



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Dec 5, 2016 – 12:05 PM EST

PDB ID : 5LJV
EMDB ID: : EMD-4062
Title : MamK double helical filament
Authors : Lowe, J.
Deposited on : 2016-07-21
Resolution : 3.65 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

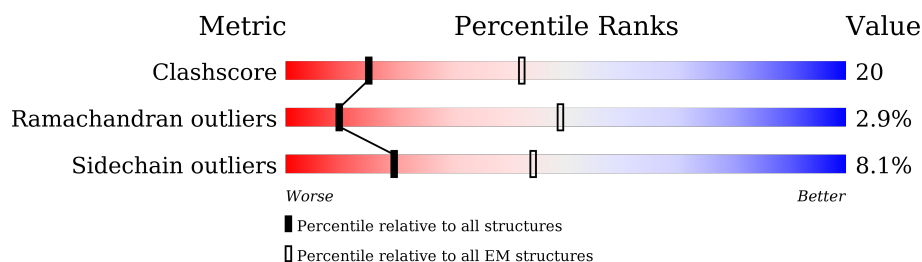
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.65 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	347	
1	B	347	
1	C	347	
1	D	347	
1	E	347	
1	F	347	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15000 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Actin-like ATPase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	325	Total	C	N	O	S	0	0
			2472	1569	425	466	12		
1	B	325	Total	C	N	O	S	0	0
			2472	1569	425	466	12		
1	C	325	Total	C	N	O	S	0	0
			2472	1569	425	466	12		
1	D	325	Total	C	N	O	S	0	0
			2472	1569	425	466	12		
1	E	325	Total	C	N	O	S	0	0
			2472	1569	425	466	12		
1	F	325	Total	C	N	O	S	0	0
			2472	1569	425	466	12		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	VAL	ILE	conflict	UNP Q2W8Q6
B	16	VAL	ILE	conflict	UNP Q2W8Q6
C	16	VAL	ILE	conflict	UNP Q2W8Q6
D	16	VAL	ILE	conflict	UNP Q2W8Q6
E	16	VAL	ILE	conflict	UNP Q2W8Q6
F	16	VAL	ILE	conflict	UNP Q2W8Q6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

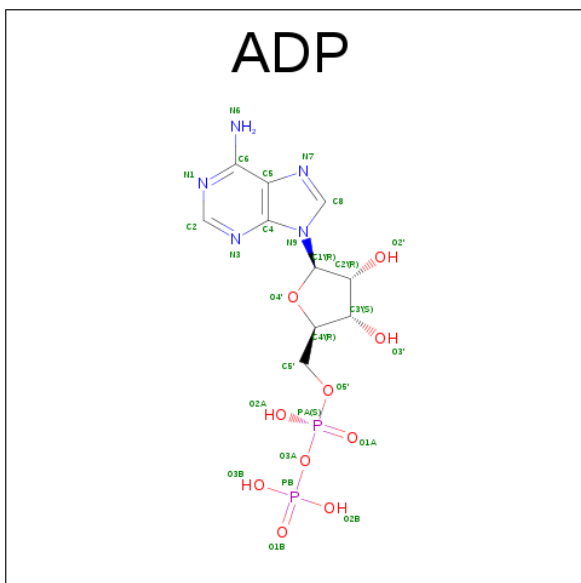
Mol	Chain	Residues	Atoms		AltConf
2	D	1	Total	Mg	0
			1	1	
2	E	1	Total	Mg	0
			1	1	
2	B	1	Total	Mg	0
			1	1	
2	C	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total Mg 1 1	0
2	F	1	Total Mg 1 1	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$).

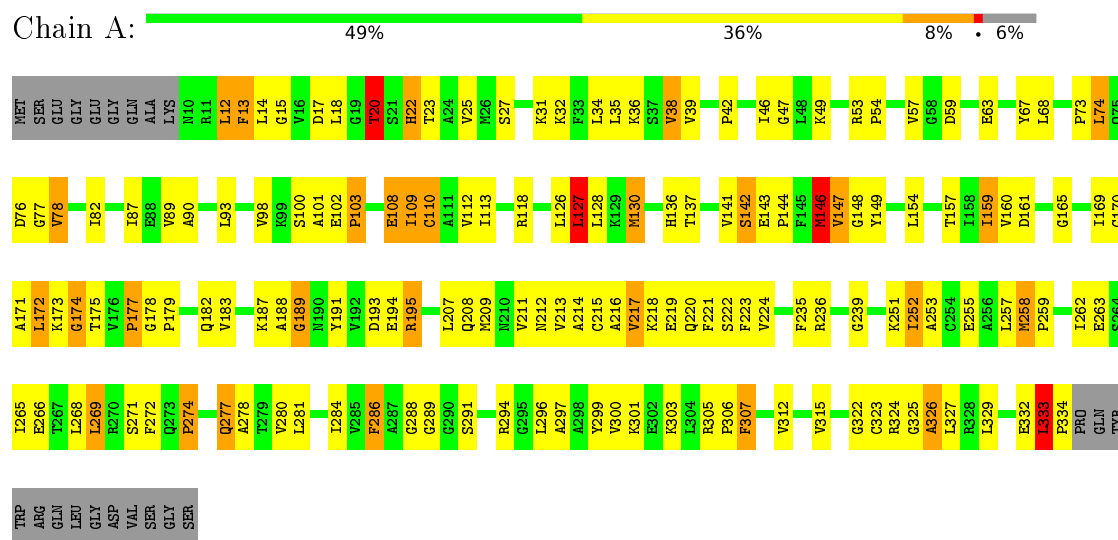


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0

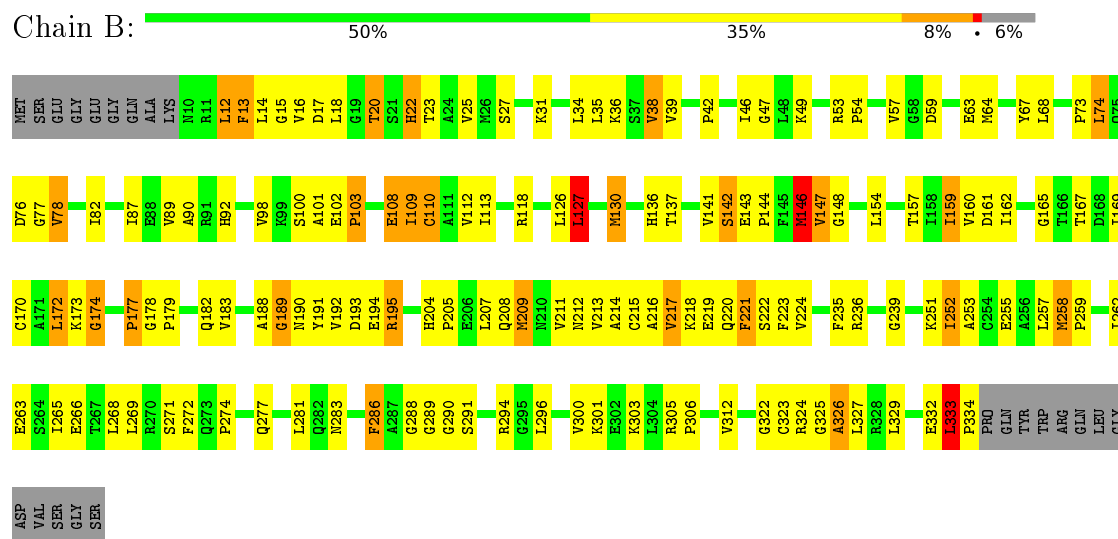
3 Residue-property plots

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. 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. 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: Actin-like ATPase

