYR:CB	1:C:119:PRO:CD	2.97	0.43
1:F:130:TRP:CH2	1:F:132:ARG:CZ	3.01	0.43
1:F:288:LEU:O	1:F:289:ASP:HB3	2.18	0.43
1:A:177:LYS:HG3	1:A:178:ASN:N	2.32	0.43
1:A:116:VAL:CG2	1:A:242:TYR:CD2	3.02	0.43
1:A:282:TYR:HB3	1:A:313:VAL:HG21	2.01	0.43
1:C:225:PHE:CZ	1:C:229:MET:CE	3.01	0.43
1:D:288:LEU:O	1:D:289:ASP:HB3	2.19	0.43
1:B:287:LYS:O	1:B:287:LYS:CG	2.63	0.42
1:E:281:HIS:O	1:E:284:SER:HB3	2.19	0.42
1:C:130:TRP:CH2	1:C:132:ARG:CZ	3.01	0.42
1:C:281:HIS:O	1:C:284:SER:HB3	2.19	0.42
1:D:362:TRP:CZ3	1:D:367:LYS:HG3	2.55	0.42
1:A:288:LEU:O	1:A:289:ASP:HB3	2.20	0.42
1:B:250:PRO:O	1:B:362:TRP:CH2	2.72	0.42
1:E:105:LEU:O	1:E:107:ASP:N	2.53	0.42
1:F:118:TYR:CB	1:F:119:PRO:CD	2.98	0.42
1:F:281:HIS:O	1:F:284:SER:HB3	2.19	0.42
1:A:255:GLU:OE2	1:F:355:MET:HE2	2.20	0.42
1:D:225:PHE:CZ	1:D:229:MET:CE	3.02	0.42
1:D:235:LYS:O	1:D:236:ASN:C	2.57	0.42
1:F:250:PRO:O	1:F:362:TRP:CH2	2.73	0.42
1:F:338:ASP:OD1	1:F:338:ASP:C	2.58	0.42
1:F:105:LEU:HD23	1:F:110:GLU:HB3	2.01	0.42
1:A:215:VAL:HG11	1:F:211:TYR:CE2	2.55	0.42
1:A:323:GLU:HA	1:A:326:GLU:CG	2.49	0.42
1:A:333:ARG:NH2	1:A:334:ALA:O	2.52	0.42
1:E:250:PRO:O	1:E:362:TRP:CH2	2.72	0.42
1:F:139:PRO:HB2	1:F:351:VAL:HG11	1.99	0.42
1:A:116:VAL:CG1	1:A:117:VAL:N	2.82	0.42
1:C:208:LEU:HD22	1:C:252:ARG:O	2.19	0.42
1:C:249:LYS:HG3	1:C:251:TRP:HE3	1.84	0.42
1:D:99:LEU:HD11	1:D:109:LYS:HG3	2.02	0.42
1:D:340:PHE:CA	1:D:343:VAL:HG22	2.49	0.42
1:C:139:PRO:HB2	1:C:351:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:THR:CB	1:E:218:GLU:HG3	2.49	0.42
1:D:362:TRP:CH2	1:D:367:LYS:CD	3.02	0.42
1:B:118:TYR:O	1:B:121:LYS:HG3	2.19	0.42
1:B:281:HIS:O	1:B:284:SER:HB3	2.20	0.42
1:B:297:LEU:O	1:B:298:ALA:C	2.58	0.42
1:C:338:ASP:C	1:C:338:ASP:OD1	2.58	0.42
1:D:158:GLU:HG3	1:D:189:LEU:CD2	2.49	0.42
1:E:225:PHE:CZ	1:E:229:MET:HE1	2.55	0.42
1:E:102:ILE:HD12	1:E:147:ILE:HG13	2.02	0.42
1:E:174:GLU:O	1:E:175:ALA:HB3	2.20	0.42
1:F:144:LYS:HE3	1:F:248:ASN:OD1	2.20	0.42
1:A:235:LYS:O	1:A:236:ASN:C	2.58	0.41
1:C:323:GLU:O	1:C:324:MET:C	2.59	0.41
1:D:103:VAL:HB	1:D:274:HIS:CE1	2.55	0.41
1:D:158:GLU:HG3	1:D:189:LEU:HD21	2.01	0.41
1:C:110:GLU:HA	1:C:113:LYS:HE3	2.02	0.41
1:C:171:TRP:NE1	1:C:177:LYS:HE2	2.35	0.41
1:C:229:MET:HE2	1:C:243:VAL:HG21	2.02	0.41
1:C:288:LEU:O	1:C:289:ASP:HB3	2.19	0.41
1:A:297:LEU:O	1:A:298:ALA:C	2.59	0.41
1:B:205:ASP:OD1	1:B:247:THR:OG1	2.25	0.41
