



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:53 PM BST

PDB ID : 3JAX  
EMDB ID: : EMD-6370  
Title : Heavy meromyosin from Schistosoma mansoni muscle thick filament by negative stain EM  
Authors : Sulbaran, G.; Alamo, L.; Pinto, A.; Marquez, G.; Mendez, F.; Padron, R.; Craig, R.  
Deposited on : 2015-07-03  
Resolution : 23.00 Å(reported)  
Based on PDB ID : 3DTP

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : unknown  
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) : trunk27241

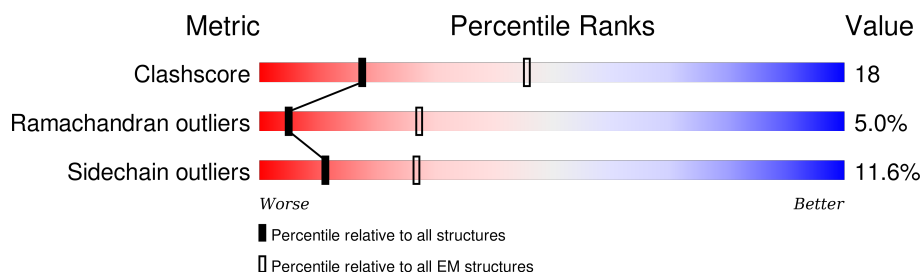
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 23.00 Å.

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



Metric	Whole archive (#Entries)	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  $\geq 3$ , 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	974	
1	B	974	
2	C	151	
2	D	151	
3	E	196	
3	F	196	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25293 atoms, of which 4713 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 myosin 2 heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	938	Total	C	H	N	O	S	0	0
			9360	4819	1759	1312	1432	38		
1	B	940	Total	C	H	N	O	S	0	0
			9379	4828	1764	1315	1434	38		

- Molecule 2 is a protein called smooth muscle myosin essential light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	148	Total	C	H	N	O	S	0	0
			1411	722	251	193	234	11		
2	D	148	Total	C	H	N	O	S	0	0
			1411	722	251	193	234	11		

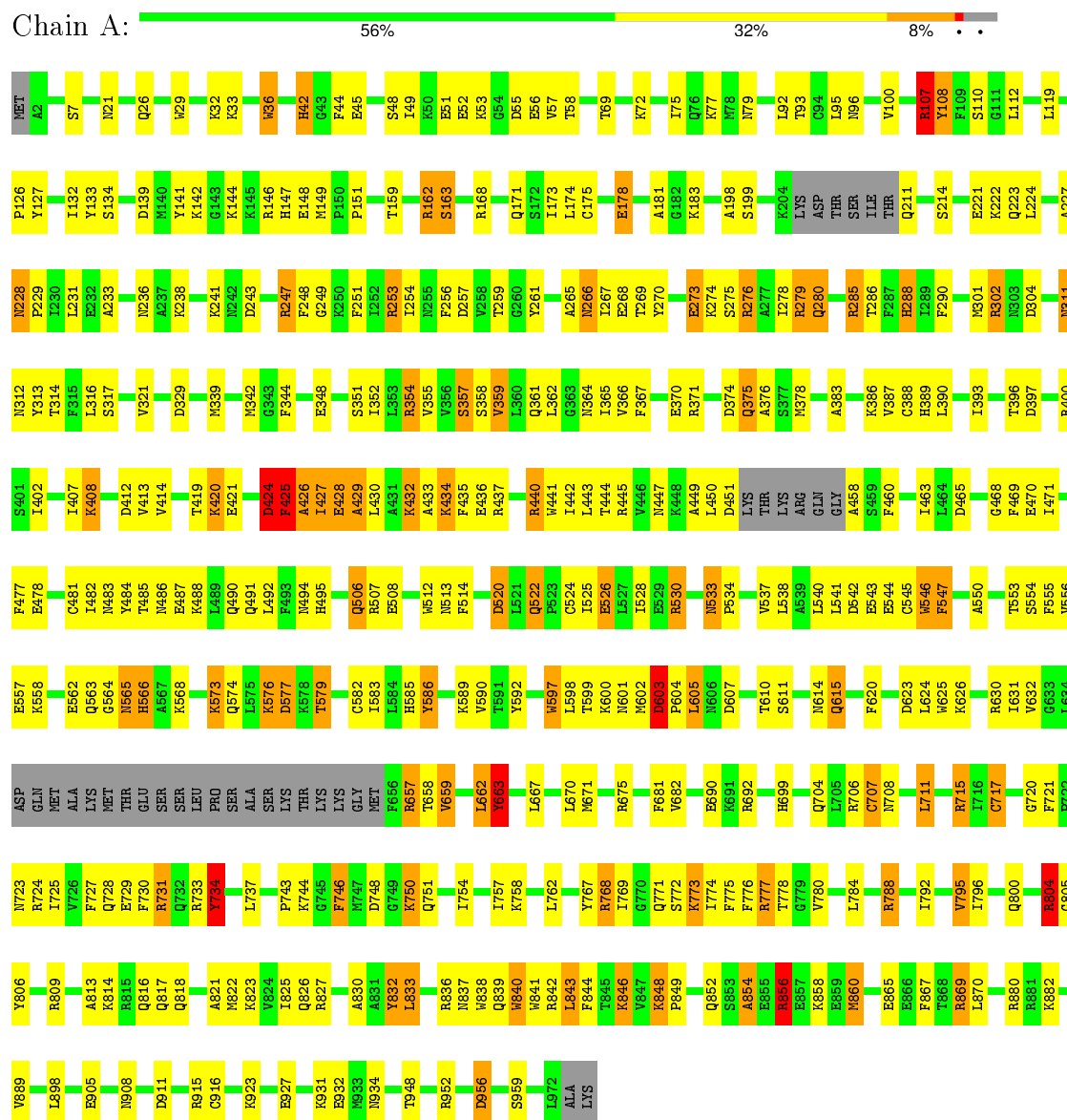
- Molecule 3 is a protein called myosin regulatory light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	196	Total	C	H	N	O	S	0	0
			1866	948	344	259	309	6		
3	F	196	Total	C	H	N	O	S	0	0
			1866	948	344	259	309	6		