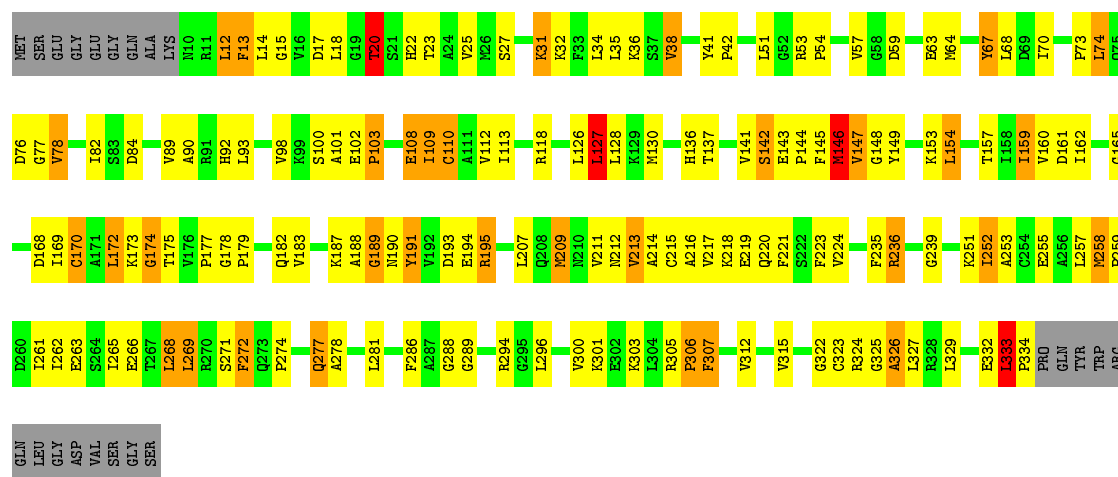


• Molecule 1: Actin-like ATPase



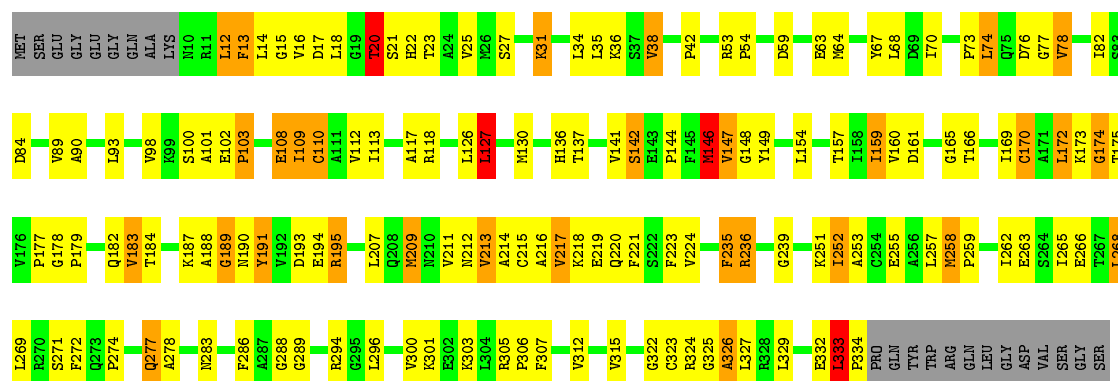
• Molecule 1: Actin-like ATPase





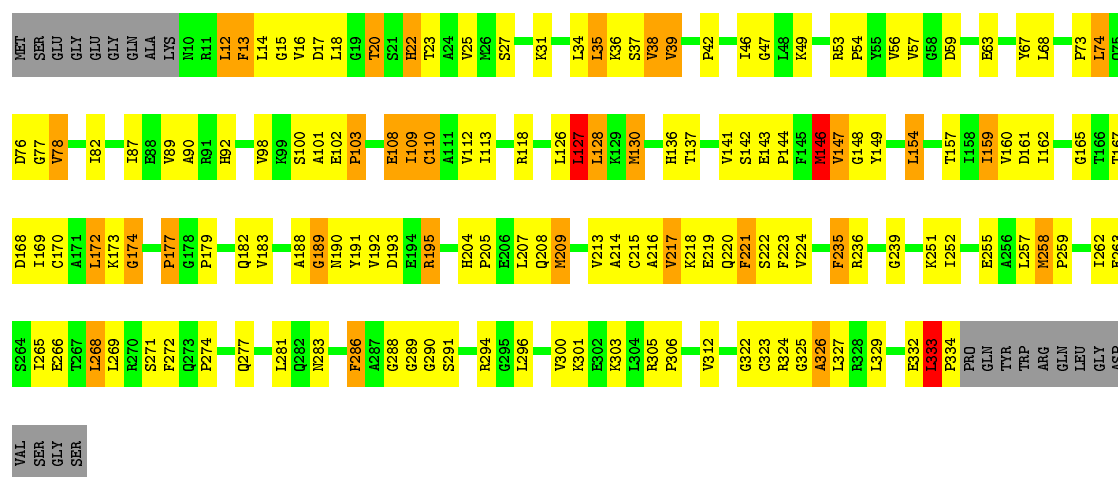
• Molecule 1: Actin-like ATPase

Chain D: 51% 33% 9% 6%

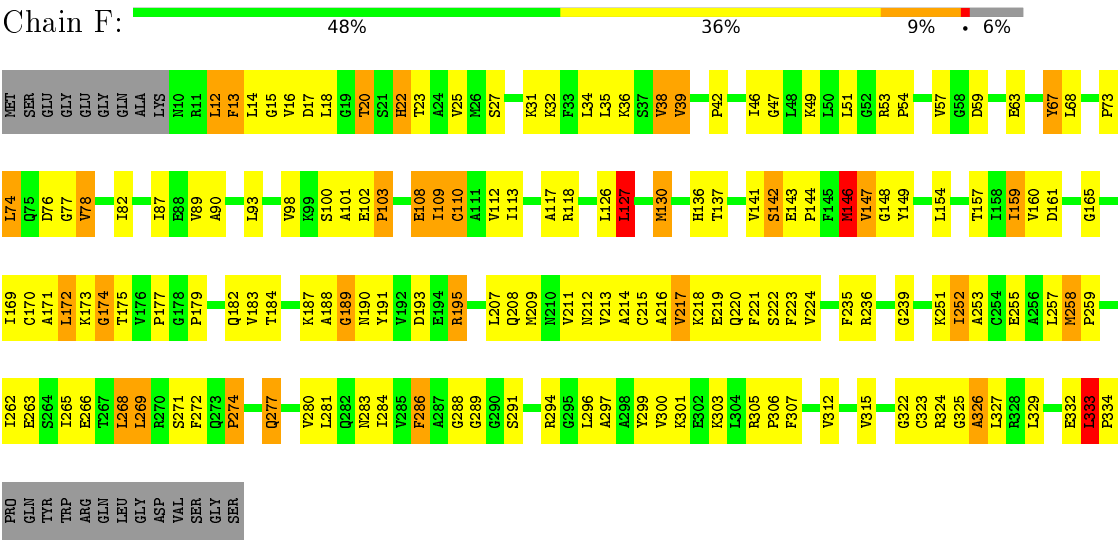


• Molecule 1: Actin-like ATPase

Chain E: 50% 34% 9% 6%



• Molecule 1: Actin-like ATPase



4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of segments used	596427	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	1.37	15/2514 (0.6%)	1.39	18/3411 (0.5%)
1	B	1.46	14/2514 (0.6%)	1.38	21/3411 (0.6%)
1	C	1.50	17/2514 (0.7%)	1.39	20/3411 (0.6%)
1	D	1.50	19/2514 (0.8%)	1.40	20/3411 (0.6%)
1	E	1.49	21/2514 (0.8%)	1.39	22/3411 (0.6%)
1	F	1.37	14/2514 (0.6%)	1.39	21/3411 (0.6%)
All	All	1.45	100/15084 (0.7%)	1.39	122/20466 (0.6%)

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	4
1	B	0	4
1	C	0	4
1	D	0	4
1	E	0	3
1	F	0	2
All	All	0	21

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	286	PHE	CB-CG	-9.62	1.34	1.51
1	D	286	PHE	CB-CG	-9.31	1.35	1.51
1	F	67	TYR	CB-CG	-7.99	1.39	1.51
1	A	67	TYR	CB-CG	-7.66	1.40	1.51
1	A	286	PHE	CB-CG	-7.24	1.39	1.51
1	F	286	PHE	CB-CG	-7.12	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	191	TYR	CB-CG	-7.04	1.41	1.51
1	D	277	GLN	CA-CB	-6.82	1.39	1.53
1	C	277	GLN	CA-CB	-6.81	1.39	1.53
1	E	274	PRO	CA-C	-6.75	1.39	1.52
1	D	221	PHE	CG-CD1	-6.63	1.28	1.38
1	F	67	TYR	CA-CB	-6.60	1.39	1.53
1	B	274	PRO	CA-C	-6.58	1.39	1.52
1	A	67	TYR	CA-CB	-6.57	1.39	1.53
1	F	272	PHE	CB-CG	-6.55	1.40	1.51
1	D	191	TYR	CB-CG	-6.45	1.42	1.51
1	D	67	TYR	CB-CG	-6.43	1.42	1.51
1	C	334	PRO	N-CA	6.43	1.58	1.47
1	B	222	SER	CB-OG	6.40	1.50	1.42
1	A	334	PRO	N-CA	6.36	1.58	1.47
1	F	222	SER	CB-OG	6.34	1.50	1.42
1	E	67	TYR	CB-CG	-6.33	1.42	1.51
1	C	67	TYR	CB-CG	-6.28	1.42	1.51
1	A	222	SER	CB-OG	6.20	1.50	1.42
1	F	274	PRO	CA-C	-6.19	1.40	1.52
1	B	286	PHE	CB-CG	-6.16	1.40	1.51
1	A	272	PHE	CB-CG	-6.16	1.40	1.51
1	A	274	PRO	CA-C	-6.14	1.40	1.52
1	E	217	VAL	C-O	-6.14	1.11	1.23
1	E	286	PHE	CB-CG	-6.11	1.41	1.51
1	E	222	SER	CB-OG	6.09	1.50	1.42
1	C	272	PHE	CA-CB	-6.09	1.40	1.53
1	B	67	TYR	CB-CG	-6.09	1.42	1.51
1	D	272	PHE	CB-CG	-6.03	1.41	1.51
1	A	299	TYR	CE1-CZ	6.01	1.46	1.38
1	D	272	PHE	CA-CB	-6.01	1.40	1.53
1	E	290	GLY	N-CA	5.98	1.55	1.46
1	F	334	PRO	N-CA	5.96	1.57	1.47
1	A	307	PHE	CB-CG	-5.94	1.41	1.51
1	B	334	PRO	N-CA	5.93	1.57	1.47
1	B	272	PHE	CB-CG	-5.92	1.41	1.51
1	D	286	PHE	CG-CD2	-5.90	1.29	1.38
1	F	307	PHE	CB-CG	-5.90	1.41	1.51
1	F	299	TYR	CE1-CZ	5.85	1.46	1.38
1	A	22	HIS	CA-C	-5.80	1.37	1.52
1	E	221	PHE	CG-CD1	-5.79	1.30	1.38
1	C	20	THR	CB-CG2	5.79	1.71	1.52
1	C	221	PHE	CG-CD1	-5.77	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	67	TYR	CA-CB	-5.75	1.41	1.53
1	F	177	PRO	N-CA	5.74	1.57	1.47
1	E	272	PHE	CB-CG	-5.72	1.41	1.51
1	F	22	HIS	CA-C	-5.71	1.38	1.52
1	A	272	PHE	CA-CB	-5.69	1.41	1.53
1	B	67	TYR	CA-CB	-5.67	1.41	1.53
1	D	235	PHE	CG-CD2	-5.65	1.30	1.38
1	E	334	PRO	N-CA	5.65	1.56	1.47
1	C	272	PHE	CB-CG	-5.65	1.41	1.51
1	A	177	PRO	N-CA	5.61	1.56	1.47
1	B	272	PHE	CA-CB	-5.59	1.41	1.53
1	D	334	PRO	N-CA	5.59	1.56	1.47
1	B	290	GLY	N-CA	5.59	1.54	1.46
1	B	277	GLN	CA-CB	-5.57	1.41	1.53
1	E	192	VAL	CB-CG1	-5.54	1.41	1.52
1	F	272	PHE	CA-CB	-5.53	1.41	1.53
1	A	277	GLN	CA-CB	-5.52	1.41	1.53
1	D	236	ARG	CZ-NH2	5.46	1.40	1.33
1	D	170	CYS	N-CA	-5.46	1.35	1.46
1	E	168	ASP	C-O	-5.45	1.13	1.23
1	D	67	TYR	CA-CB	-5.42	1.42	1.53
1	E	272	PHE	CA-CB	-5.41	1.42	1.53
1	C	67	TYR	CA-CB	-5.38	1.42	1.53
1	F	39	VAL	N-CA	-5.37	1.35	1.46
1	C	177	PRO	N-CA	5.35	1.56	1.47
1	E	277	GLN	CA-CB	-5.32	1.42	1.53
1	E	177	PRO	N-CA	5.26	1.56	1.47
1	D	20	THR	CB-CG2	5.26	1.69	1.52
1	C	170	CYS	N-CA	-5.26	1.35	1.46
1	C	307	PHE	CB-CG	-5.24	1.42	1.51
1	B	22	HIS	CA-C	-5.23	1.39	1.52
1	F	277	GLN	CA-CB	-5.23	1.42	1.53
1	C	57	VAL	CA-CB	-5.19	1.43	1.54
1	C	286	PHE	CG-CD2	-5.19	1.30	1.38
1	E	22	HIS	CA-C	-5.18	1.39	1.52
1	D	307	PHE	CB-CG	-5.17	1.42	1.51
1	E	39	VAL	N-CA	-5.14	1.36	1.46
1	E	128	LEU	N-CA	-5.14	1.36	1.46
1	D	183	VAL	CA-CB	-5.14	1.44	1.54
1	B	221	PHE	CG-CD1	-5.12	1.31	1.38
1	D	177	PRO	N-CA	5.12	1.55	1.47
1	A	334	PRO	CA-C	5.11	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	192	VAL	CB-CG1	-5.09	1.42	1.52
1	C	41	TYR	CB-CG	-5.09	1.44	1.51
1	B	177	PRO	N-CA	5.08	1.55	1.47
1	D	221	PHE	CB-CG	-5.04	1.42	1.51
1	D	67	TYR	N-CA	-5.03	1.36	1.46
1	E	67	TYR	N-CA	-5.03	1.36	1.46
1	E	235	PHE	CG-CD2	-5.03	1.31	1.38
1	E	268	LEU	CA-CB	-5.03	1.42	1.53
1	A	20	THR	CB-CG2	5.01	1.68	1.52
1	C	236	ARG	CZ-NH2	5.00	1.39	1.33