1:C:116:VAL:HG12	1:C:242:TYR:CD2	2.55	0.41
1:E:362:TRP:C	1:E:362:TRP:CD1	2.93	0.41
1:C:106:GLU:O	1:C:107:ASP:HB3	2.21	0.41
1:C:177:LYS:HG3	1:C:178:ASN:N	2.35	0.41
1:C:297:LEU:O	1:C:298:ALA:C	2.58	0.41
1:F:297:LEU:O	1:F:298:ALA:C	2.58	0.41
1:A:250:PRO:HB2	1:A:362:TRP:CH2	2.55	0.41
1:D:218:GLU:O	1:D:220:ARG:N	2.54	0.41
1:F:229:MET:HE2	1:F:243:VAL:HG21	2.03	0.41
1:A:145:THR:HG23	1:A:200:PHE:CE2	2.55	0.41
1:A:137:TYR:CD2	1:A:362:TRP:HZ3	2.39	0.41
1:B:181:LYS:HA	1:B:184:LYS:HB2	2.03	0.41
1:C:324:MET:SD	1:D:125:LEU:HD21	2.61	0.41
1:E:97:VAL:CG2	1:E:101:GLU:OE2	2.68	0.41
1:E:181:LYS:HA	1:E:184:LYS:HB2	2.02	0.41
1:B:322:LYS:HA	1:B:322:LYS:HD3	1.89	0.41
1:C:340:PHE:HA	1:C:343:VAL:HG12	2.02	0.41
1:D:214:GLU:OE1	1:E:215:VAL:HG23	2.21	0.41
1:E:235:LYS:O	1:E:236:ASN:C	2.58	0.41
1:A:290:PRO:O	1:A:291:ASN:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:THR:OG1	1:E:218:GLU:HG3	2.20	0.41
1:D:297:LEU:O	1:D:298:ALA:C	2.59	0.41
1:C:283:SER:O	1:C:285:LYS:N	2.54	0.41
1:E:118:TYR:CB	1:E:119:PRO:CD	2.99	0.41
1:F:235:LYS:O	1:F:236:ASN:C	2.59	0.41
1:F:340:PHE:HA	1:F:343:VAL:HG12	2.02	0.41
1:A:323:GLU:O	1:A:324:MET:C	2.60	0.40
1:D:106:GLU:O	1:D:109:LYS:N	2.54	0.40
1:D:145:THR:HG23	1:D:200:PHE:CE2	2.56	0.40
1:E:177:LYS:HG3	1:E:178:ASN:N	2.35	0.40
1:E:218:GLU:O	1:E:220:ARG:N	2.54	0.40
1:E:283:SER:O	1:E:284:SER:C	2.59	0.40
1:F:218:GLU:O	1:F:220:ARG:N	2.54	0.40
1:F:250:PRO:HB2	1:F:362:TRP:CE2	2.56	0.40
1:A:218:GLU:O	1:A:220:ARG:N	2.54	0.40
1:B:105:LEU:O	1:B:107:ASP:N	2.54	0.40
1:D:103:VAL:O	1:D:105:LEU:N	2.54	0.40
1:D:118:TYR:CB	1:D:119:PRO:CD	2.99	0.40
1:D:264:ARG:NH1	1:D:366:PHE:O	2.54	0.40
1:A:340:PHE:HA	1:A:343:VAL:HG12	2.03	0.40
1:B:112:LEU:HG	1:B:151:VAL:HG11	2.02	0.40
1:B:260:ARG:N	1:B:260:ARG:HD2	2.36	0.40
1:B:291:ASN:OD1	1:B:337:MET:HB2	2.21	0.40
1:B:324:MET:CE	1:C:125:LEU:HD21	2.51	0.40
1:D:216:GLY:HA3	1:D:218:GLU:CD	2.42	0.40
1:A:286:VAL:O	1:A:286:VAL:HG23	2.21	0.40
1:B:177:LYS:HG3	1:B:178:ASN:N	2.36	0.40
1:B:340:PHE:HA	1:B:343:VAL:HG12	2.02	0.40
1:C:235:LYS:O	1:C:236:ASN:C	2.59	0.40
1:F:158:GLU:HG3	1:F:189:LEU:CG	2.52	0.40
1:F:256:PRO:O	1:F:260:ARG:NH1	2.55	0.40
1:F:362:TRP:CD1	1:F:362:TRP:C	2.94	0.40
1:A:336:ASN:OD1	1:A:337:MET:N	2.53	0.40
1:B:218:GLU:O	1:B:220:ARG:N	2.54	0.40
1:B:283:SER:O	1:B:284:SER:C	2.60	0.40
1:C:317:HIS:HA	1:C:335:ILE:HD11	2.03	0.40
1:F:286:VAL:HG23	1:F:286:VAL:O	2.22	0.40