### 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.

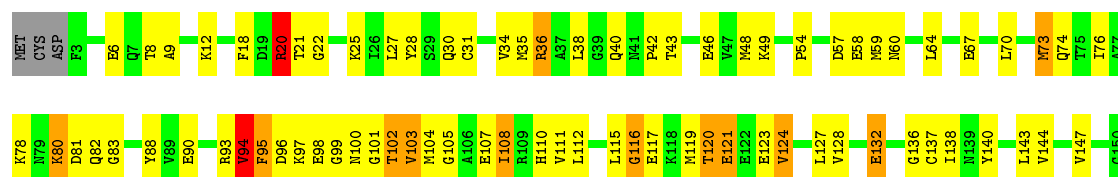
- Molecule 1: myosin 2 heavy chain



- Molecule 1: myosin 2 heavy chain

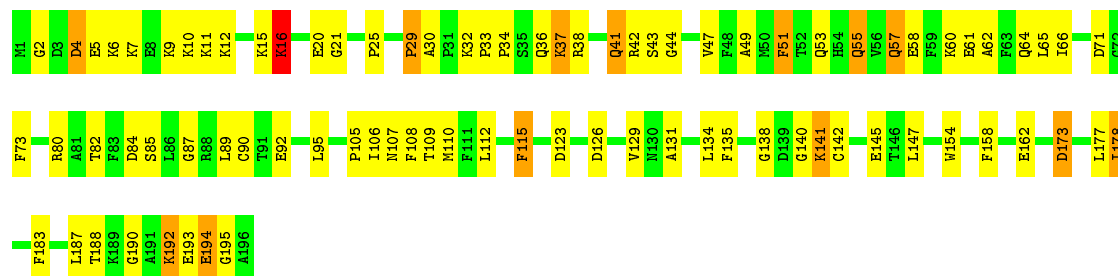






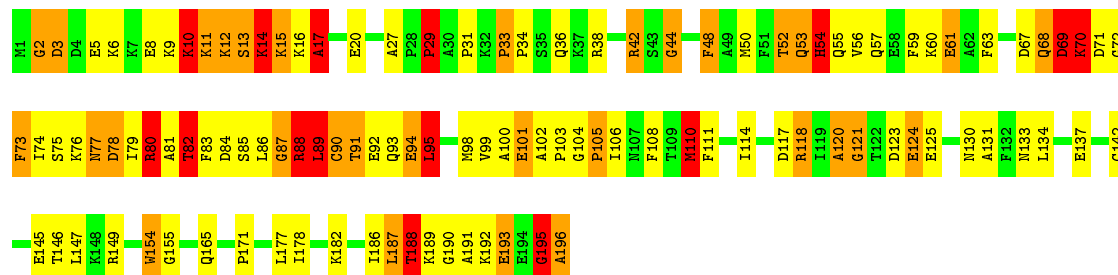
• Molecule 3: myosin regulatory light chain

Chain E: 57% 36% 7%



• Molecule 3: myosin regulatory light chain

Chain F: 43% 34% 16% 8%



## 4 Experimental information

Property	Value	Source
Reconstruction method	HELICAL	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	9500	Depositor
Resolution determination method	FSC 0.5	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI/PHILIPS CM120T	Depositor
Voltage (kV)	80	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	10	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	42000	Depositor
Image detector	TVIPS TEMCAM-F224 (2k x 2k)	Depositor

## 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	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.66	0/7730	1.43	80/10402 (0.8%)
1	B	0.66	0/7744	1.42	77/10420 (0.7%)
2	C	0.63	0/1175	1.19	2/1575 (0.1%)
2	D	0.65	0/1175	1.33	5/1575 (0.3%)
3	E	0.65	0/1546	1.34	10/2071 (0.5%)
3	F	0.68	0/1546	1.57	21/2071 (1.0%)
All	All	0.66	0/20916	1.41	195/28114 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	22
1	B	0	31
2	D	0	7
3	E	0	3
3	F	0	16
All	All	0	79

There are no bond length outliers.