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	269	LEU	CB-CG-CD2	-9.41	95.01	111.00
1	F	269	LEU	CB-CG-CD2	-9.35	95.11	111.00
1	C	269	LEU	CB-CG-CD2	-9.33	95.14	111.00
1	A	269	LEU	CB-CG-CD2	-9.30	95.18	111.00
1	C	172	LEU	CA-CB-CG	-8.85	94.94	115.30
1	D	172	LEU	CA-CB-CG	-8.77	95.13	115.30
1	E	269	LEU	CB-CG-CD2	-8.28	96.92	111.00
1	E	161	ASP	CB-CG-OD2	8.05	125.55	118.30
1	B	161	ASP	CB-CG-OD2	8.05	125.54	118.30
1	B	269	LEU	CB-CG-CD2	-8.04	97.33	111.00
1	A	333	LEU	CB-CG-CD1	7.90	124.42	111.00
1	F	333	LEU	CB-CG-CD1	7.87	124.38	111.00
1	A	172	LEU	CA-CB-CG	-7.85	97.24	115.30
1	F	172	LEU	CA-CB-CG	-7.75	97.47	115.30
1	E	333	LEU	CB-CG-CD1	7.70	124.08	111.00
1	A	161	ASP	CB-CG-OD2	7.70	125.23	118.30
1	B	333	LEU	CB-CG-CD1	7.64	124.00	111.00
1	C	333	LEU	CB-CG-CD1	7.54	123.81	111.00
1	F	161	ASP	CB-CG-OD2	7.52	125.07	118.30
1	D	333	LEU	CB-CG-CD1	7.51	123.76	111.00
1	B	172	LEU	CA-CB-CG	-7.33	98.44	115.30
1	C	127	LEU	CA-CB-CG	-7.29	98.53	115.30
1	E	172	LEU	CA-CB-CG	-7.29	98.53	115.30
1	D	127	LEU	CA-CB-CG	-7.20	98.74	115.30
1	A	17	ASP	N-CA-C	-7.07	91.91	111.00
1	C	161	ASP	CB-CG-OD2	7.04	124.63	118.30
1	D	161	ASP	CB-CG-OD2	7.02	124.62	118.30
1	C	258	MET	CA-CB-CG	-6.96	101.47	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	LEU	CA-CB-CG	-6.95	99.31	115.30
1	F	127	LEU	CA-CB-CG	-6.92	99.38	115.30
1	D	258	MET	CA-CB-CG	-6.86	101.64	113.30
1	F	258	MET	CA-CB-CG	-6.71	101.89	113.30
1	A	258	MET	CA-CB-CG	-6.67	101.96	113.30
1	F	17	ASP	N-CA-C	-6.66	93.01	111.00
1	E	161	ASP	CB-CG-OD1	-6.62	112.34	118.30
1	B	127	LEU	CA-CB-CG	-6.62	100.08	115.30
1	E	147	VAL	CB-CA-C	-6.60	98.86	111.40
1	C	17	ASP	N-CA-C	-6.60	93.19	111.00
1	C	154	LEU	CA-CB-CG	-6.56	100.21	115.30
1	E	35	LEU	CB-CG-CD1	6.55	122.14	111.00
1	B	17	ASP	N-CA-C	-6.50	93.45	111.00
1	B	147	VAL	CB-CA-C	-6.49	99.08	111.40
1	B	35	LEU	CB-CG-CD1	6.47	122.00	111.00
1	D	154	LEU	CA-CB-CG	-6.46	100.44	115.30
1	E	127	LEU	CA-CB-CG	-6.46	100.44	115.30
1	B	146	MET	CB-CG-SD	6.38	131.54	112.40
1	D	147	VAL	CB-CA-C	-6.34	99.35	111.40
1	E	146	MET	CB-CG-SD	6.34	131.44	112.40
1	A	146	MET	CB-CG-SD	6.33	131.38	112.40
1	F	146	MET	CB-CG-SD	6.28	131.25	112.40
1	B	161	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	D	17	ASP	N-CA-C	-6.21	94.23	111.00
1	F	161	ASP	CB-CG-OD1	-6.20	112.72	118.30
1	C	146	MET	CB-CG-SD	6.20	131.00	112.40
1	E	17	ASP	N-CA-C	-6.18	94.31	111.00
1	C	147	VAL	CB-CA-C	-6.15	99.72	111.40
1	D	146	MET	CB-CG-SD	6.15	130.84	112.40
1	B	258	MET	CA-CB-CG	-6.12	102.89	113.30
1	D	35	LEU	CB-CG-CD1	6.12	121.41	111.00
1	E	258	MET	CA-CB-CG	-6.07	102.99	113.30
1	E	16	VAL	N-CA-C	-6.03	94.71	111.00
1	E	127	LEU	CB-CA-C	-5.99	98.81	110.20
1	B	217	VAL	CA-CB-CG2	-5.97	101.94	110.90
1	F	147	VAL	CB-CA-C	-5.96	100.08	111.40
1	A	159	ILE	CB-CA-C	-5.95	99.69	111.60
1	F	35	LEU	CB-CG-CD1	5.93	121.08	111.00
1	B	154	LEU	CA-CB-CG	-5.92	101.69	115.30
1	F	159	ILE	CB-CA-C	-5.88	99.83	111.60
1	D	286	PHE	CB-CG-CD1	-5.87	116.69	120.80
1	E	154	LEU	CA-CB-CG	-5.87	101.81	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	35	LEU	CB-CG-CD1	5.84	120.93	111.00
1	A	147	VAL	CB-CA-C	-5.83	100.32	111.40
1	D	161	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	A	35	LEU	CB-CG-CD1	5.80	120.87	111.00
1	A	161	ASP	CB-CG-OD1	-5.79	113.09	118.30
1	D	195	ARG	CG-CD-NE	-5.79	99.65	111.80
1	F	127	LEU	CB-CA-C	-5.77	99.24	110.20
1	B	127	LEU	CB-CA-C	-5.74	99.29	110.20
1	E	217	VAL	CA-CB-CG2	-5.74	102.29	110.90
1	C	159	ILE	CB-CA-C	-5.66	100.28	111.60
1	F	195	ARG	CG-CD-NE	-5.65	99.93	111.80
1	A	127	LEU	CB-CA-C	-5.62	99.52	110.20
1	D	159	ILE	CB-CA-C	-5.62	100.36	111.60
1	D	127	LEU	CB-CA-C	-5.59	99.58	110.20
1	C	127	LEU	CB-CA-C	-5.58	99.60	110.20
1	F	16	VAL	N-CA-C	-5.57	95.97	111.00
1	A	217	VAL	CA-CB-CG2	-5.56	102.56	110.90
1	B	16	VAL	N-CA-C	-5.52	96.09	111.00
1	E	195	ARG	CG-CD-NE	-5.50	100.25	111.80
1	C	195	ARG	CG-CD-NE	-5.46	100.33	111.80
1	C	161	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	A	195	ARG	CG-CD-NE	-5.42	100.43	111.80
1	F	217	VAL	CA-CB-CG2	-5.38	102.83	110.90
1	E	162	ILE	CB-CA-C	-5.38	100.84	111.60
1	A	154	LEU	CA-CB-CG	-5.37	102.95	115.30
1	E	159	ILE	CB-CA-C	-5.36	100.88	111.60
1	F	154	LEU	CA-CB-CG	-5.36	102.97	115.30
1	E	56	VAL	CB-CA-C	-5.33	101.27	111.40
1	C	286	PHE	CB-CG-CD1	-5.28	117.10	120.80
1	F	272	PHE	CB-CA-C	-5.28	99.84	110.40
1	B	159	ILE	CB-CA-C	-5.28	101.05	111.60
1	D	213	VAL	CB-CA-C	-5.25	101.42	111.40
1	B	162	ILE	CB-CA-C	-5.24	101.12	111.60
1	E	268	LEU	CA-CB-CG	-5.23	103.27	115.30
1	A	32	LYS	N-CA-C	-5.20	96.97	111.00
1	B	195	ARG	CG-CD-NE	-5.19	100.91	111.80
1	B	167	THR	N-CA-C	-5.18	97.02	111.00
1	B	268	LEU	CA-CB-CG	-5.17	103.42	115.30
1	C	32	LYS	N-CA-C	-5.13	97.13	111.00
1	B	268	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	C	168	ASP	CB-CG-OD2	5.12	122.91	118.30
1	E	167	THR	N-CA-C	-5.10	97.22	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	PHE	CB-CA-C	-5.09	100.21	110.40
1	D	16	VAL	N-CA-C	-5.07	97.30	111.00
1	C	268	LEU	CB-CA-C	-5.07	100.56	110.20
1	F	32	LYS	N-CA-C	-5.05	97.38	111.00
1	E	268	LEU	CB-CG-CD1	-5.02	102.46	111.00
1	D	217	VAL	CA-CB-CG1	5.02	118.43	110.90
1	C	213	VAL	CB-CA-C	-5.01	101.88	111.40
1	D	268	LEU	CB-CA-C	-5.01	100.68	110.20
1	F	268	LEU	CA-CB-CG	-5.00	103.80	115.30
1	F	268	LEU	CB-CA-C	-5.00	100.69	110.20

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	GLY	Peptide
1	A	177	PRO	Peptide
1	A	178	GLY	Peptide
1	A	333	LEU	Peptide
1	B	174	GLY	Peptide
1	B	177	PRO	Peptide
1	B	178	GLY	Peptide
1	B	209	MET	Peptide
1	C	174	GLY	Peptide
1	C	178	GLY	Peptide
1	C	209	MET	Peptide
1	C	31	LYS	Peptide
1	D	174	GLY	Peptide
1	D	178	GLY	Peptide
1	D	209	MET	Peptide
1	D	31	LYS	Peptide
1	E	174	GLY	Peptide
1	E	177	PRO	Peptide
1	E	209	MET	Peptide
1	F	174	GLY	Peptide
1	F	333	LEU	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	2472	0	2524	110	0
1	B	2472	0	2524	101	0
1	C	2472	0	2524	110	0
1	D	2472	0	2524	101	0
1	E	2472	0	2524	97	0
1	F	2472	0	2524	114	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	27	0	12	2	0
3	B	27	0	12	1	0
3	C	27	0	12	2	0
3	D	27	0	12	3	0
3	E	27	0	12	1	0
3	F	27	0	12	2	0
All	All	15000	0	15216	598	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 20.