All (1) 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:C:126:PHE:O	1:F:330:GLN:NE2[2_665]	2.19	0.01

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	263/316 (83%)	207 (79%)	34 (13%)	22 (8%)	1	10
1	B	249/316 (79%)	204 (82%)	31 (12%)	14 (6%)	2	19
1	C	270/316 (85%)	218 (81%)	35 (13%)	17 (6%)	1	17
1	D	271/316 (86%)	210 (78%)	38 (14%)	23 (8%)	1	10
1	E	256/316 (81%)	207 (81%)	32 (12%)	17 (7%)	1	16
1	F	272/316 (86%)	214 (79%)	39 (14%)	19 (7%)	1	14
All	All	1581/1896 (83%)	1260 (80%)	209 (13%)	112 (7%)	1	14

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	101	GLU
1	A	106	GLU
1	A	215	VAL
1	A	238	ILE
1	A	284	SER
1	A	328	ASN
1	B	103	VAL
1	B	106	GLU
1	B	174	GLU
1	B	284	SER
1	B	337	MET
1	C	103	VAL
1	C	172	LEU
1	C	235	LYS

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Mol	Chain	Res	Type
1	C	284	SER
1	D	104	GLY
1	D	106	GLU
1	D	172	LEU
1	D	238	ILE
1	D	284	SER
1	D	329	LEU
1	D	366	PHE
1	E	103	VAL
1	E	106	GLU
1	E	238	ILE
1	E	284	SER
1	F	104	GLY
1	F	106	GLU
1	F	172	LEU
1	F	215	VAL
1	F	238	ILE
1	F	284	SER
1	A	219	ALA
1	A	233	ALA
1	A	236	ASN
1	A	237	GLU
1	A	325	PHE
1	A	334	ALA
1	B	219	ALA
1	C	171	TRP
1	C	219	ALA
1	C	233	ALA
1	C	236	ASN
1	C	293	ASN
1	D	171	TRP
1	D	219	ALA
1	D	233	ALA
1	D	236	ASN
1	D	237	GLU
1	D	293	ASN
1	D	328	ASN
1	E	219	ALA
1	E	233	ALA
1	E	236	ASN
1	E	237	GLU
1	F	171	TRP