All (195) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	ARG	NE-CZ-NH2	-16.82	111.89	120.30
1	A	107	ARG	NE-CZ-NH1	11.83	126.22	120.30
2	C	36	ARG	NE-CZ-NH2	-10.39	115.10	120.30
1	A	285	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	B	484	TYR	CB-CG-CD2	-9.59	115.25	121.00
1	A	441	TRP	CD1-CG-CD2	9.03	113.52	106.30
1	B	441	TRP	CD1-CG-CD2	8.68	113.24	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	TYR	CB-CG-CD2	-8.67	115.80	121.00
1	B	840	TRP	CD1-CG-CD2	8.63	113.21	106.30
1	A	428	GLU	CA-CB-CG	8.62	132.36	113.40
1	B	546	TRP	CD1-CG-CD2	8.53	113.12	106.30
3	E	154	TRP	CD1-CG-CD2	8.51	113.11	106.30
1	A	597	TRP	CD1-CG-CD2	8.48	113.09	106.30
1	A	827	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	B	838	TRP	CD1-CG-CD2	8.46	113.06	106.30
1	A	546	TRP	CD1-CG-CD2	8.41	113.03	106.30
1	A	445	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	A	302	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	A	840	TRP	CD1-CG-CD2	8.27	112.92	106.30
1	B	512	TRP	CD1-CG-CD2	8.27	112.91	106.30
1	B	441	TRP	CE2-CD2-CG	-8.18	100.75	107.30
1	A	36	TRP	CD1-CG-CD2	8.15	112.82	106.30
1	B	36	TRP	CE2-CD2-CG	-8.12	100.80	107.30
3	F	14	LYS	N-CA-C	8.11	132.91	111.00
1	A	625	TRP	CD1-CG-CD2	8.07	112.76	106.30
1	B	840	TRP	CE2-CD2-CG	-8.03	100.88	107.30
1	A	841	TRP	CD1-CG-CD2	7.97	112.68	106.30
1	A	441	TRP	CE2-CD2-CG	-7.94	100.95	107.30
1	A	597	TRP	CE2-CD2-CG	-7.88	101.00	107.30
1	B	597	TRP	CD1-CG-CD2	7.87	112.60	106.30
1	A	36	TRP	CE2-CD2-CG	-7.84	101.03	107.30
1	B	546	TRP	CE2-CD2-CG	-7.81	101.05	107.30
1	A	804	ARG	NE-CZ-NH2	7.80	124.20	120.30
1	B	29	TRP	CD1-CG-CD2	7.80	112.54	106.30
1	B	841	TRP	CD1-CG-CD2	7.79	112.54	106.30
1	B	512	TRP	CE2-CD2-CG	-7.72	101.13	107.30
1	B	625	TRP	CD1-CG-CD2	7.71	112.46	106.30
1	A	838	TRP	CD1-CG-CD2	7.69	112.45	106.30
1	A	840	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	B	838	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	B	841	TRP	CE2-CD2-CG	-7.67	101.17	107.30
1	B	715	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	A	788	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	A	546	TRP	CE2-CD2-CG	-7.63	101.19	107.30
1	A	734	TYR	CB-CG-CD2	-7.59	116.45	121.00
1	A	29	TRP	CD1-CG-CD2	7.58	112.36	106.30
3	E	42	ARG	NE-CZ-NH2	-7.57	116.51	120.30
1	A	856	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	B	29	TRP	CE2-CD2-CG	-7.54	101.26	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	154	TRP	CE2-CD2-CG	-7.51	101.29	107.30
1	A	512	TRP	CE2-CD2-CG	-7.48	101.31	107.30
1	B	597	TRP	CE2-CD2-CG	-7.48	101.32	107.30
3	F	154	TRP	CD1-CG-CD2	7.46	112.27	106.30
1	A	838	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	A	777	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	A	512	TRP	CD1-CG-CD2	7.35	112.18	106.30
1	B	781	LEU	CA-C-N	-7.35	101.03	117.20
1	B	253	ARG	NE-CZ-NH2	-7.35	116.63	120.30
1	B	36	TRP	CD1-CG-CD2	7.29	112.14	106.30
2	D	36	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	29	TRP	CE2-CD2-CG	-7.23	101.52	107.30
1	A	841	TRP	CE2-CD2-CG	-7.21	101.53	107.30
1	A	625	TRP	CE2-CD2-CG	-7.20	101.54	107.30
1	B	394	ASN	CA-C-N	-7.20	101.36	117.20
2	D	94	VAL	CA-CB-CG1	7.12	121.58	110.90
1	A	253	ARG	NE-CZ-NH2	-7.08	116.76	120.30
3	E	16	LYS	CA-CB-CG	7.06	128.94	113.40
1	B	625	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	A	731	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	425	PHE	N-CA-CB	6.97	123.15	110.60
1	B	285	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	428	GLU	N-CA-CB	6.89	123.00	110.60
1	B	782	ALA	N-CA-CB	-6.88	100.47	110.10
1	A	663	TYR	CB-CG-CD2	-6.88	116.87	121.00
3	F	91	THR	CA-C-N	6.86	132.28	117.20
1	A	228	ASN	N-CA-C	6.81	129.38	111.00
1	B	437	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	B	302	ARG	NE-CZ-NH2	-6.65	116.98	120.30
3	F	195	GLY	O-C-N	-6.61	112.12	122.70
3	E	192	LYS	O-C-N	-6.56	112.21	122.70
1	A	276	ARG	NE-CZ-NH1	6.54	123.57	120.30
2	D	93	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	788	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	B	441	TRP	CB-CG-CD1	-6.46	118.61	127.00
3	F	154	TRP	CE2-CD2-CG	-6.44	102.15	107.30
3	E	16	LYS	N-CA-CB	6.41	122.13	110.60
1	B	469	PHE	CA-C-N	-6.35	103.24	117.20
1	A	869	ARG	NE-CZ-NH2	-6.34	117.13	120.30
3	F	196	ALA	N-CA-C	6.33	128.10	111.00
1	A	425	PHE	CA-C-N	6.33	131.12	117.20
1	A	276	ARG	NE-CZ-NH2	-6.32	117.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	733	ARG	NE-CZ-NH2	6.27	123.43	120.30
1	B	809	ARG	NE-CZ-NH1	6.23	123.42	120.30
3	F	195	GLY	CA-C-N	6.23	130.91	117.20
1	B	468	GLY	CA-C-N	-6.22	103.51	117.20
1	B	856	ARG	N-CA-C	6.18	127.69	111.00
1	B	869	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	B	484	TYR	CB-CG-CD1	6.13	124.68	121.00
1	A	253	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	428	GLU	OE1-CD-OE2	-6.07	116.02	123.30
1	A	36	TRP	CG-CD2-CE3	6.06	139.35	133.90
2	D	20	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	484	TYR	CA-CB-CG	6.03	124.85	113.40
1	B	512	TRP	CB-CG-CD1	-6.02	119.17	127.00
1	A	659	VAL	CA-CB-CG2	5.99	119.89	110.90
1	B	836	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	36	TRP	CB-CG-CD1	-5.94	119.28	127.00
3	E	80	ARG	NE-CZ-NH2	5.93	123.26	120.30
1	A	285	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	659	VAL	CB-CA-C	-5.92	100.16	111.40
1	A	279	ARG	CA-CB-CG	5.91	126.39	113.40
3	F	54	HIS	CA-CB-CG	5.89	123.62	113.60
1	B	706	ARG	NE-CZ-NH2	-5.88	117.36	120.30
3	F	54	HIS	N-CA-CB	5.87	121.16	110.60
1	B	441	TRP	CG-CD2-CE3	5.85	139.16	133.90
1	B	253	ARG	NE-CZ-NH1	5.79	123.20	120.30
2	C	88	TYR	CB-CG-CD2	-5.79	117.53	121.00
1	B	881	ARG	NE-CZ-NH2	-5.76	117.42	120.30
3	E	57	GLN	CA-C-N	-5.73	104.59	117.20
3	F	94	GLU	CA-CB-CG	5.72	126.00	113.40
1	A	36	TRP	CB-CG-CD1	-5.72	119.57	127.00
1	B	168	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	465	ASP	CA-C-N	-5.70	104.65	117.20
3	F	187	LEU	N-CA-C	5.70	126.38	111.00
1	A	795	VAL	CA-CB-CG1	5.69	119.43	110.90
1	A	795	VAL	O-C-N	-5.69	113.60	122.70
3	F	14	LYS	CA-C-N	5.67	129.68	117.20
1	B	718	ARG	NE-CZ-NH1	5.66	123.13	120.30
3	F	188	THR	N-CA-C	5.66	126.28	111.00
1	B	36	TRP	CG-CD2-CE3	5.63	138.97	133.90
3	F	82	THR	CA-CB-CG2	5.61	120.26	112.40
1	A	273	GLU	N-CA-CB	5.61	120.70	110.60
1	B	856	ARG	NE-CZ-NH2	-5.59	117.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	718	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	B	546	TRP	CB-CG-CD1	-5.53	119.81	127.00
1	A	465	ASP	CB-CG-OD1	5.53	123.27	118.30
1	A	440	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	A	441	TRP	CG-CD1-NE1	-5.50	104.60	110.10
1	A	795	VAL	N-CA-C	5.47	125.78	111.00
1	B	840	TRP	CG-CD2-CE3	5.47	138.82	133.90
1	B	624	LEU	CA-CB-CG	5.47	127.87	115.30
1	A	827	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	659	VAL	N-CA-CB	5.46	123.51	111.50
2	D	124	VAL	CA-CB-CG2	5.46	119.09	110.90
3	F	73	PHE	CB-CG-CD1	-5.45	116.99	120.80
3	F	80	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	B	840	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	A	227	ALA	N-CA-C	5.39	125.56	111.00
1	B	795	VAL	CA-C-N	5.39	129.06	117.20
1	B	718	ARG	CA-CB-CG	5.38	125.25	113.40
1	B	841	TRP	CG-CD2-CE3	5.38	138.74	133.90
1	B	14	PHE	CB-CA-C	-5.38	99.64	110.40
1	A	168	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	838	TRP	CG-CD1-NE1	-5.37	104.73	110.10
1	A	512	TRP	CB-CG-CD1	-5.37	120.02	127.00
1	B	838	TRP	CG-CD2-CE3	5.36	138.73	133.90
1	A	838	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	A	424	ASP	O-C-N	-5.34	114.15	122.70
1	A	750	LYS	CA-CB-CG	5.34	125.14	113.40
1	A	248	PHE	CA-C-N	5.29	126.79	116.20
3	E	154	TRP	CG-CD1-NE1	-5.28	104.83	110.10
3	F	80	ARG	NE-CZ-NH2	5.27	122.93	120.30
1	A	441	TRP	CB-CG-CD1	-5.26	120.16	127.00
1	B	827	ARG	CA-CB-CG	5.22	124.90	113.40
1	B	839	GLN	N-CA-C	5.22	125.10	111.00
1	B	869	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	463	ILE	CA-C-N	5.22	128.68	117.20
1	A	530	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	520	ASP	N-CA-C	-5.21	96.94	111.00
1	B	711	LEU	CA-CB-CG	5.21	127.27	115.30
1	A	777	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	840	TRP	CG-CD1-NE1	-5.19	104.91	110.10
1	B	276	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	406	ARG	CA-CB-CG	5.16	124.74	113.40
1	B	936	ARG	NE-CZ-NH2	-5.15	117.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	PRO	N-CA-CB	-5.15	96.93	102.60
1	A	229	PRO	N-CA-C	5.14	125.46	112.10
3	F	87	GLY	CA-C-N	5.13	128.50	117.20
3	F	89	LEU	CB-CG-CD1	-5.13	102.28	111.00
1	B	441	TRP	CG-CD1-NE1	-5.12	104.98	110.10
1	B	546	TRP	CG-CD2-CE3	5.12	138.50	133.90
1	A	675	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	806	TYR	CB-CG-CD1	-5.10	117.94	121.00
3	F	154	TRP	CG-CD1-NE1	-5.09	105.01	110.10
1	A	441	TRP	CG-CD2-CE3	5.07	138.47	133.90
1	B	726	VAL	CG1-CB-CG2	-5.05	102.81	110.90
1	A	546	TRP	CG-CD2-CE3	5.05	138.44	133.90
1	A	706	ARG	NE-CZ-NH2	-5.05	117.78	120.30
3	F	91	THR	O-C-N	-5.05	114.63	122.70
3	E	192	LYS	CA-C-N	5.04	128.28	117.20
1	A	408	LYS	CA-CB-CG	5.03	124.46	113.40
1	A	841	TRP	CG-CD1-NE1	-5.02	105.08	110.10
1	B	597	TRP	CG-CD2-CE3	5.02	138.42	133.90
1	B	546	TRP	CG-CD1-NE1	-5.01	105.09	110.10
1	A	546	TRP	CG-CD1-NE1	-5.00	105.10	110.10

There are no chirality outliers.