All (598) 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:49:LYS:NZ	1:C:149:TYR:OH	2.07	0.88
1:D:149:TYR:OH	1:F:49:LYS:NZ	2.07	0.87
1:A:149:TYR:OH	1:B:49:LYS:NZ	2.11	0.83
1:D:332:GLU:C	1:D:333:LEU:HD12	1.99	0.83
1:C:332:GLU:C	1:C:333:LEU:HD12	1.98	0.83
1:E:49:LYS:NZ	1:F:149:TYR:OH	2.13	0.81
1:F:332:GLU:C	1:F:333:LEU:HD12	2.04	0.78
1:F:258:MET:SD	1:F:296:LEU:CD1	2.72	0.77
1:A:258:MET:SD	1:A:296:LEU:CD1	2.73	0.77
1:A:332:GLU:C	1:A:333:LEU:HD12	2.04	0.77
1:C:82:ILE:HG22	1:C:82:ILE:O	1.86	0.76
1:D:258:MET:SD	1:D:296:LEU:CD1	2.75	0.75
1:B:82:ILE:HG22	1:B:82:ILE:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:MET:SD	1:C:296:LEU:CD1	2.75	0.75
1:D:82:ILE:HG22	1:D:82:ILE:O	1.86	0.74
1:E:258:MET:SD	1:E:296:LEU:CD1	2.75	0.74
1:B:332:GLU:C	1:B:333:LEU:HD12	2.07	0.74
1:E:82:ILE:O	1:E:82:ILE:HG22	1.86	0.74
1:B:258:MET:SD	1:B:296:LEU:CD1	2.75	0.73
1:E:332:GLU:C	1:E:333:LEU:HD12	2.09	0.73
1:C:332:GLU:O	1:C:333:LEU:HD12	1.89	0.72
1:D:325:GLY:O	1:D:326:ALA:C	2.27	0.72
1:A:82:ILE:O	1:A:82:ILE:HG22	1.88	0.72
1:F:82:ILE:O	1:F:82:ILE:HG22	1.88	0.72
1:C:159:ILE:HG22	1:C:160:VAL:N	2.05	0.72
1:D:332:GLU:O	1:D:333:LEU:HD12	1.90	0.71
1:F:112:VAL:HB	1:F:326:ALA:HB1	1.72	0.71
1:F:325:GLY:O	1:F:326:ALA:C	2.28	0.71
1:C:325:GLY:O	1:C:326:ALA:C	2.28	0.71
1:A:236:ARG:NH1	1:A:239:GLY:O	2.24	0.70
1:B:325:GLY:O	1:B:326:ALA:C	2.29	0.70
1:B:332:GLU:O	1:B:333:LEU:HD12	1.92	0.69
1:A:325:GLY:O	1:A:326:ALA:C	2.30	0.69
1:D:112:VAL:HB	1:D:326:ALA:HB1	1.74	0.69
1:E:224:VAL:HG12	1:E:255:GLU:HG3	1.73	0.69
1:F:332:GLU:O	1:F:333:LEU:HD12	1.92	0.69
1:A:332:GLU:O	1:A:333:LEU:HD12	1.91	0.69
1:B:236:ARG:NH1	1:B:239:GLY:O	2.26	0.69
1:F:236:ARG:NH1	1:F:239:GLY:O	2.25	0.69
1:E:332:GLU:O	1:E:333:LEU:HD12	1.92	0.68
1:F:224:VAL:HG12	1:F:255:GLU:HG3	1.75	0.68
1:D:224:VAL:HG12	1:D:255:GLU:HG3	1.75	0.68
1:D:159:ILE:HG22	1:D:160:VAL:N	2.06	0.68
1:A:112:VAL:HB	1:A:326:ALA:HB1	1.74	0.68
1:A:159:ILE:HG22	1:A:160:VAL:N	2.08	0.68
1:B:224:VAL:HG12	1:B:255:GLU:HG3	1.74	0.68
1:E:236:ARG:NH1	1:E:239:GLY:O	2.26	0.68
1:A:224:VAL:HG12	1:A:255:GLU:HG3	1.75	0.67
1:C:224:VAL:HG12	1:C:255:GLU:HG3	1.75	0.67
1:F:325:GLY:O	1:F:327:LEU:N	2.27	0.67
1:E:113:ILE:HD13	1:E:127:LEU:HD22	1.76	0.67
1:B:113:ILE:HD13	1:B:127:LEU:HD22	1.76	0.67
1:E:325:GLY:O	1:E:326:ALA:C	2.28	0.67
1:A:325:GLY:O	1:A:327:LEU:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:GLY:O	1:D:327:LEU:N	2.28	0.66
1:C:325:GLY:O	1:C:327:LEU:N	2.28	0.66
1:A:113:ILE:HD13	1:A:127:LEU:HD22	1.77	0.66
1:C:112:VAL:HB	1:C:326:ALA:HB1	1.77	0.66
1:E:325:GLY:O	1:E:327:LEU:N	2.29	0.66
1:E:112:VAL:HB	1:E:326:ALA:HB1	1.78	0.65
1:F:113:ILE:HD13	1:F:127:LEU:HD22	1.77	0.65
1:F:159:ILE:HG22	1:F:160:VAL:N	2.10	0.65
1:D:18:LEU:HD12	1:D:23:THR:OG1	1.97	0.65
1:E:18:LEU:HD12	1:E:23:THR:OG1	1.97	0.64
1:F:18:LEU:HD12	1:F:23:THR:OG1	1.97	0.64
1:B:18:LEU:HD12	1:B:23:THR:OG1	1.98	0.64
1:B:325:GLY:O	1:B:327:LEU:N	2.30	0.64
1:F:223:PHE:HE1	1:F:251:LYS:HG3	1.62	0.64
1:A:223:PHE:HE1	1:A:251:LYS:HG3	1.63	0.64
1:A:18:LEU:HD12	1:A:23:THR:OG1	1.98	0.64
1:C:236:ARG:NH1	1:C:239:GLY:O	2.31	0.64
1:B:112:VAL:HB	1:B:326:ALA:HB1	1.79	0.63
1:C:223:PHE:HE1	1:C:251:LYS:HG3	1.64	0.63
1:C:18:LEU:HD12	1:C:23:THR:OG1	1.98	0.63
1:C:141:VAL:HG23	1:C:146:MET:HE3	1.81	0.63
1:D:236:ARG:NH1	1:D:239:GLY:O	2.31	0.63
1:B:159:ILE:HG22	1:B:160:VAL:N	2.14	0.62
1:E:108:GLU:HG2	1:E:136:HIS:NE2	2.14	0.62
1:C:113:ILE:HD13	1:C:127:LEU:HD22	1.82	0.62
1:D:141:VAL:HG23	1:D:146:MET:HE3	1.82	0.62
1:D:223:PHE:HE1	1:D:251:LYS:HG3	1.64	0.61
1:D:113:ILE:HD13	1:D:127:LEU:HD22	1.82	0.61
1:E:191:TYR:CD2	1:E:191:TYR:C	2.74	0.61
1:E:159:ILE:HG22	1:E:160:VAL:N	2.14	0.60
1:F:108:GLU:HG2	1:F:136:HIS:NE2	2.16	0.60
1:D:191:TYR:CD2	1:D:191:TYR:C	2.73	0.60
1:B:108:GLU:HG2	1:B:136:HIS:NE2	2.14	0.60
1:B:191:TYR:C	1:B:191:TYR:CD2	2.75	0.60
1:F:141:VAL:HG23	1:F:146:MET:HE3	1.84	0.60
1:C:20:THR:OG1	1:C:20:THR:O	2.18	0.60
1:E:223:PHE:HE1	1:E:251:LYS:HG3	1.67	0.60
1:F:20:THR:O	1:F:20:THR:OG1	2.19	0.60
1:D:20:THR:O	1:D:20:THR:OG1	2.18	0.60
1:B:223:PHE:HE1	1:B:251:LYS:HG3	1.67	0.59
1:A:108:GLU:HG2	1:A:136:HIS:NE2	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:GLU:HG2	1:D:136:HIS:NE2	2.17	0.59
1:A:53:ARG:HB2	1:A:54:PRO:HD2	1.84	0.59
1:C:191:TYR:C	1:C:191:TYR:CD2	2.74	0.59
1:A:141:VAL:HG23	1:A:146:MET:HE3	1.84	0.59
1:B:20:THR:OG1	1:B:20:THR:O	2.18	0.59
1:A:20:THR:O	1:A:20:THR:OG1	2.19	0.59
1:C:53:ARG:HB2	1:C:54:PRO:HD2	1.84	0.59
1:F:146:MET:HG3	1:F:326:ALA:H	1.68	0.59
1:D:82:ILE:CG2	1:D:82:ILE:O	2.51	0.58
1:C:108:GLU:HG2	1:C:136:HIS:NE2	2.17	0.58
1:D:53:ARG:HB2	1:D:54:PRO:HD2	1.84	0.58
1:B:82:ILE:CG2	1:B:82:ILE:O	2.52	0.58
1:F:218:LYS:HE2	3:F:402:ADP:N3	2.18	0.57
1:A:218:LYS:HE2	3:A:402:ADP:N3	2.19	0.57
1:C:82:ILE:CG2	1:C:82:ILE:O	2.51	0.57
1:D:20:THR:HG21	1:D:165:GLY:HA3	1.87	0.57
1:B:53:ARG:HB2	1:B:54:PRO:HD2	1.86	0.57
1:C:188:ALA:O	1:C:189:GLY:C	2.43	0.57
1:F:191:TYR:CD2	1:F:191:TYR:C	2.77	0.57
1:F:53:ARG:HB2	1:F:54:PRO:HD2	1.85	0.57
1:A:146:MET:HG3	1:A:326:ALA:H	1.69	0.57
1:A:191:TYR:CD2	1:A:191:TYR:C	2.78	0.57
1:E:147:VAL:HG12	1:E:148:GLY:N	2.20	0.57
1:E:141:VAL:HG23	1:E:146:MET:HE3	1.87	0.57
1:C:20:THR:HG21	1:C:165:GLY:HA3	1.86	0.57
1:B:141:VAL:HG23	1:B:146:MET:HE3	1.86	0.56
1:F:82:ILE:O	1:F:82:ILE:CG2	2.53	0.56
1:F:42:PRO:HA	1:F:68:LEU:HD23	1.86	0.56
1:E:82:ILE:O	1:E:82:ILE:CG2	2.52	0.56
1:B:157:THR:HB	1:B:172:LEU:HB2	1.88	0.56
1:C:216:ALA:O	1:C:217:VAL:C	2.40	0.56
1:D:188:ALA:O	1:D:189:GLY:C	2.42	0.56
1:A:82:ILE:CG2	1:A:82:ILE:O	2.53	0.56
1:E:49:LYS:HZ1	1:F:333:LEU:CD1	2.18	0.56
1:E:53:ARG:HB2	1:E:54:PRO:HD2	1.87	0.56
1:A:300:VAL:O	1:A:301:LYS:C	2.44	0.56
1:A:42:PRO:HA	1:A:68:LEU:HD23	1.88	0.56
1:D:73:PRO:HD2	1:D:74:LEU:H	1.71	0.56
1:E:73:PRO:HD2	1:E:74:LEU:H	1.70	0.55
1:C:73:PRO:HD2	1:C:74:LEU:H	1.71	0.55
1:A:239:GLY:HA2	1:C:277:GLN:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:VAL:HG12	1:B:148:GLY:N	2.20	0.55
1:C:157:THR:HB	1:C:172:LEU:HB2	1.89	0.55
1:E:157:THR:HB	1:E:172:LEU:HB2	1.88	0.55
1:F:188:ALA:O	1:F:189:GLY:C	2.45	0.55
1:C:323:CYS:O	1:C:324:ARG:C	2.45	0.55
1:A:188:ALA:O	1:A:189:GLY:C	2.44	0.55
1:D:157:THR:HB	1:D:172:LEU:HB2	1.89	0.55
1:E:102:GLU:O	1:E:102:GLU:HG3	2.07	0.55
1:D:277:GLN:OE1	1:F:239:GLY:HA2	2.07	0.55
1:D:102:GLU:HG3	1:D:102:GLU:O	2.08	0.54
1:F:102:GLU:O	1:F:102:GLU:HG3	2.08	0.54
1:F:300:VAL:O	1:F:301:LYS:C	2.45	0.54
1:F:157:THR:HB	1:F:172:LEU:HB2	1.89	0.54
1:D:146:MET:HG3	1:D:326:ALA:H	1.73	0.54
1:D:323:CYS:O	1:D:324:ARG:C	2.45	0.54
1:A:333:LEU:CD1	1:B:49:LYS:HZ1	2.20	0.54
1:B:188:ALA:O	1:B:189:GLY:C	2.46	0.54
1:B:73:PRO:HD2	1:B:74:LEU:H	1.72	0.54
1:A:157:THR:HB	1:A:172:LEU:HB2	1.90	0.54
1:E:20:THR:O	1:E:20:THR:OG1	2.18	0.53
1:C:146:MET:HG3	1:C:326:ALA:H	1.73	0.53
1:C:14:LEU:HD23	1:C:27:SER:HA	1.91	0.53
1:E:42:PRO:HA	1:E:68:LEU:HD23	1.89	0.53
1:A:102:GLU:O	1:A:102:GLU:HG3	2.08	0.53
1:B:102:GLU:HG3	1:B:102:GLU:O	2.07	0.53
1:B:42:PRO:HA	1:B:68:LEU:HD23	1.91	0.53
1:A:14:LEU:HD23	1:A:27:SER:HA	1.91	0.53
1:C:102:GLU:HG3	1:C:102:GLU:O	2.07	0.53
1:B:14:LEU:HD23	1:B:27:SER:HA	1.91	0.53
1:B:214:ALA:O	1:B:215:CYS:C	2.46	0.53
1:F:31:LYS:HE3	1:F:102:GLU:HG2	1.91	0.52
1:D:31:LYS:HE3	1:D:102:GLU:HG2	1.92	0.52
1:A:277:GLN:OE1	1:B:239:GLY:HA2	2.09	0.52
1:D:14:LEU:HD23	1:D:27:SER:HA	1.92	0.52
1:B:218:LYS:HE2	3:B:402:ADP:N3	2.25	0.52
1:C:305:ARG:N	1:C:306:PRO:CD	2.73	0.52
1:E:188:ALA:O	1:E:189:GLY:C	2.48	0.52
1:A:218:LYS:O	1:A:219:GLU:C	2.47	0.51
1:B:326:ALA:O	1:B:329:LEU:HB3	2.10	0.51
1:C:182:GLN:O	1:C:183:VAL:HG23	2.09	0.51
1:A:323:CYS:O	1:A:324:ARG:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:VAL:O	1:A:303:LYS:N	2.43	0.51
1:E:265:ILE:O	1:E:266:GLU:C	2.48	0.51
1:B:22:HIS:HB3	1:B:34:LEU:HD11	1.92	0.51
1:E:73:PRO:CD	1:E:74:LEU:H	2.23	0.51
1:E:14:LEU:HD23	1:E:27:SER:HA	1.91	0.51
1:E:31:LYS:HE3	1:E:102:GLU:HG2	1.92	0.51
1:F:160:VAL:HG13	1:F:169:ILE:HG12	1.92	0.51
1:E:214:ALA:O	1:E:215:CYS:C	2.46	0.51
1:A:31:LYS:HE3	1:A:102:GLU:HG2	1.91	0.51
1:D:182:GLN:O	1:D:183:VAL:HG23	2.10	0.51
1:E:22:HIS:HB3	1:E:34:LEU:HD11	1.92	0.51
1:E:89:VAL:O	1:E:90:ALA:C	2.45	0.51
1:F:323:CYS:O	1:F:324:ARG:C	2.49	0.51
1:C:31:LYS:HE3	1:C:102:GLU:HG2	1.92	0.51
1:E:216:ALA:O	1:E:217:VAL:C	2.46	0.51
1:F:218:LYS:O	1:F:219:GLU:C	2.47	0.51
1:E:239:GLY:HA2	1:F:277:GLN:OE1	2.11	0.51
1:B:89:VAL:O	1:B:90:ALA:C	2.47	0.51
1:B:31:LYS:HE3	1:B:102:GLU:HG2	1.91	0.50
1:B:216:ALA:O	1:B:217:VAL:C	2.47	0.50
1:D:305:ARG:N	1:D:306:PRO:CD	2.73	0.50
1:F:14:LEU:HD23	1:F:27:SER:HA	1.92	0.50
1:E:188:ALA:HA	1:E:257:LEU:HD21	1.93	0.50