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Mol	Chain	Res	Type
1	F	210	SER
1	F	219	ALA
1	F	233	ALA
1	F	236	ASN
1	F	237	GLU
1	A	193	GLU
1	A	240	LYS
1	A	293	ASN
1	A	333	ARG
1	A	338	ASP
1	B	193	GLU
1	B	240	LYS
1	B	293	ASN
1	C	193	GLU
1	C	210	SER
1	C	214	GLU
1	C	240	LYS
1	D	193	GLU
1	D	210	SER
1	D	240	LYS
1	D	326	GLU
1	E	193	GLU
1	E	240	LYS
1	E	293	ASN
1	F	193	GLU
1	F	240	LYS
1	F	293	ASN
1	A	289	ASP
1	A	368	ALA
1	B	184	LYS
1	B	289	ASP
1	B	336	ASN
1	C	289	ASP
1	D	215	VAL
1	D	289	ASP
1	E	98	THR
1	E	184	LYS
1	E	289	ASP
1	F	289	ASP
1	F	184	LYS
1	A	184	LYS
1	C	99	LEU

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Mol	Chain	Res	Type
1	C	184	LYS
1	D	184	LYS
1	D	217	GLY
1	E	97	VAL
1	E	105	LEU
1	A	256	PRO
1	B	104	GLY
1	C	256	PRO
1	D	256	PRO
1	F	256	PRO
1	B	256	PRO
1	E	256	PRO
1	F	97	VAL

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	232/273 (85%)	202 (87%)	30 (13%)	4 24
1	B	221/273 (81%)	191 (86%)	30 (14%)	3 22
1	C	234/273 (86%)	209 (89%)	25 (11%)	6 32
1	D	235/273 (86%)	211 (90%)	24 (10%)	7 34
1	E	227/273 (83%)	199 (88%)	28 (12%)	4 26
1	F	235/273 (86%)	211 (90%)	24 (10%)	7 34
All	All	1384/1638 (84%)	1223 (88%)	161 (12%)	5 29

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	LEU
1	A	101	GLU
1	A	105	LEU
1	A	109	LYS
1	A	112	LEU

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Mol	Chain	Res	Type
1	A	116	VAL
1	A	122	ARG
1	A	132	ARG
1	A	168	MET
1	A	190	SER
1	A	195	LYS
1	A	205	ASP
1	A	214	GLU
1	A	215	VAL
1	A	222	ARG
1	A	223	ASN
1	A	252	ARG
1	A	254	ASP
1	A	257	PHE
1	A	260	ARG
1	A	276	LEU
1	A	287	LYS
1	A	291	ASN
1	A	296	GLU
1	A	312	ILE
1	A	326	GLU
1	A	328	ASN
1	A	366	PHE
1	A	367	LYS
1	A	369	LEU
1	B	105	LEU
1	B	109	LYS
1	B	122	ARG
1	B	132	ARG
1	B	168	MET
1	B	190	SER
1	B	205	ASP
1	B	215	VAL
1	B	218	GLU
1	B	220	ARG
1	B	223	ASN
1	B	252	ARG
1	B	254	ASP
1	B	257	PHE
1	B	260	ARG
1	B	265	ILE
1	B	269	LEU

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Mol	Chain	Res	Type
1	B	272	LYS
1	B	276	LEU
1	B	277	GLU
1	B	287	LYS
1	B	293	ASN
1	B	296	GLU
1	B	301	THR
1	B	322	LYS
1	B	324	MET
1	B	337	MET
1	B	353	GLN
1	B	354	ASP
1	B	367	LYS
1	C	101	GLU
1	C	102	ILE
1	C	122	ARG
1	C	132	ARG
1	C	168	MET
1	C	190	SER
1	C	205	ASP
1	C	214	GLU
1	C	215	VAL
1	C	218	GLU
1	C	222	ARG
1	C	238	ILE
1	C	252	ARG
1	C	254	ASP
1	C	257	PHE
1	C	260	ARG
1	C	276	LEU
1	C	285	LYS
1	C	296	GLU
1	C	309	ILE
1	C	324	MET
1	C	337	MET
1	C	351	VAL
1	C	353	GLN
1	C	367	LYS
1	D	99	LEU
1	D	103	VAL
1	D	105	LEU
1	D	122	ARG