All (79) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ARG	Sidechain
1	A	108	TYR	Sidechain
1	A	127	TYR	Sidechain
1	A	133	TYR	Sidechain
1	A	249	GLY	Peptide
1	A	270	TYR	Sidechain
1	A	276	ARG	Sidechain
1	A	313	TYR	Sidechain
1	A	354	ARG	Sidechain
1	A	359	VAL	Peptide
1	A	362	LEU	Peptide
1	A	424	ASP	Peptide
1	A	427	ILE	Peptide
1	A	432	LYS	Peptide
1	A	663	TYR	Sidechain
1	A	715	ARG	Sidechain
1	A	734	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	A	746	PHE	Sidechain
1	A	768	ARG	Sidechain
1	A	773	LYS	Peptide
1	A	804	ARG	Sidechain
1	A	832	TYR	Sidechain
1	B	116	TYR	Sidechain
1	B	127	TYR	Sidechain
1	B	141	TYR	Sidechain
1	B	146	ARG	Sidechain
1	B	193	TYR	Sidechain
1	B	211	GLN	Peptide
1	B	270	TYR	Sidechain
1	B	276	ARG	Sidechain
1	B	302	ARG	Sidechain
1	B	313	TYR	Sidechain
1	B	372	ASN	Peptide
1	B	377	SER	Peptide
1	B	467	ALA	Peptide
1	B	630	ARG	Sidechain
1	B	657	ARG	Sidechain
1	B	683	ARG	Peptide
1	B	691	LYS	Peptide
1	B	719	GLN	Peptide
1	B	733	ARG	Sidechain
1	B	734	TYR	Sidechain
1	B	767	TYR	Sidechain
1	B	768	ARG	Sidechain
1	B	776	PHE	Sidechain
1	B	781	LEU	Peptide
1	B	792	ILE	Peptide
1	B	815	ARG	Sidechain
1	B	817	GLN	Peptide
1	B	832	TYR	Sidechain
1	B	844	PHE	Peptide
1	B	848	LYS	Peptide
1	B	915	ARG	Sidechain
2	D	120	THR	Peptide
2	D	20	ARG	Sidechain
2	D	28	TYR	Sidechain
2	D	36	ARG	Sidechain
2	D	67	GLU	Peptide
2	D	95	PHE	Sidechain