1:D:42:PRO:HA	1:D:68:LEU:HD23	1.93	0.50
1:E:218:LYS:HE2	3:E:402:ADP:N3	2.27	0.50
1:A:216:ALA:O	1:A:217:VAL:C	2.46	0.50
1:E:326:ALA:O	1:E:329:LEU:HB3	2.10	0.50
1:B:15:GLY:O	1:B:25:VAL:HA	2.11	0.50
1:F:265:ILE:O	1:F:266:GLU:C	2.49	0.50
1:F:258:MET:SD	1:F:296:LEU:HD12	2.51	0.50
1:A:326:ALA:O	1:A:329:LEU:HB3	2.11	0.50
1:E:323:CYS:O	1:E:324:ARG:C	2.50	0.50
1:C:159:ILE:CG2	1:C:160:VAL:N	2.75	0.50
1:D:265:ILE:O	1:D:266:GLU:C	2.49	0.50
1:B:300:VAL:O	1:B:303:LYS:N	2.45	0.50
1:B:300:VAL:O	1:B:301:LYS:C	2.50	0.50
1:B:73:PRO:CD	1:B:74:LEU:H	2.25	0.50
1:C:265:ILE:O	1:C:266:GLU:C	2.48	0.50
1:C:22:HIS:HB3	1:C:34:LEU:HD11	1.93	0.50
1:F:326:ALA:O	1:F:329:LEU:HB3	2.11	0.50
1:B:188:ALA:HA	1:B:257:LEU:HD21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:HIS:HB3	1:D:34:LEU:HD11	1.94	0.49
1:F:188:ALA:HA	1:F:257:LEU:HD21	1.94	0.49
1:B:108:GLU:HG2	1:B:136:HIS:CE1	2.47	0.49
1:C:288:GLY:O	1:C:289:GLY:C	2.50	0.49
1:F:300:VAL:O	1:F:303:LYS:N	2.45	0.49
1:A:265:ILE:O	1:A:266:GLU:C	2.49	0.49
1:E:108:GLU:HG2	1:E:136:HIS:CE1	2.47	0.49
1:E:160:VAL:HG13	1:E:169:ILE:HG12	1.95	0.49
1:F:20:THR:HG21	1:F:165:GLY:HA3	1.94	0.49
1:F:147:VAL:HG12	1:F:148:GLY:N	2.27	0.49
1:B:218:LYS:O	1:B:219:GLU:C	2.50	0.49
1:C:326:ALA:O	1:C:329:LEU:HB3	2.12	0.49
1:D:326:ALA:O	1:D:329:LEU:HB3	2.13	0.49
1:C:300:VAL:O	1:C:301:LYS:C	2.50	0.49
1:E:20:THR:HG21	1:E:165:GLY:HA3	1.95	0.49
1:B:20:THR:HG21	1:B:165:GLY:HA3	1.95	0.49
1:A:20:THR:HG21	1:A:165:GLY:HA3	1.94	0.49
1:A:160:VAL:HG13	1:A:169:ILE:HG12	1.93	0.49
1:D:258:MET:SD	1:D:296:LEU:HD12	2.53	0.49
1:E:300:VAL:O	1:E:303:LYS:N	2.45	0.49
1:C:42:PRO:HA	1:C:68:LEU:HD23	1.95	0.49
1:E:300:VAL:O	1:E:301:LYS:C	2.51	0.48
1:A:208:GLN:CB	1:C:274:PRO:HG3	2.44	0.48
1:D:188:ALA:HA	1:D:257:LEU:HD21	1.95	0.48
1:F:182:GLN:O	1:F:183:VAL:HG23	2.13	0.48
1:D:333:LEU:CD1	1:F:49:LYS:HZ1	2.26	0.48
1:E:146:MET:HG3	1:E:326:ALA:H	1.79	0.48
1:A:182:GLN:O	1:A:183:VAL:HG23	2.12	0.48
1:A:258:MET:SD	1:A:296:LEU:HD12	2.51	0.48
1:D:147:VAL:HG12	1:D:148:GLY:N	2.28	0.48
1:F:223:PHE:C	1:F:223:PHE:CD1	2.87	0.48
1:F:89:VAL:O	1:F:90:ALA:C	2.50	0.48
1:B:323:CYS:O	1:B:324:ARG:C	2.50	0.48
1:E:15:GLY:O	1:E:25:VAL:HA	2.13	0.48
1:B:13:PHE:HA	1:B:110:CYS:O	2.14	0.48
1:D:300:VAL:O	1:D:301:LYS:C	2.51	0.48
1:C:147:VAL:HG12	1:C:148:GLY:N	2.28	0.48
1:D:288:GLY:O	1:D:289:GLY:C	2.50	0.48
1:A:108:GLU:HG2	1:A:136:HIS:CE1	2.49	0.48
1:A:188:ALA:HA	1:A:257:LEU:HD21	1.96	0.48
1:A:147:VAL:HG12	1:A:148:GLY:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ILE:O	1:B:266:GLU:C	2.49	0.48
1:C:173:LYS:HZ1	1:C:271:SER:CB	2.27	0.48
1:F:144:PRO:HB2	1:F:170:CYS:HB3	1.96	0.48
1:A:15:GLY:O	1:A:25:VAL:HA	2.14	0.47
1:E:13:PHE:HA	1:E:110:CYS:O	2.14	0.47
1:B:146:MET:HG3	1:B:326:ALA:H	1.80	0.47
1:E:218:LYS:O	1:E:219:GLU:C	2.50	0.47
1:B:73:PRO:HB3	1:B:89:VAL:HG12	1.96	0.47
1:D:108:GLU:HG2	1:D:136:HIS:CE1	2.49	0.47
1:D:274:PRO:HG3	1:F:208:GLN:CB	2.43	0.47
1:A:159:ILE:CG2	1:A:160:VAL:N	2.77	0.47
1:C:15:GLY:O	1:C:25:VAL:HA	2.15	0.47
1:C:332:GLU:C	1:C:333:LEU:CD1	2.78	0.47
1:C:73:PRO:HB3	1:C:89:VAL:HG12	1.97	0.47
1:A:22:HIS:HB3	1:A:34:LEU:HD11	1.95	0.47
1:C:258:MET:SD	1:C:296:LEU:HD12	2.53	0.47
1:B:262:ILE:HG22	1:B:263:GLU:N	2.29	0.47
1:A:47:GLY:HA2	1:C:175:THR:HG21	1.97	0.47
1:F:22:HIS:HB3	1:F:34:LEU:HD11	1.96	0.47
1:C:188:ALA:HA	1:C:257:LEU:HD21	1.97	0.47
1:D:159:ILE:CG2	1:D:160:VAL:N	2.75	0.47
1:E:189:GLY:O	1:E:190:ASN:C	2.51	0.47
1:E:73:PRO:CD	1:E:74:LEU:N	2.77	0.47
1:A:73:PRO:HB3	1:A:89:VAL:HG12	1.96	0.47
1:D:175:THR:HG21	1:F:47:GLY:HA2	1.96	0.47
1:D:216:ALA:O	1:D:217:VAL:C	2.42	0.47
1:E:73:PRO:HB3	1:E:89:VAL:HG12	1.96	0.47
1:A:13:PHE:HA	1:A:110:CYS:O	2.15	0.47
1:A:223:PHE:CD1	1:A:223:PHE:C	2.88	0.47
1:A:76:ASP:O	1:A:78:VAL:N	2.48	0.47
1:E:258:MET:SD	1:E:296:LEU:HD12	2.54	0.47
1:F:108:GLU:HG2	1:F:136:HIS:CE1	2.49	0.47
1:C:108:GLU:HG2	1:C:136:HIS:CE1	2.50	0.47
1:E:288:GLY:O	1:E:289:GLY:C	2.52	0.47
1:E:49:LYS:HZ1	1:F:333:LEU:HD11	1.79	0.47
1:B:160:VAL:HG13	1:B:169:ILE:HG12	1.97	0.46
1:D:332:GLU:C	1:D:333:LEU:CD1	2.78	0.46
1:F:15:GLY:O	1:F:25:VAL:HA	2.15	0.46
1:D:15:GLY:O	1:D:25:VAL:HA	2.15	0.46
1:A:193:ASP:OD1	1:A:218:LYS:CD	2.63	0.46
1:F:13:PHE:HA	1:F:110:CYS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:GLY:O	1:A:289:GLY:C	2.54	0.46
1:C:218:LYS:O	1:C:219:GLU:C	2.52	0.46
1:E:182:GLN:O	1:E:183:VAL:HG23	2.16	0.46
1:F:216:ALA:O	1:F:217:VAL:C	2.47	0.46
1:B:182:GLN:O	1:B:183:VAL:HG23	2.15	0.46
1:C:300:VAL:O	1:C:303:LYS:N	2.48	0.46
1:D:73:PRO:HB3	1:D:89:VAL:HG12	1.97	0.46
1:D:218:LYS:HE2	3:D:402:ADP:N3	2.30	0.46
1:F:193:ASP:OD1	1:F:218:LYS:CD	2.64	0.46
1:A:89:VAL:O	1:A:90:ALA:C	2.51	0.46
1:F:73:PRO:HB3	1:F:89:VAL:HG12	1.96	0.46
1:A:144:PRO:HB2	1:A:170:CYS:HB3	1.98	0.46
1:B:257:LEU:HD23	1:B:257:LEU:HA	1.76	0.46
1:F:214:ALA:O	1:F:215:CYS:C	2.52	0.46
1:A:236:ARG:HH21	1:C:278:ALA:N	2.14	0.45
1:A:305:ARG:N	1:A:306:PRO:CD	2.79	0.45
1:B:73:PRO:CD	1:B:74:LEU:N	2.79	0.45
1:F:281:LEU:HD23	1:F:281:LEU:HA	1.68	0.45
1:A:333:LEU:HD11	1:B:49:LYS:HZ1	1.80	0.45
1:F:289:GLY:HA3	3:F:402:ADP:O5'	2.14	0.45
1:A:36:LYS:HB3	1:A:38:VAL:CG1	2.46	0.45
1:B:288:GLY:O	1:B:289:GLY:C	2.51	0.45
1:B:305:ARG:N	1:B:306:PRO:CD	2.79	0.45
1:C:281:LEU:HD23	1:C:281:LEU:HA	1.60	0.45
1:D:218:LYS:O	1:D:219:GLU:C	2.51	0.45
1:D:73:PRO:CD	1:D:74:LEU:H	2.26	0.45
1:F:305:ARG:N	1:F:306:PRO:CD	2.79	0.45
1:D:73:PRO:CD	1:D:74:LEU:N	2.79	0.45
1:B:143:GLU:N	1:B:144:PRO:HD2	2.31	0.45
1:D:300:VAL:O	1:D:303:LYS:N	2.49	0.45
1:C:193:ASP:OD1	1:C:218:LYS:CD	2.65	0.45
1:E:144:PRO:HB2	1:E:170:CYS:HB3	1.98	0.45
1:F:76:ASP:O	1:F:78:VAL:N	2.48	0.45
1:A:220:GLN:HG2	1:A:221:PHE:CE2	2.52	0.45
1:B:207:LEU:HD22	1:B:235:PHE:HB3	1.98	0.45
1:E:110:CYS:HA	1:E:137:THR:O	2.17	0.45
1:E:143:GLU:N	1:E:144:PRO:HD2	2.32	0.45
1:E:172:LEU:O	1:E:174:GLY:N	2.49	0.45
1:E:46:ILE:HB	1:F:175:THR:HB	1.98	0.45
1:F:143:GLU:N	1:F:144:PRO:HD2	2.31	0.45
1:D:193:ASP:OD1	1:D:218:LYS:CD	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:TYR:HH	1:F:49:LYS:NZ	2.13	0.45
1:A:110:CYS:HA	1:A:137:THR:O	2.17	0.44
1:A:173:LYS:HZ1	1:A:271:SER:CB	2.29	0.44
1:A:289:GLY:HA3	3:A:402:ADP:O5'	2.16	0.44
1:A:49:LYS:NZ	1:C:149:TYR:HH	2.11	0.44
1:A:175:THR:HB	1:B:46:ILE:HB	1.99	0.44
1:A:49:LYS:HZ1	1:C:333:LEU:CD1	2.30	0.44
1:F:110:CYS:HA	1:F:137:THR:O	2.17	0.44
1:F:36:LYS:HB3	1:F:38:VAL:CG1	2.46	0.44
1:A:257:LEU:HA	1:A:257:LEU:HD23	1.83	0.44
1:A:274:PRO:HG3	1:B:208:GLN:CB	2.48	0.44
1:C:218:LYS:HE2	3:C:402:ADP:N3	2.31	0.44
1:E:207:LEU:HD22	1:E:235:PHE:HB3	1.98	0.44
1:A:211:VAL:HG23	1:A:212:ASN:N	2.32	0.44
1:B:172:LEU:O	1:B:174:GLY:N	2.50	0.44
1:F:173:LYS:HZ1	1:F:271:SER:CB	2.31	0.44
1:A:214:ALA:O	1:A:215:CYS:C	2.53	0.44
1:B:110:CYS:HA	1:B:137:THR:O	2.17	0.44
1:C:207:LEU:HD22	1:C:235:PHE:HB3	1.99	0.44
1:C:76:ASP:O	1:C:78:VAL:N	2.50	0.44
1:F:172:LEU:HD23	1:F:172:LEU:HA	1.93	0.44
1:B:14:LEU:HA	1:B:14:LEU:HD23	1.81	0.44
1:B:258:MET:SD	1:B:296:LEU:HD12	2.54	0.44
1:D:278:ALA:N	1:F:236:ARG:HH21	2.14	0.44
1:B:144:PRO:HB2	1:B:170:CYS:HB3	1.99	0.44
1:B:220:GLN:HG2	1:B:221:PHE:CE2	2.53	0.44
1:B:281:LEU:HD23	1:B:281:LEU:HA	1.59	0.44
1:C:172:LEU:HA	1:C:172:LEU:HD23	1.89	0.44
1:D:160:VAL:HG13	1:D:169:ILE:HG12	1.99	0.44
1:E:262:ILE:HG22	1:E:263:GLU:N	2.30	0.44
1:E:286:PHE:HB3	1:E:291:SER:HB2	2.00	0.44
1:F:220:GLN:HG2	1:F:221:PHE:CE2	2.52	0.44
1:A:220:GLN:O	1:A:294:ARG:NH2	2.51	0.44
1:B:173:LYS:HZ1	1:B:271:SER:CB	2.31	0.44
1:C:13:PHE:HA	1:C:110:CYS:O	2.18	0.44
1:C:269:LEU:HA	1:C:269:LEU:HD12	1.80	0.44
1:C:73:PRO:CD	1:C:74:LEU:N	2.80	0.44
1:D:13:PHE:HA	1:D:110:CYS:O	2.18	0.44
1:D:300:VAL:HG12	1:D:312:VAL:HG21	1.99	0.44
1:A:143:GLU:N	1:A:144:PRO:HD2	2.33	0.44
1:B:220:GLN:O	1:B:294:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:PRO:HB2	1:D:170:CYS:HB3	2.00	0.44
1:E:220:GLN:O	1:E:294:ARG:NH2	2.50	0.44
1:E:305:ARG:N	1:E:306:PRO:CD	2.80	0.44
1:F:189:GLY:O	1:F:190:ASN:C	2.55	0.44
1:C:262:ILE:HG22	1:C:263:GLU:N	2.33	0.44
1:C:73:PRO:HG2	1:C:74:LEU:HG	2.00	0.44
1:B:36:LYS:HB3	1:B:38:VAL:CG1	2.48	0.43
1:D:193:ASP:OD1	1:D:218:LYS:HD3	2.18	0.43
1:D:193:ASP:O	1:D:194:GLU:C	2.54	0.43
1:A:31:LYS:CE	1:A:102:GLU:HG2	2.48	0.43
1:B:193:ASP:O	1:B:194:GLU:C	2.55	0.43
1:C:160:VAL:HG13	1:C:169:ILE:HG12	1.99	0.43
1:C:220:GLN:O	1:C:294:ARG:NH2	2.50	0.43
1:C:325:GLY:C	1:C:327:LEU:N	2.72	0.43
1:D:207:LEU:HD22	1:D:235:PHE:HB3	1.99	0.43
1:D:257:LEU:HA	1:D:257:LEU:HD23	1.80	0.43
1:D:258:MET:SD	1:D:296:LEU:HD11	2.58	0.43
1:E:223:PHE:C	1:E:223:PHE:CD1	2.91	0.43
1:E:76:ASP:O	1:E:78:VAL:N	2.49	0.43
1:F:268:LEU:HD23	1:F:268:LEU:HA	1.75	0.43