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Mol	Chain	Res	Type
1	D	132	ARG
1	D	168	MET
1	D	171	TRP
1	D	190	SER
1	D	195	LYS
1	D	205	ASP
1	D	218	GLU
1	D	223	ASN
1	D	228	GLU
1	D	252	ARG
1	D	254	ASP
1	D	257	PHE
1	D	260	ARG
1	D	269	LEU
1	D	276	LEU
1	D	285	LYS
1	D	296	GLU
1	D	324	MET
1	D	329	LEU
1	D	347	ARG
1	E	106	GLU
1	E	109	LYS
1	E	122	ARG
1	E	132	ARG
1	E	168	MET
1	E	190	SER
1	E	205	ASP
1	E	215	VAL
1	E	218	GLU
1	E	220	ARG
1	E	223	ASN
1	E	252	ARG
1	E	254	ASP
1	E	257	PHE
1	E	260	ARG
1	E	265	ILE
1	E	269	LEU
1	E	276	LEU
1	E	277	GLU
1	E	290	PRO
1	E	301	THR
1	E	322	LYS

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Mol	Chain	Res	Type
1	E	324	MET
1	E	347	ARG
1	E	351	VAL
1	E	353	GLN
1	E	354	ASP
1	E	367	LYS
1	F	121	LYS
1	F	122	ARG
1	F	132	ARG
1	F	144	LYS
1	F	146	MET
1	F	168	MET
1	F	171	TRP
1	F	190	SER
1	F	205	ASP
1	F	215	VAL
1	F	218	GLU
1	F	223	ASN
1	F	228	GLU
1	F	251	TRP
1	F	252	ARG
1	F	254	ASP
1	F	257	PHE
1	F	269	LEU
1	F	276	LEU
1	F	285	LYS
1	F	322	LYS
1	F	337	MET
1	F	351	VAL
1	F	369	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	C	100	ASN
1	D	161	HIS
1	D	274	HIS
1	E	274	HIS
1	E	293	ASN

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	210:SER	C	211:TYR	N	2.55

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	269/316 (85%)	-0.04	11 (4%)	37	24	84, 149, 228, 279	0
1	B	257/316 (81%)	-0.05	9 (3%)	44	29	71, 135, 218, 262	0
1	C	272/316 (86%)	-0.19	5 (1%)	68	53	86, 134, 200, 216	0
1	D	273/316 (86%)	-0.22	3 (1%)	80	68	81, 135, 208, 251	0
1	E	262/316 (82%)	-0.18	6 (2%)	60	44	61, 133, 216, 275	0
1	F	274/316 (86%)	-0.21	4 (1%)	73	60	73, 126, 193, 246	0
All	All	1607/1896 (84%)	-0.15	38 (2%)	59	42	61, 134, 214, 279	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	197	ALA	9.4
1	F	192	LYS	8.5
1	A	217	GLY	5.3
1	B	196	PRO	4.4
1	C	192	LYS	4.0
1	A	192	LYS	4.0
1	D	192	LYS	3.9
1	D	171	TRP	3.6
1	F	171	TRP	3.2
1	E	216	GLY	3.1
1	F	214	GLU	3.1
1	E	194	ASN	3.0
1	A	301	THR	2.9
1	D	170	LYS	2.9
1	C	197	ALA	2.9
1	A	297	LEU	2.9
1	A	322	LYS	2.8
1	B	216	GLY	2.8
1	B	103	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	340	PHE	2.7
1	A	282	TYR	2.7
1	E	96	LYS	2.7
1	A	170	LYS	2.7
1	E	196	PRO	2.5
1	B	217	GLY	2.5
1	F	106	GLU	2.5
1	E	103	VAL	2.4
1	B	102	ILE	2.4
1	C	160	ILE	2.3
1	B	192	LYS	2.3
1	A	216	GLY	2.3
1	E	217	GLY	2.2
1	A	293	ASN	2.1
1	B	240	LYS	2.1
1	C	358	ALA	2.0
1	A	295	GLU	2.0
1	C	210	SER	2.0
1	B	100	ASN	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.