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Mol	Chain	Res	Type	Group
2	D	99	GLY	Peptide
3	E	138	GLY	Peptide
3	E	21	GLY	Peptide
3	E	25	PRO	Peptide
3	F	10	LYS	Peptide
3	F	101	GLU	Peptide
3	F	17	ALA	Peptide
3	F	2	GLY	Peptide
3	F	38	ARG	Sidechain
3	F	52	THR	Peptide
3	F	53	GLN	Peptide
3	F	54	HIS	Peptide
3	F	68	GLN	Peptide
3	F	69	ASP	Peptide
3	F	70	LYS	Peptide
3	F	71	ASP	Peptide
3	F	78	ASP	Peptide
3	F	80	ARG	Peptide
3	F	88	ARG	Peptide
3	F	89	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	7601	1759	7638	236	0
1	B	7615	1764	7656	339	0
2	C	1160	251	1126	17	0
2	D	1160	251	1126	57	0
3	E	1522	344	1492	59	0
3	F	1522	344	1492	109	0
All	All	20580	4713	20530	726	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (726) 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)
3:E:12:LYS:HA	3:F:68:GLN:HG3	1.41	0.99
1:B:238:LYS:HB3	1:B:285:ARG:HB2	1.43	0.98
1:B:375:GLN:HA	1:B:419:THR:HA	1.43	0.98
1:B:178:GLU:HA	1:B:469:PHE:HB3	1.42	0.98
1:A:273:GLU:HA	1:A:478:GLU:HG2	1.46	0.97
3:F:88:ARG:HD2	3:F:89:LEU:HB2	1.45	0.97
1:B:856:ARG:HA	1:B:859:GLU:HB2	1.47	0.96
1:A:728:GLN:HG3	1:B:395:VAL:HB	1.46	0.96
1:A:33:LYS:HB3	1:A:49:ILE:HB	1.52	0.91
1:B:118:GLY:HA3	1:B:717:CYS:HB3	1.54	0.90
1:B:122:VAL:HA	1:B:683:ARG:HB2	1.52	0.90
1:B:147:HIS:HB3	1:B:782:ALA:HB3	1.54	0.89
3:E:9:LYS:HD3	3:F:81:ALA:HA	1.58	0.86
1:A:238:LYS:HB3	1:A:285:ARG:HB2	1.61	0.83
1:A:367:PHE:HB2	1:A:424:ASP:HB2	1.60	0.83
1:A:487:GLU:HG3	1:A:525:ILE:HG12	1.58	0.83
1:B:729:GLU:HG2	2:D:107:GLU:HG2	1.60	0.81
1:B:732:GLN:HB3	2:D:94:VAL:HA	1.63	0.80
3:E:142:CYS:HB3	3:E:147:LEU:HD21	1.63	0.80
1:B:123:VAL:HG21	1:B:682:VAL:HG12	1.62	0.80
1:B:731:ARG:HB2	1:B:753:CYS:HB2	1.63	0.80
1:B:736:ILE:HG12	1:B:795:VAL:HB	1.63	0.80
3:F:3:ASP:HA	3:F:6:LYS:HB2	1.66	0.78
1:A:822:MET:HA	1:A:825:ILE:HD12	1.65	0.77
3:E:57:GLN:HG3	3:E:58:GLU:HG3	1.65	0.77
1:B:727:PHE:HB2	1:B:774:ILE:HB	1.69	0.75
1:B:3:GLN:HG3	1:B:17:LYS:HD3	1.67	0.75
1:B:123:VAL:HG11	1:B:186:ASN:HD21	1.50	0.75
1:B:15:VAL:HG12	1:B:112:LEU:HD13	1.68	0.75
3:F:60:LYS:HA	3:F:63:PHE:HB2	1.69	0.74
1:A:231:LEU:HD21	1:A:442:ILE:HG13	1.69	0.74
1:B:33:LYS:HB3	1:B:49:ILE:HB	1.68	0.74
1:A:355:VAL:HA	1:A:358:SER:HB2	1.69	0.73
1:B:524:CYS:HB2	1:B:568:LYS:HD3	1.70	0.72
1:A:428:GLU:HB2	1:A:432:LYS:HE3	1.71	0.72
2:D:83:GLY:HA3	2:D:88:TYR:HE2	1.54	0.72
1:B:801:ALA:HB2	2:D:43:THR:HG22	1.72	0.72
1:A:428:GLU:O	1:A:432:LYS:HG2	1.90	0.72
3:E:6:LYS:HE2	3:E:32:LYS:HA	1.72	0.72
3:F:54:HIS:HB3	3:F:57:GLN:HB2	1.72	0.71
1:A:268:GLU:HA	1:A:443:LEU:HD21	1.73	0.71
1:B:382:THR:HA	1:B:385:GLN:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:THR:HG21	1:A:631:ILE:HG13	1.73	0.70
2:D:20:ARG:HH21	2:D:27:LEU:HD11	1.54	0.70
1:A:352:ILE:HA	1:A:355:VAL:HB	1.73	0.70
1:A:840:TRP:HA	3:E:195:GLY:HA3	1.73	0.70
1:A:792:ILE:HD12	2:C:94:VAL:HG13	1.72	0.70
1:B:265:ALA:HB3	1:B:450:LEU:HB3	1.73	0.70
1:A:754:ILE:HA	1:A:757:ILE:HB	1.74	0.70
1:A:860:MET:SD	1:B:863:MET:SD	2.90	0.70
3:F:52:THR:HG21	3:F:56:VAL:HB	1.72	0.69
1:B:402:ILE:HG12	1:B:427:ILE:HD13	1.74	0.69
1:B:138:ILE:HG21	1:B:196:VAL:HG13	1.74	0.69
1:B:496:THR:HB	1:B:679:PRO:HG3	1.73	0.69
3:F:11:LYS:HB3	3:F:104:GLY:HA3	1.73	0.69
1:A:491:GLN:HB2	1:A:525:ILE:HD12	1.74	0.69
3:F:111:PHE:HA	3:F:114:ILE:HG12	1.75	0.68
2:D:119:MET:HB3	2:D:123:GLU:HB2	1.73	0.68
1:B:843:LEU:HA	3:F:192:LYS:HA	1.76	0.68
1:B:164:MET:HE2	1:B:171:GLN:HG3	1.76	0.68
1:A:339:MET:SD	1:A:352:ILE:HG21	2.34	0.68
3:F:15:LYS:HG2	3:F:102:ALA:HA	1.77	0.67
1:A:524:CYS:SG	1:A:585:HIS:HA	2.34	0.67
1:A:424:ASP:HA	1:A:427:ILE:HG22	1.74	0.67
1:B:817:GLN:HB2	3:F:134:LEU:HD13	1.76	0.67
1:B:124:ILE:HG13	1:B:685:ILE:HB	1.74	0.67
2:D:95:PHE:HB2	2:D:103:VAL:HG13	1.77	0.67
1:B:671:MET:SD	1:B:674:LEU:HD12	2.35	0.67
1:B:671:MET:HG3	1:B:675:ARG:NH1	2.10	0.66
1:A:880:ARG:HB3	1:B:881:ARG:HD2	1.77	0.66
3:F:74:ILE:HB	3:F:106:ILE:HB	1.76	0.66
2:D:95:PHE:HD1	2:D:107:GLU:HG3	1.61	0.66
1:B:176:THR:OG1	1:B:683:ARG:HA	1.95	0.66
1:B:763:ASP:HB3	1:B:766:LEU:HD12	1.77	0.66
2:D:54:PRO:HB2	2:D:59:MET:HG2	1.78	0.66
1:B:789:ASP:HB3	2:D:116:GLY:HA2	1.78	0.66
3:F:11:LYS:HA	3:F:103:PRO:O	1.96	0.66
1:B:269:THR:HG22	1:B:443:LEU:HD22	1.77	0.66
3:F:106:ILE:HA	3:F:110:MET:HB3	1.78	0.65
1:A:898:LEU:HD21	1:B:899:GLN:HE21	1.60	0.65
1:A:437:ARG:HA	1:A:440:ARG:HB2	1.77	0.65
1:A:139:ASP:HA	1:A:142:LYS:HB2	1.77	0.65
1:A:768:ARG:HB3	1:A:775:PHE:HB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:GLN:HB3	1:B:96:ASN:HD21	1.61	0.65