1:F:288:GLY:O	1:F:289:GLY:C	2.55	0.43
1:B:223:PHE:C	1:B:223:PHE:CD1	2.91	0.43
1:C:300:VAL:HG12	1:C:312:VAL:HG21	1.99	0.43
1:D:141:VAL:CG2	1:D:146:MET:HE3	2.49	0.43
1:E:204:HIS:N	1:E:205:PRO:CD	2.81	0.43
1:E:281:LEU:HD23	1:E:281:LEU:HA	1.59	0.43
1:F:220:GLN:O	1:F:294:ARG:NH2	2.51	0.43
1:A:296:LEU:O	1:A:297:ALA:C	2.57	0.43
1:B:189:GLY:O	1:B:190:ASN:C	2.54	0.43
1:A:175:THR:HG21	1:B:47:GLY:HA2	2.01	0.43
1:C:89:VAL:O	1:C:90:ALA:C	2.56	0.43
1:D:268:LEU:HD23	1:D:268:LEU:HA	1.71	0.43
1:D:73:PRO:HG3	1:D:93:LEU:HD22	2.00	0.43
1:E:208:GLN:CB	1:F:274:PRO:HG3	2.48	0.43
1:E:220:GLN:HG2	1:E:221:PHE:CE2	2.53	0.43
1:F:325:GLY:C	1:F:327:LEU:N	2.72	0.43
1:B:193:ASP:OD1	1:B:218:LYS:CD	2.66	0.43
1:D:220:GLN:O	1:D:294:ARG:NH2	2.50	0.43
1:A:46:ILE:HB	1:C:175:THR:HB	2.01	0.43
1:C:193:ASP:OD1	1:C:218:LYS:HD3	2.18	0.43
1:D:89:VAL:O	1:D:90:ALA:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:MET:HG2	1:E:213:VAL:CG1	2.49	0.43
1:E:268:LEU:HA	1:E:268:LEU:HD23	1.70	0.43
1:E:36:LYS:HB3	1:E:38:VAL:CG1	2.48	0.43
1:F:51:LEU:HD12	1:F:51:LEU:HA	1.83	0.43
1:A:128:LEU:HD12	1:A:128:LEU:HA	1.84	0.43
1:A:193:ASP:OD1	1:A:218:LYS:HD3	2.18	0.43
1:A:286:PHE:HB3	1:A:291:SER:HB2	2.01	0.43
1:B:204:HIS:N	1:B:205:PRO:CD	2.81	0.43
1:B:87:ILE:HG23	1:B:130:MET:CE	2.49	0.43
1:C:110:CYS:HA	1:C:137:THR:O	2.19	0.43
1:C:73:PRO:CD	1:C:74:LEU:H	2.27	0.43
1:D:73:PRO:HG2	1:D:74:LEU:HG	2.00	0.43
1:E:73:PRO:HG2	1:E:74:LEU:HG	2.00	0.43
1:C:36:LYS:HB3	1:C:38:VAL:CG1	2.49	0.43
1:D:189:GLY:O	1:D:190:ASN:C	2.52	0.43
1:B:98:VAL:O	1:B:101:ALA:HB3	2.19	0.43
1:C:142:SER:OG	1:C:144:PRO:HG2	2.18	0.43
1:C:209:MET:HG2	1:C:213:VAL:CG1	2.49	0.43
1:D:110:CYS:HA	1:D:137:THR:O	2.19	0.43
1:D:223:PHE:C	1:D:223:PHE:CD1	2.92	0.43
1:F:209:MET:HG2	1:F:213:VAL:CG1	2.49	0.43
1:A:209:MET:HG2	1:A:213:VAL:CG1	2.49	0.43
1:B:31:LYS:CE	1:B:102:GLU:HG2	2.49	0.43
1:C:31:LYS:CE	1:C:102:GLU:HG2	2.49	0.43
1:C:189:GLY:O	1:C:190:ASN:C	2.53	0.43
1:C:193:ASP:O	1:C:194:GLU:C	2.54	0.43
1:D:289:GLY:HA3	3:D:402:ADP:O5'	2.19	0.43
1:D:76:ASP:O	1:D:78:VAL:N	2.50	0.43
1:E:31:LYS:CE	1:E:102:GLU:HG2	2.49	0.43
1:E:12:LEU:HD23	1:E:109:ILE:HG23	1.99	0.43
1:F:73:PRO:HG3	1:F:93:LEU:HD22	2.01	0.43
1:A:258:MET:SD	1:A:296:LEU:HD11	2.57	0.42
1:A:325:GLY:C	1:A:327:LEU:N	2.73	0.42
1:B:12:LEU:HD23	1:B:109:ILE:HG23	1.99	0.42
1:D:173:LYS:HZ1	1:D:271:SER:CB	2.32	0.42
1:E:193:ASP:OD1	1:E:218:LYS:CD	2.67	0.42
1:F:31:LYS:CE	1:F:102:GLU:HG2	2.48	0.42
1:A:73:PRO:HG2	1:A:74:LEU:HG	2.01	0.42
1:B:209:MET:HG2	1:B:213:VAL:CG1	2.48	0.42
1:B:76:ASP:O	1:B:78:VAL:N	2.49	0.42
1:D:12:LEU:HD23	1:D:109:ILE:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:LEU:HD23	1:A:281:LEU:HA	1.67	0.42
1:C:144:PRO:HB2	1:C:170:CYS:HB3	2.01	0.42
1:D:169:ILE:HG21	1:D:169:ILE:HD13	1.70	0.42
1:D:209:MET:HG2	1:D:213:VAL:CG1	2.50	0.42
1:E:258:MET:SD	1:E:296:LEU:HD11	2.57	0.42
1:E:325:GLY:C	1:E:327:LEU:N	2.72	0.42
1:F:211:VAL:HG23	1:F:212:ASN:N	2.34	0.42
1:F:73:PRO:CD	1:F:74:LEU:H	2.33	0.42
1:A:172:LEU:O	1:A:174:GLY:N	2.53	0.42
1:B:286:PHE:HB3	1:B:291:SER:HB2	2.00	0.42
1:C:143:GLU:O	1:C:144:PRO:C	2.57	0.42
1:C:258:MET:SD	1:C:296:LEU:HD11	2.59	0.42
1:C:98:VAL:O	1:C:101:ALA:HB3	2.20	0.42
1:E:98:VAL:O	1:E:101:ALA:HB3	2.19	0.42
1:C:257:LEU:HD23	1:C:257:LEU:HA	1.80	0.42
1:C:70:ILE:HG13	1:C:70:ILE:O	2.20	0.42
1:E:87:ILE:HG23	1:E:130:MET:CE	2.48	0.42
1:F:172:LEU:O	1:F:174:GLY:N	2.52	0.42
1:F:286:PHE:HB3	1:F:291:SER:HB2	2.00	0.42
1:C:67:TYR:CD1	1:C:67:TYR:C	2.93	0.42
1:C:73:PRO:HG3	1:C:93:LEU:HD22	2.00	0.42
1:D:262:ILE:HG22	1:D:263:GLU:N	2.33	0.42
1:F:12:LEU:HD23	1:F:109:ILE:HG23	2.01	0.42
1:F:193:ASP:OD1	1:F:218:LYS:HD3	2.19	0.42
1:A:193:ASP:O	1:A:194:GLU:C	2.58	0.42
1:B:102:GLU:N	1:B:103:PRO:HD3	2.35	0.42
1:E:47:GLY:HA2	1:F:175:THR:HG21	2.01	0.42
1:F:141:VAL:CG2	1:F:146:MET:HE3	2.50	0.42
1:F:262:ILE:HG22	1:F:263:GLU:N	2.35	0.42
1:A:207:LEU:HD22	1:A:235:PHE:HB3	2.02	0.42
1:E:89:VAL:O	1:E:92:HIS:N	2.53	0.42
1:F:284:ILE:HG22	1:F:312:VAL:HG13	2.01	0.42
1:B:325:GLY:C	1:B:327:LEU:N	2.73	0.42
1:D:117:ALA:O	1:D:184:THR:OG1	2.36	0.42
1:D:70:ILE:O	1:D:70:ILE:HG13	2.20	0.42
1:E:14:LEU:HD23	1:E:14:LEU:HA	1.80	0.42
1:F:98:VAL:O	1:F:101:ALA:HB3	2.20	0.42
1:A:73:PRO:HG3	1:A:93:LEU:HD22	2.02	0.42
1:B:73:PRO:HG2	1:B:74:LEU:HG	2.01	0.42
1:D:98:VAL:O	1:D:101:ALA:HB3	2.20	0.42
1:B:252:ILE:HG22	1:B:253:ALA:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:MET:SD	1:B:296:LEU:HD11	2.58	0.41
1:B:332:GLU:C	1:B:333:LEU:CD1	2.85	0.41
1:D:142:SER:OG	1:D:144:PRO:HG2	2.20	0.41
1:E:102:GLU:N	1:E:103:PRO:HD3	2.35	0.41
1:B:193:ASP:OD1	1:B:218:LYS:HD3	2.20	0.41
1:C:268:LEU:HD23	1:C:268:LEU:HA	1.71	0.41
1:E:173:LYS:HZ1	1:E:271:SER:CB	2.32	0.41
1:F:296:LEU:O	1:F:297:ALA:C	2.57	0.41
1:A:102:GLU:N	1:A:103:PRO:HD3	2.35	0.41
1:A:14:LEU:HA	1:A:14:LEU:HD23	1.85	0.41
1:A:98:VAL:O	1:A:101:ALA:HB3	2.20	0.41
1:B:89:VAL:O	1:B:92:HIS:N	2.53	0.41
1:D:31:LYS:CE	1:D:102:GLU:HG2	2.49	0.41
1:D:274:PRO:HG3	1:F:208:GLN:HB2	2.02	0.41
1:E:169:ILE:HG21	1:E:169:ILE:HD13	1.70	0.41
1:F:51:LEU:HD22	1:F:68:LEU:HD22	2.02	0.41
1:F:73:PRO:HG2	1:F:74:LEU:HG	2.01	0.41
1:B:169:ILE:HG21	1:B:169:ILE:HD13	1.69	0.41
1:A:278:ALA:N	1:B:236:ARG:HH21	2.19	0.41
1:C:211:VAL:HG23	1:C:212:ASN:N	2.35	0.41
1:C:173:LYS:HZ1	1:C:271:SER:HB2	1.85	0.41
1:C:289:GLY:HA3	3:C:402:ADP:O5'	2.20	0.41
1:D:175:THR:HB	1:F:46:ILE:HB	2.01	0.41
1:E:149:TYR:HA	1:E:154:LEU:HD11	2.02	0.41
1:A:12:LEU:HD23	1:A:109:ILE:HG23	2.01	0.41
1:A:252:ILE:HG22	1:A:253:ALA:N	2.34	0.41
1:F:159:ILE:CG2	1:F:160:VAL:N	2.77	0.41
1:A:262:ILE:HG22	1:A:263:GLU:N	2.35	0.41
1:B:87:ILE:HG23	1:B:130:MET:HE1	2.02	0.41
1:C:214:ALA:O	1:C:215:CYS:C	2.58	0.41
1:C:281:LEU:HD11	1:C:307:PHE:CB	2.50	0.41
1:A:142:SER:OG	1:A:144:PRO:HG2	2.20	0.41
1:A:284:ILE:HG22	1:A:312:VAL:HG13	2.02	0.41
1:B:172:LEU:HD23	1:B:172:LEU:HA	1.98	0.41
1:D:274:PRO:HG3	1:F:208:GLN:HB3	2.03	0.41
1:D:36:LYS:HB3	1:D:38:VAL:CG1	2.50	0.41
1:D:21:SER:N	3:D:402:ADP:O3B	2.50	0.41
1:F:300:VAL:HG12	1:F:312:VAL:HG21	2.01	0.41
1:A:208:GLN:HB2	1:C:274:PRO:HG3	2.02	0.41
1:B:39:VAL:HG22	1:B:57:VAL:HG13	2.03	0.41
1:D:157:THR:HA	1:D:283:ASN:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:ALA:O	1:F:184:THR:OG1	2.36	0.41
1:F:171:ALA:HB2	1:F:268:LEU:HD13	2.03	0.41
1:B:142:SER:OG	1:B:144:PRO:HG2	2.21	0.41
1:B:159:ILE:CG2	1:B:160:VAL:N	2.82	0.41
1:C:12:LEU:HD23	1:C:109:ILE:HG23	2.02	0.41
1:D:172:LEU:O	1:D:174:GLY:N	2.54	0.41
1:D:214:ALA:O	1:D:215:CYS:C	2.56	0.41
1:A:208:GLN:HB3	1:C:274:PRO:HG3	2.03	0.41
1:A:87:ILE:HG23	1:A:130:MET:CE	2.51	0.41
1:B:211:VAL:HG23	1:B:212:ASN:N	2.36	0.41
1:C:153:LYS:C	1:C:154:LEU:HG	2.41	0.41
1:C:271:SER:OG	1:C:272:PHE:N	2.54	0.41
1:D:300:VAL:CG1	1:D:312:VAL:HG21	2.51	0.41
1:E:300:VAL:HG12	1:E:312:VAL:HG21	2.02	0.41
1:A:171:ALA:HB2	1:A:268:LEU:HD13	2.02	0.41
1:A:268:LEU:HD23	1:A:268:LEU:HA	1.76	0.41
1:A:39:VAL:HG22	1:A:57:VAL:HG13	2.02	0.41
1:C:223:PHE:C	1:C:223:PHE:CD1	2.94	0.41
1:C:252:ILE:HG22	1:C:253:ALA:N	2.35	0.41
1:F:102:GLU:N	1:F:103:PRO:HD3	2.35	0.41
1:F:39:VAL:HG22	1:F:57:VAL:HG13	2.02	0.41
1:A:300:VAL:HG12	1:A:312:VAL:HG21	2.02	0.40
1:B:300:VAL:HG12	1:B:312:VAL:HG21	2.02	0.40
1:C:102:GLU:N	1:C:103:PRO:HD3	2.36	0.40
1:C:136:HIS:CE1	1:C:137:THR:HG1	2.38	0.40
1:D:102:GLU:N	1:D:103:PRO:HD3	2.36	0.40
1:D:211:VAL:HG23	1:D:212:ASN:N	2.36	0.40
1:E:300:VAL:CG1	1:E:312:VAL:HG21	2.51	0.40
1:E:37:SER:C	1:E:38:VAL:HG12	2.40	0.40
1:F:252:ILE:HG22	1:F:253:ALA:N	2.36	0.40
1:F:36:LYS:HB3	1:F:38:VAL:HG12	2.03	0.40
1:A:281:LEU:HD11	1:A:307:PHE:CB	2.51	0.40
1:C:92:HIS:O	1:C:93:LEU:C	2.58	0.40
1:D:325:GLY:C	1:D:327:LEU:N	2.72	0.40
1:E:128:LEU:HD12	1:E:128:LEU:HA	1.84	0.40
1:E:332:GLU:C	1:E:333:LEU:CD1	2.86	0.40
1:E:39:VAL:HG22	1:E:57:VAL:HG13	2.02	0.40
1:F:87:ILE:HG23	1:F:130:MET:CE	2.50	0.40
1:F:207:LEU:HD22	1:F:235:PHE:HB3	2.02	0.40
1:A:269:LEU:CD1	1:A:280:VAL:HG11	2.51	0.40
1:C:128:LEU:HD12	1:C:128:LEU:HA	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:VAL:CG1	1:C:312:VAL:HG21	2.50	0.40
1:C:51:LEU:HA	1:C:51:LEU:HD12	1.84	0.40
1:F:169:ILE:HD13	1:F:169:ILE:HG21	1.73	0.40
1:F:269:LEU:CD1	1:F:280:VAL:HG11	2.51	0.40
1:F:67:TYR:C	1:F:67:TYR:CD1	2.94	0.40
1:C:172:LEU:O	1:C:174:GLY:N	2.55	0.40
1:C:162:ILE:HD11	1:C:261:ILE:HD13	2.04	0.40
1:D:252:ILE:HG22	1:D:253:ALA:N	2.36	0.40
1:E:23:THR:HB	1:E:35:LEU:HD12	2.04	0.40
1:F:142:SER:OG	1:F:144:PRO:HG2	2.22	0.40
1:F:258:MET:SD	1:F:296:LEU:HD11	2.57	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 PDB entries followed by that with respect to all EM entries.