1:B:393:ILE:HD11	1:B:398:PHE:HD1	1.61	0.65
1:B:704:GLN:HA	1:B:707:CYS:SG	2.36	0.64
3:F:80:ARG:HD2	3:F:95:LEU:HD21	1.80	0.64
1:A:49:ILE:HG23	1:A:57:VAL:HG11	1.79	0.64
1:B:554:SER:HA	1:B:557:GLU:HG2	1.80	0.64
1:B:797:ILE:HG12	2:D:117:GLU:HG2	1.79	0.64
1:B:362:LEU:HD13	1:B:431:ALA:HA	1.78	0.63
2:C:54:PRO:HB3	2:C:58:GLU:HG2	1.80	0.63
3:F:78:ASP:O	3:F:82:THR:HB	1.99	0.63
1:B:610:THR:HG22	1:B:628:VAL:HG22	1.81	0.63
1:B:278:ILE:HG12	1:B:432:LYS:HE2	1.81	0.62
2:D:80:LYS:HD2	2:D:81:ASP:H	1.62	0.62
1:A:53:LYS:HB2	1:A:56:GLU:HB2	1.80	0.62
1:A:407:ILE:HG13	1:A:414:VAL:HB	1.82	0.62
1:A:658:THR:O	1:A:662:LEU:HB3	1.99	0.62
3:F:68:GLN:NE2	3:F:78:ASP:HB2	2.14	0.62
2:C:54:PRO:HB2	2:C:59:MET:HG2	1.81	0.62
1:A:485:THR:HG23	1:A:667:LEU:HD11	1.82	0.62
1:B:173:ILE:HG12	1:B:680:ASN:HB2	1.82	0.62
2:D:111:VAL:HG13	2:D:115:LEU:HD22	1.82	0.62
1:A:737:LEU:HD21	1:A:788:ARG:HA	1.82	0.61
1:B:859:GLU:HB3	1:B:863:MET:SD	2.41	0.61
1:B:184:THR:O	1:B:188:LYS:HE3	2.01	0.61
2:D:70:LEU:HG	2:D:74:GLN:HE21	1.65	0.61
1:A:447:ASN:HA	1:A:450:LEU:HB2	1.80	0.61
1:B:535:PRO:HB2	1:B:540:LEU:HG	1.82	0.61
3:F:8:GLU:HA	3:F:11:LYS:HD2	1.83	0.61
1:A:771:GLN:O	1:B:379:PRO:HA	1.99	0.61
1:A:667:LEU:O	1:A:671:MET:HB2	2.01	0.61
1:B:503:GLU:HA	1:B:506:GLN:HB2	1.81	0.61
3:E:66:ILE:HA	3:E:82:THR:HG21	1.82	0.61
1:A:425:PHE:CE2	1:A:428:GLU:HG3	2.36	0.60
1:B:223:GLN:HB3	1:B:342:MET:SD	2.41	0.60
3:F:130:ASN:HA	3:F:133:ASN:HB3	1.82	0.60
1:A:729:GLU:HG3	1:B:396:THR:HB	1.82	0.60
1:A:426:ALA:HA	1:A:429:ALA:HB3	1.83	0.60
1:B:266:ASN:HA	1:B:447:ASN:OD1	2.00	0.60
1:A:275:SER:OG	1:A:600:LYS:HE2	2.02	0.60
3:F:13:SER:HA	3:F:15:LYS:N	2.17	0.60
1:B:238:LYS:HD3	1:B:285:ARG:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:804:ARG:NH2	2:D:119:MET:SD	2.75	0.60
3:F:44:GLY:O	3:F:120:ALA:HA	2.01	0.60
1:B:510:ILE:HD12	1:B:768:ARG:HG2	1.84	0.59
1:B:146:ARG:HB2	1:B:723:ASN:OD1	2.01	0.59
1:B:735:GLU:HA	1:B:756:MET:CE	2.32	0.59
1:B:49:ILE:HG23	1:B:57:VAL:HG11	1.83	0.59
1:B:845:THR:HB	3:F:189:LYS:HA	1.84	0.59
3:E:4:ASP:HA	3:E:7:LYS:HD2	1.83	0.59
1:B:153:ILE:HG12	1:B:186:ASN:O	2.01	0.59
1:B:164:MET:SD	1:B:459:SER:HB2	2.43	0.59
3:E:61:GLU:HA	3:E:64:GLN:OE1	2.03	0.59
1:A:817:GLN:HG3	3:E:134:LEU:HB3	1.84	0.59
3:F:69:ASP:HB2	3:F:73:PHE:HB2	1.85	0.59
1:B:301:MET:HA	1:B:304:ASP:HB2	1.84	0.59
1:A:175:CYS:SG	1:A:682:VAL:HB	2.43	0.59
1:B:437:ARG:HB3	1:B:624:LEU:HB3	1.85	0.59
1:B:483:ASN:HA	1:B:486:ASN:HB2	1.85	0.58
1:A:911:ASP:HB3	1:A:915:ARG:HH21	1.68	0.58
1:B:852:GLN:O	1:B:853:SER:HB2	2.02	0.58
1:A:77:LYS:HD2	1:A:77:LYS:H	1.68	0.58
3:E:37:LYS:HB2	3:F:89:LEU:HD21	1.84	0.58
1:B:793:THR:HA	1:B:797:ILE:HB	1.83	0.58
1:B:354:ARG:HB2	1:B:390:LEU:HD22	1.85	0.58
1:B:843:LEU:HD13	3:F:196:ALA:HB3	1.85	0.58
1:A:492:LEU:HD22	1:A:671:MET:SD	2.43	0.58
1:B:388:CYS:HA	1:B:391:MET:HB2	1.85	0.58
1:A:707:CYS:SG	1:A:708:ASN:N	2.77	0.58
1:A:119:LEU:HB2	1:A:717:CYS:SG	2.43	0.58
2:C:38:LEU:HD12	2:C:73:MET:HG3	1.86	0.57
1:B:727:PHE:HA	1:B:730:PHE:HB2	1.85	0.57
3:E:62:ALA:HA	3:E:65:LEU:HB2	1.86	0.57
1:A:163:SER:HB3	1:A:171:GLN:NE2	2.18	0.57
1:A:870:LEU:HB3	1:B:870:LEU:HB3	1.86	0.57
1:B:306:LEU:HB3	1:B:386:LYS:HE3	1.87	0.57
1:B:223:GLN:HG2	1:B:342:MET:HA	1.87	0.57
1:A:605:LEU:HD21	1:A:662:LEU:HD22	1.87	0.57
3:F:14:LYS:HB3	3:F:103:PRO:HB2	1.87	0.57
1:A:723:ASN:HB2	1:A:776:PHE:HB2	1.87	0.57
1:A:553:THR:HA	1:A:579:THR:HG21	1.87	0.57
1:A:107:ARG:HG2	1:A:112:LEU:HB2	1.85	0.57
1:B:614:ASN:HB2	1:B:628:VAL:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:104:MET:HB3	2:D:107:GLU:HB3	1.85	0.57
2:D:42:PRO:HB3	2:D:76:ILE:HG21	1.86	0.57
1:A:556:VAL:HB	1:A:579:THR:HG22	1.87	0.56
1:B:576:LYS:HD2	1:B:577:ASP:H	1.70	0.56
1:A:290:PHE:HD1	1:A:316:LEU:HD21	1.69	0.56
1:B:735:GLU:HA	1:B:756:MET:HE1	1.87	0.56
1:A:856:ARG:NH2	1:B:856:ARG:HB3	2.20	0.56
1:B:726:VAL:HA	1:B:773:LYS:HA	1.87	0.56
1:B:137:ILE:O	1:B:141:TYR:HB2	2.06	0.56
1:A:576:LYS:HD2	1:A:577:ASP:H	1.70	0.56
1:B:173:ILE:O	1:B:463:ILE:HA	2.06	0.56
1:B:502:GLN:HG2	1:B:512:TRP:CD1	2.41	0.56
1:A:842:ARG:NH1	3:E:194:GLU:HB2	2.21	0.55
1:B:194:LEU:HD12	1:B:198:ALA:HB2	1.87	0.55
1:A:573:LYS:HD2	1:A:573:LYS:H	1.70	0.55
1:A:247:ARG:HG3	1:A:273:GLU:HB3	1.88	0.55
1:A:144:LYS:HD2	1:A:148:GLU:HB2	1.89	0.55
3:F:9:LYS:HG2	3:F:12:LYS:HB2	1.89	0.55
2:D:18:PHE:HB3	2:D:30:GLN:NE2	2.21	0.55
1:A:108:TYR:HE1	1:A:126:PRO:HA	1.71	0.55
1:B:614:ASN:ND2	1:B:626:LYS:HA	2.21	0.55
3:F:117:ASP:HA	3:F:120:ALA:HB3	1.87	0.55
1:B:814:LYS:HD3	3:F:137:GLU:HA	1.89	0.55
1:A:141:TYR:HA	1:A:149:MET:HG3	1.88	0.55
1:A:274:LYS:HB2	1:A:432:LYS:HB2	1.88	0.55
1:B:768:ARG:HB3	1:B:775:PHE:HB2	1.89	0.55
1:B:833:LEU:HD22	1:B:833:LEU:H	1.72	0.55
1:B:306:LEU:HD11	1:B:389:HIS:HD2	1.72	0.54
2:C:35:MET:SD	2:C:76:ILE:HD12	2.47	0.54
1:A:704:GLN:HA	1:A:707:CYS:SG	2.48	0.54
1:B:492:LEU:HD13	1:B:675:ARG:HH21	1.73	0.54
1:B:722:PRO:HD2	1:B:777:ARG:HA	1.88	0.54
1:B:580:GLU:HB3	1:B:593:ASN:HD22	1.72	0.54
1:A:402:ILE:HG12	1:A:427:ILE:HD13	1.90	0.54
1:A:734:TYR:HB3	1:A:737:LEU:HD12	1.89	0.54
1:A:809:ARG:HB3	2:C:37:ALA:HA	1.89	0.54
1:B:253:ARG:O	1:B:265:ALA:HA	2.08	0.54
1:A:178:GLU:O	1:A:183:LYS:NZ	2.41	0.54
1:B:846:LYS:NZ	3:F:191:ALA:HA	2.23	0.54
1:B:768:ARG:O	1:B:774:ILE:HA	2.08	0.54
1:B:610:THR:HG21	1:B:631:ILE:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ASN:HA	1:A:447:ASN:OD1	2.08	0.54
1:B:845:THR:HG21	3:F:188:THR:O	2.08	0.54
1:B:323:ILE:HG21	1:B:326:GLN:NE2	2.23	0.54
1:A:351:SER:HA	1:A:354:ARG:HG2	1.88	0.54
1:A:814:LYS:O	1:A:817:GLN:HG2	2.08	0.54
1:B:844:PHE:HB3	1:B:845:THR:HG23	1.90	0.53
3:E:112:LEU:HA	3:E:115:PHE:HB2	1.89	0.53
1:A:253:ARG:O	1:A:265:ALA:HA	2.08	0.53
1:B:788:ARG:HG2	1:B:792:ILE:HG12	1.90	0.53
1:B:101:LEU:HD13	1:B:702:LEU:HD13	1.90	0.53
1:A:491:GLN:HB2	1:A:525:ILE:CD1	2.38	0.53
1:A:818:GLN:O	1:A:821:ALA:HB3	2.09	0.53
1:B:496:THR:HA	1:B:500:LEU:HB2	1.91	0.53
1:B:145:LYS:HB3	1:B:782:ALA:HB1	1.90	0.53
1:B:821:ALA:HB1	3:F:131:ALA:HA	1.89	0.53
3:F:42:ARG:NH1	3:F:121:GLY:O	2.42	0.53
1:B:433:ALA:O	1:B:437:ARG:HG2	2.08	0.53
3:E:16:LYS:HB3	3:F:68:GLN:O	2.08	0.53
3:E:38:ARG:HG2	3:F:88:ARG:HD3	1.90	0.53
1:A:728:GLN:HE22	1:B:385:GLN:HG3	1.74	0.53
1:A:800:GLN:O	1:A:804:ARG:HG3	2.08	0.53
3:F:106:ILE:HD13	3:F:114:ILE:HG21	1.90	0.53
1:A:839:GLN:HA	3:E:194:GLU:HG2	1.91	0.53
3:E:90:CYS:HB2	3:E:95:LEU:HG	1.89	0.53
3:F:106:ILE:HD13	3:F:114:ILE:HD13	1.91	0.53
1:A:33:LYS:O	1:A:48:SER:HA	2.09	0.53
2:D:111:VAL:HA	2:D:115:LEU:HD13	1.91	0.53
3:F:8:GLU:O	3:F:11:LYS:HB2	2.09	0.53
1:B:191:ILE:HG23	1:B:224:LEU:HG	1.91	0.53
1:B:430:LEU:HD11	1:B:613:LEU:HD11	1.91	0.52
1:A:528:ILE:HG12	1:A:538:LEU:HG	1.91	0.52
2:C:15:PHE:HD2	2:C:34:VAL:HG11	1.75	0.52
2:D:132:GLU:HB2	2:D:136:GLY:HA2	1.90	0.52
1:A:198:ALA:O	1:A:261:TYR:HA	2.09	0.52
2:C:8:THR:O	2:C:12:LYS:HG3	2.09	0.52
3:E:73:PHE:HA	3:E:107:ASN:HA	1.91	0.52
1:A:830:ALA:HA	1:A:833:LEU:HD22	1.90	0.52
1:B:819:LEU:HD12	2:D:22:GLY:HA2	1.92	0.52
1:B:99:SER:HA	1:B:102:HIS:HB3	1.91	0.52
1:B:140:MET:HB3	1:B:149:MET:HE1	1.90	0.52
1:B:172:SER:HA	1:B:462:GLY:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ALA:HA	1:A:436:GLU:HB2	1.92	0.52
2:D:54:PRO:HB3	2:D:58:GLU:HG2	1.92	0.52
1:A:814:LYS:HE3	3:E:134:LEU:O	2.10	0.52
3:F:68:GLN:HB2	3:F:78:ASP:CG	2.30	0.52
1:A:49:ILE:HD11	1:A:75:ILE:HD12	1.92	0.52
1:A:425:PHE:CD2	1:A:428:GLU:HG3	2.45	0.52
3:E:109:THR:OG1	3:F:70:LYS:HB3	2.10	0.52
1:A:750:LYS:HG3	1:A:769:ILE:HG21	1.91	0.51
1:B:800:GLN:O	1:B:804:ARG:HG3	2.10	0.51
1:B:480:LEU:HD23	1:B:481:CYS:SG	2.50	0.51
1:B:764:PRO:HA	1:B:767:TYR:HE2	1.75	0.51
1:B:466:ILE:HD13	1:B:489:LEU:HD23	1.92	0.51
1:B:674:LEU:HA	1:B:677:THR:OG1	2.09	0.51
1:B:809:ARG:NH2	2:D:40:GLN:O	2.42	0.51
1:B:247:ARG:HG3	1:B:273:GLU:HB3	1.90	0.51
1:B:671:MET:HG3	1:B:675:ARG:HH12	1.76	0.51
1:A:582:CYS:HA	1:A:590:VAL:O	2.09	0.51
3:F:73:PHE:O	3:F:74:ILE:HG13	2.10	0.51
1:A:425:PHE:O	1:A:429:ALA:N	2.44	0.51
1:B:183:LYS:HG2	1:B:466:ILE:HG13	1.92	0.51
3:F:83:PHE:HB3	3:F:88:ARG:O	2.10	0.51
1:B:735:GLU:N	1:B:756:MET:SD	2.84	0.51
1:A:42:HIS:HD2	1:A:45:GLU:HB3	1.75	0.51
3:E:82:THR:HA	3:E:85:SER:OG	2.11	0.51
1:B:545:CYS:SG	1:B:602:MET:HB2	2.51	0.51
1:A:233:ALA:O	1:A:288:HIS:HB2	2.11	0.51
1:A:767:TYR:CD1	1:A:769:ILE:HG12	2.46	0.51
1:B:222:LYS:O	1:B:226:GLN:HG2	2.11	0.51
1:A:545:CYS:SG	1:A:602:MET:SD	3.02	0.50
1:B:252:ILE:HB	1:B:463:ILE:HB	1.92	0.50
3:F:75:SER:HA	3:F:105:PRO:HA	1.94	0.50
1:B:358:SER:HB3	1:B:390:LEU:HB2	1.94	0.50
1:B:494:ASN:HD22	1:B:494:ASN:N	2.09	0.50
1:B:583:ILE:HG12	1:B:592:TYR:HE2	1.76	0.50
1:A:729:GLU:OE2	1:B:396:THR:HA	2.12	0.50
3:F:88:ARG:CD	3:F:89:LEU:HB2	2.32	0.50
1:B:847:VAL:HG12	1:B:851:LEU:HD21	1.94	0.50
1:B:148:GLU:O	1:B:150:PRO:HD3	2.12	0.50
3:E:9:LYS:NZ	3:F:80:ARG:HA	2.27	0.50
3:F:69:ASP:CB	3:F:73:PHE:HB2	2.40	0.50
2:D:108:ILE:HD12	2:D:128:VAL:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:734:TYR:CD2	1:B:788:ARG:HD3	2.47	0.50
1:B:150:PRO:O	1:B:155:ALA:HB2	2.10	0.50