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	323/347 (93%)	290 (90%)	23 (7%)	10 (3%)	5	46
1	B	323/347 (93%)	289 (90%)	26 (8%)	8 (2%)	7	49
1	C	323/347 (93%)	291 (90%)	22 (7%)	10 (3%)	5	46
1	D	323/347 (93%)	291 (90%)	22 (7%)	10 (3%)	5	46
1	E	323/347 (93%)	289 (90%)	26 (8%)	8 (2%)	7	49
1	F	323/347 (93%)	289 (90%)	24 (7%)	10 (3%)	5	46
All	All	1938/2082 (93%)	1739 (90%)	143 (7%)	56 (3%)	9	47

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	PRO

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Mol	Chain	Res	Type
1	A	179	PRO
1	B	103	PRO
1	B	179	PRO
1	C	103	PRO
1	C	179	PRO
1	D	103	PRO
1	D	179	PRO
1	E	103	PRO
1	E	179	PRO
1	F	103	PRO
1	F	179	PRO
1	A	77	GLY
1	A	333	LEU
1	C	77	GLY
1	D	77	GLY
1	D	333	LEU
1	F	77	GLY
1	F	333	LEU
1	A	326	ALA
1	B	333	LEU
1	C	326	ALA
1	C	333	LEU
1	D	326	ALA
1	E	333	LEU
1	F	326	ALA
1	A	187	LYS
1	B	326	ALA
1	E	326	ALA
1	F	187	LYS
1	B	77	GLY
1	C	187	LYS
1	E	77	GLY
1	A	189	GLY
1	A	322	GLY
1	C	78	VAL
1	D	78	VAL
1	D	187	LYS
1	A	78	VAL
1	C	189	GLY
1	D	189	GLY
1	F	78	VAL
1	F	189	GLY

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Mol	Chain	Res	Type
1	F	322	GLY
1	A	315	VAL
1	B	189	GLY
1	C	322	GLY
1	D	322	GLY
1	E	189	GLY
1	F	315	VAL
1	B	322	GLY
1	E	78	VAL
1	E	322	GLY
1	B	78	VAL
1	D	315	VAL
1	C	315	VAL

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 PDB entries followed by that with respect to all EM entries.

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	268/285 (94%)	248 (92%)	20 (8%)	17	58
1	B	268/285 (94%)	246 (92%)	22 (8%)	14	54
1	C	268/285 (94%)	244 (91%)	24 (9%)	12	50
1	D	268/285 (94%)	245 (91%)	23 (9%)	13	53
1	E	268/285 (94%)	247 (92%)	21 (8%)	16	56
1	F	268/285 (94%)	247 (92%)	21 (8%)	16	56
All	All	1608/1710 (94%)	1477 (92%)	131 (8%)	19	54

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	13	PHE
1	A	20	THR
1	A	38	VAL
1	A	59	ASP

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Mol	Chain	Res	Type
1	A	63	GLU
1	A	74	LEU
1	A	100	SER
1	A	108	GLU
1	A	109	ILE
1	A	110	CYS
1	A	118	ARG
1	A	126	LEU
1	A	127	LEU
1	A	130	MET
1	A	142	SER
1	A	146	MET
1	A	195	ARG
1	A	252	ILE
1	A	259	PRO
1	B	12	LEU
1	B	13	PHE
1	B	20	THR
1	B	38	VAL
1	B	59	ASP
1	B	63	GLU
1	B	64	MET
1	B	74	LEU
1	B	100	SER
1	B	108	GLU
1	B	109	ILE
1	B	110	CYS
1	B	118	ARG
1	B	126	LEU
1	B	127	LEU
1	B	130	MET
1	B	142	SER
1	B	146	MET
1	B	195	ARG
1	B	252	ILE
1	B	259	PRO
1	B	283	ASN
1	C	12	LEU
1	C	13	PHE
1	C	20	THR
1	C	38	VAL
1	C	59	ASP

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Mol	Chain	Res	Type
1	C	63	GLU
1	C	64	MET
1	C	74	LEU
1	C	84	ASP
1	C	100	SER
1	C	108	GLU
1	C	109	ILE
1	C	110	CYS
1	C	118	ARG
1	C	126	LEU
1	C	127	LEU
1	C	130	MET
1	C	142	SER
1	C	145	PHE
1	C	146	MET
1	C	195	ARG
1	C	252	ILE
1	C	259	PRO
1	C	306	PRO
1	D	12	LEU
1	D	13	PHE
1	D	20	THR
1	D	38	VAL
1	D	59	ASP
1	D	63	GLU
1	D	64	MET
1	D	74	LEU
1	D	84	ASP
1	D	100	SER
1	D	108	GLU
1	D	109	ILE
1	D	110	CYS
1	D	118	ARG
1	D	126	LEU
1	D	127	LEU
1	D	130	MET
1	D	142	SER
1	D	146	MET
1	D	166	THR
1	D	195	ARG
1	D	252	ILE
1	D	259	PRO

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Mol	Chain	Res	Type
1	E	12	LEU
1	E	13	PHE
1	E	20	THR
1	E	38	VAL
1	E	59	ASP
1	E	63	GLU
1	E	74	LEU
1	E	100	SER
1	E	108	GLU
1	E	109	ILE
1	E	110	CYS
1	E	118	ARG
1	E	126	LEU
1	E	127	LEU
1	E	130	MET
1	E	142	SER
1	E	146	MET
1	E	195	ARG
1	E	252	ILE
1	E	259	PRO
1	E	283	ASN
1	F	12	LEU
1	F	13	PHE
1	F	20	THR
1	F	38	VAL
1	F	59	ASP
1	F	63	GLU
1	F	74	LEU
1	F	100	SER
1	F	108	GLU
1	F	109	ILE
1	F	110	CYS
1	F	118	ARG
1	F	126	LEU
1	F	127	LEU
1	F	130	MET
1	F	142	SER
1	F	146	MET
1	F	195	ARG
1	F	252	ILE
1	F	259	PRO
1	F	283	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	123	ASN
1	B	92	HIS
1	B	123	ASN
1	C	92	HIS
1	C	123	ASN
1	D	92	HIS
1	D	123	ASN
1	E	92	HIS
1	E	123	ASN
1	F	92	HIS
1	F	123	ASN

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](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	A	402	2	24,29,29	1.26	2 (8%)	23,45,45	3.24	6 (26%)
3	ADP	B	402	2	24,29,29	1.36	5 (20%)	23,45,45	3.73	10 (43%)
3	ADP	C	402	2	24,29,29	1.43	3 (12%)	23,45,45	3.17	8 (34%)
3	ADP	D	402	2	24,29,29	1.43	5 (20%)	23,45,45	3.07	9 (39%)
3	ADP	E	402	2	24,29,29	1.42	5 (20%)	23,45,45	3.87	10 (43%)
3	ADP	F	402	2	24,29,29	1.32	3 (12%)	23,45,45	3.29	7 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	402	2	-	0/12/32/32	0/3/3/3
3	ADP	B	402	2	-	0/12/32/32	0/3/3/3
3	ADP	C	402	2	-	0/12/32/32	0/3/3/3
3	ADP	D	402	2	-	0/12/32/32	0/3/3/3
3	ADP	E	402	2	-	0/12/32/32	0/3/3/3
3	ADP	F	402	2	-	0/12/32/32	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	402	ADP	O4'-C4'	-2.54	1.39	1.45
3	C	402	ADP	C2'-C3'	-2.40	1.47	1.53
3	D	402	ADP	C2'-C3'	-2.34	1.47	1.53
3	B	402	ADP	O4'-C4'	-2.33	1.39	1.45
3	D	402	ADP	O4'-C4'	-2.23	1.39	1.45
3	D	402	ADP	C4-N3	-2.11	1.32	1.35
3	E	402	ADP	PA-O2A	-2.05	1.46	1.55
3	B	402	ADP	C2-N1	2.02	1.37	1.33
3	F	402	ADP	C3'-C4'	2.11	1.58	1.53
3	B	402	ADP	PB-O1B	2.17	1.57	1.50
3	B	402	ADP	O2'-C2'	2.28	1.48	1.43
3	A	402	ADP	PB-O1B	2.31	1.58	1.50
3	E	402	ADP	O2'-C2'	2.42	1.48	1.43
3	E	402	ADP	PB-O1B	2.47	1.58	1.50
3	F	402	ADP	PB-O1B	2.51	1.58	1.50
3	C	402	ADP	PB-O1B	2.61	1.59	1.50
3	E	402	ADP	C5-C4	2.66	1.46	1.40
3	B	402	ADP	C5-C4	2.73	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	ADP	PB-O1B	2.79	1.59	1.50
3	A	402	ADP	C5-C4	2.95	1.47	1.40
3	D	402	ADP	C5-C4	3.05	1.47	1.40
3	F	402	ADP	C5-C4	3.09	1.47	1.40
3	C	402	ADP	C5-C4	3.19	1.47	1.40

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	402	ADP	C1'-N9-C4	-11.65	113.81	126.81
3	A	402	ADP	C1'-N9-C4	-11.64	113.81	126.81
3	E	402	ADP	N3-C2-N1	-10.70	120.46	128.87
3	B	402	ADP	N3-C2-N1	-9.83	121.15	128.87
3	B	402	ADP	C1'-N9-C4	-9.58	116.11	126.81
3	E	402	ADP	C1'-N9-C4	-9.51	116.19	126.81
3	C	402	ADP	C1'-N9-C4	-9.02	116.74	126.81
3	D	402	ADP	C1'-N9-C4	-8.76	117.03	126.81
3	C	402	ADP	N3-C2-N1	-7.55	122.94	128.87
3	D	402	ADP	N3-C2-N1	-7.00	123.37	128.87
3	F	402	ADP	N3-C2-N1	-4.53	125.31	128.87
3	A	402	ADP	C4'-O4'-C1'	-4.51	104.87	109.64
3	F	402	ADP	C4'-O4'-C1'	-4.48	104.90	109.64
3	D	402	ADP	C2'-C1'-N9	-4.34	101.86	113.47
3	C	402	ADP	C2'-C1'-N9	-4.25	102.09	113.47
3	E	402	ADP	C2'-C1'-N9	-4.19	102.24	113.47
3	A	402	ADP	N3-C2-N1	-4.14	125.62	128.87
3	B	402	ADP	C2'-C1'-N9	-4.01	102.74	113.47
3	F	402	ADP	C2'-C1'-N9	-3.93	102.95	113.47
3	E	402	ADP	C4'-O4'-C1'	-3.88	105.53	109.64
3	A	402	ADP	C2'-C1'-N9	-3.65	103.70	113.47
3	B	402	ADP	C4'-O4'-C1'	-3.58	105.85	109.64
3	C	402	ADP	C4'-O4'-C1'	-2.96	106.51	109.64
3	D	402	ADP	C4'-O4'-C1'	-2.60	106.89	109.64
3	C	402	ADP	O3'-C3'-C2'	-2.43	104.01	111.86
3	D	402	ADP	O3'-C3'-C2'	-2.40	104.08	111.86
3	B	402	ADP	O3'-C3'-C2'	-2.35	104.27	111.86
3	D	402	ADP	O5'-PA-O1A	2.08	117.73	109.21
3	E	402	ADP	O2'-C2'-C3'	2.21	119.01	111.86
3	D	402	ADP	C2'-C3'-C4'	2.26	107.26	102.64
3	C	402	ADP	O5'-PA-O1A	2.27	118.51	109.21
3	B	402	ADP	O5'-PA-O1A	2.30	118.64	109.21
3	F	402	ADP	O2'-C2'-C3'	2.31	119.33	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	402	ADP	O5'-PA-O1A	2.34	118.81	109.21
3	E	402	ADP	O3B-PB-O2B	2.35	116.07	107.44
3	B	402	ADP	O3B-PB-O2B	2.38	116.19	107.44
3	D	402	ADP	C2-N1-C6	2.42	123.08	118.77
3	F	402	ADP	O2B-PB-O1B	2.48	118.73	110.63
3	A	402	ADP	O2B-PB-O1B	2.62	119.17	110.63
3	C	402	ADP	C2-N1-C6	2.62	123.45	118.77
3	B	402	ADP	C2'-C3'-C4'	2.66	108.08	102.64
3	E	402	ADP	C2'-C3'-C4'	2.81	108.39	102.64
3	B	402	ADP	C2-N1-C6	3.83	125.60	118.77
3	E	402	ADP	C2-N1-C6	3.94	125.80	118.77
3	A	402	ADP	N6-C6-N1	5.34	127.47	118.52
3	C	402	ADP	N6-C6-N1	5.42	127.61	118.52
3	F	402	ADP	N6-C6-N1	5.47	127.70	118.52
3	D	402	ADP	N6-C6-N1	5.56	127.84	118.52
3	B	402	ADP	N6-C6-N1	7.10	130.43	118.52
3	E	402	ADP	N6-C6-N1	7.30	130.75	118.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	ADP	2	0
3	B	402	ADP	1	0
3	C	402	ADP	2	0
3	D	402	ADP	3	0
3	E	402	ADP	1	0
3	F	402	ADP	2	0

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.