3:F:177:LEU:HD11	3:F:182:LYS:HD2	1.93	0.50
1:A:507:ARG:HG2	1:B:372:ASN:ND2	2.26	0.50
3:F:78:ASP:HA	3:F:81:ALA:HB3	1.94	0.50
1:B:138:ILE:HG23	1:B:197:VAL:HG23	1.94	0.50
1:A:537:VAL:HG13	1:A:555:PHE:HZ	1.76	0.50
1:B:405:PRO:HB3	1:B:606:ASN:HD21	1.76	0.50
1:B:108:TYR:HD1	1:B:113:ILE:HG22	1.77	0.50
1:A:821:ALA:HB1	3:E:131:ALA:HA	1.94	0.49
1:B:511:GLU:O	1:B:768:ARG:NH1	2.45	0.49
1:B:766:LEU:HD13	1:B:780:VAL:HG21	1.94	0.49
1:B:152:HIS:HB3	1:B:155:ALA:H	1.76	0.49
1:B:141:TYR:HB3	1:B:193:TYR:HE2	1.77	0.49
1:A:931:LYS:HA	1:A:934:ASN:HD22	1.76	0.49
3:E:62:ALA:O	3:E:66:ILE:HB	2.12	0.49
1:B:620:PHE:O	1:B:624:LEU:HG	2.13	0.49
1:B:74:ASP:O	1:B:76:GLN:HG3	2.12	0.49
1:A:49:ILE:HG23	1:A:57:VAL:CG1	2.42	0.49
1:A:367:PHE:CE1	1:A:427:ILE:HG21	2.47	0.49
1:B:730:PHE:CD1	1:B:774:ILE:HG21	2.47	0.49
1:B:919:LEU:HA	1:B:922:ASN:HB3	1.94	0.49
3:E:141:LYS:HE2	3:E:178:ILE:HB	1.94	0.49
1:B:731:ARG:HD2	1:B:756:MET:HE3	1.95	0.49
1:A:119:LEU:HD12	1:A:717:CYS:SG	2.52	0.49
1:A:36:TRP:HA	1:A:45:GLU:O	2.12	0.49
1:B:851:LEU:HA	3:E:53:GLN:NE2	2.28	0.49
1:A:813:ALA:HA	1:A:816:GLN:OE1	2.13	0.49
1:A:848:LYS:H	1:A:849:PRO:HD2	1.77	0.49
1:A:223:GLN:NE2	1:A:449:ALA:HB1	2.28	0.49
1:B:302:ARG:HA	1:B:307:LEU:HD12	1.94	0.49
2:D:140:TYR:O	2:D:144:VAL:HG23	2.13	0.49
3:E:60:LYS:HE2	3:F:60:LYS:HD3	1.94	0.49
1:B:141:TYR:HB3	1:B:193:TYR:CE2	2.47	0.49
3:E:51:PHE:HB3	3:F:61:GLU:HG3	1.94	0.49
1:B:178:GLU:O	1:B:183:LYS:NZ	2.46	0.48
1:B:727:PHE:HB3	1:B:772:SER:O	2.13	0.48
1:A:889:VAL:HG11	1:B:258:VAL:HG22	1.95	0.48
1:B:805:GLY:O	1:B:809:ARG:HG2	2.13	0.48
1:A:351:SER:HB3	1:A:390:LEU:HD11	1.94	0.48
2:C:121:GLU:HA	2:C:124:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:813:ALA:O	1:B:816:GLN:HG2	2.12	0.48
1:A:174:LEU:O	1:A:681:PHE:HA	2.13	0.48
1:B:731:ARG:HD2	1:B:756:MET:CE	2.43	0.48
3:F:48:PHE:HB2	3:F:56:VAL:HG23	1.96	0.48
2:D:127:LEU:HD11	2:D:147:VAL:HG12	1.96	0.48
3:F:79:ILE:HG23	3:F:83:PHE:HB2	1.95	0.48
1:A:659:VAL:HA	1:A:662:LEU:HD23	1.94	0.48
1:B:732:GLN:CB	2:D:94:VAL:HA	2.38	0.48
1:A:370:GLU:HB2	1:A:376:ALA:HA	1.94	0.48
1:B:364:ASN:HB2	1:B:383:ALA:HA	1.96	0.48
1:B:404:THR:HG22	1:B:417:ALA:HA	1.95	0.48
1:A:238:LYS:HG3	1:A:243:ASP:HA	1.95	0.48
1:B:726:VAL:HG13	1:B:772:SER:O	2.14	0.48
1:B:237:ALA:HB3	1:B:247:ARG:HD3	1.96	0.48
1:A:603:ASP:O	1:A:605:LEU:HD22	2.13	0.48
3:F:15:LYS:N	3:F:103:PRO:HD2	2.29	0.48
1:B:339:MET:HB3	1:B:344:PHE:HB2	1.96	0.48
1:A:421:GLU:O	1:A:425:PHE:HB2	2.14	0.47
1:A:542:ASP:O	1:A:545:CYS:SG	2.72	0.47
1:A:522:GLN:O	1:A:526:GLU:HG2	2.14	0.47
1:B:727:PHE:CE1	1:B:769:ILE:HD12	2.49	0.47
1:A:923:LYS:HG2	1:B:926:LEU:HD11	1.95	0.47
1:B:290:PHE:HB3	1:B:360:LEU:HD21	1.94	0.47
1:B:178:GLU:CA	1:B:469:PHE:HB3	2.29	0.47
1:A:367:PHE:O	1:A:420:LYS:HG3	2.13	0.47
1:B:881:ARG:HH11	1:B:881:ARG:HG2	1.78	0.47
1:B:617:SER:HB2	2:C:99:GLY:HA3	1.94	0.47
1:B:7:SER:H	1:B:10:GLU:HB2	1.79	0.47
1:A:383:ALA:HA	1:A:386:LYS:HD2	1.94	0.47
1:B:123:VAL:HG11	1:B:186:ASN:ND2	2.24	0.47
1:A:275:SER:CB	1:A:600:LYS:HE2	2.45	0.47
1:A:483:ASN:HB2	1:A:592:TYR:OH	2.14	0.47
1:B:854:ALA:O	3:F:55:GLN:HB2	2.14	0.47
1:B:707:CYS:SG	1:B:708:ASN:N	2.88	0.47
1:A:956:ASP:O	1:A:959:SER:HB3	2.14	0.47
1:A:95:LEU:HD22	1:A:100:VAL:HG22	1.97	0.47
1:A:843:LEU:HA	3:E:192:LYS:HA	1.97	0.47
3:E:84:ASP:HB2	3:E:89:LEU:HD21	1.97	0.47
1:B:406:ARG:HB3	1:B:608:ASN:HD21	1.79	0.47
1:B:789:ASP:OD1	2:D:115:LEU:HA	2.14	0.47
1:B:480:LEU:HG	1:B:528:ILE:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:THR:HA	1:B:69:THR:HA	1.97	0.47
1:B:104:LEU:HD12	1:B:710:VAL:HG11	1.97	0.47
1:B:783:HIS:CE1	1:B:787:GLU:HG3	2.50	0.47
1:B:121:CYS:O	1:B:123:VAL:HG23	2.15	0.47
1:A:269:THR:O	1:A:440:ARG:NH1	2.47	0.47
1:B:323:ILE:HG21	1:B:326:GLN:HE21	1.80	0.47
1:A:58:THR:HA	1:A:69:THR:HA	1.96	0.47
1:A:626:LYS:HB2	1:A:626:LYS:HE3	1.74	0.47
1:A:541:LEU:HA	1:A:544:GLU:HB2	1.97	0.47
2:D:8:THR:HG22	2:D:12:LYS:HE3	1.96	0.47
3:F:90:CYS:HA	3:F:94:GLU:HB2	1.96	0.47
1:A:355:VAL:O	1:A:359:VAL:HG23	2.15	0.46
1:B:815:ARG:O	2:D:18:PHE:HA	2.15	0.46
1:B:801:ALA:CB	2:D:43:THR:HG22	2.43	0.46
1:B:800:GLN:NE2	2:D:112:LEU:HA	2.29	0.46
1:A:236:ASN:O	1:A:288:HIS:HD2	1.98	0.46
1:B:150:PRO:HB2	1:B:151:PRO:HD2	1.96	0.46
1:A:301:MET:HA	1:A:304:ASP:HB2	1.96	0.46
1:A:533:ASN:HB3	1:A:534:PRO:HD2	1.96	0.46
3:E:20:GLU:HG2	3:E:110:MET:HB2	1.96	0.46
1:A:524:CYS:SG	1:A:585:HIS:ND1	2.88	0.46
2:D:80:LYS:HD2	2:D:81:ASP:N	2.28	0.46
3:E:92:GLU:HA	3:E:95:LEU:HD12	1.97	0.46
1:A:547:PHE:HB3	1:A:550:ALA:HB2	1.96	0.46
3:F:2:GLY:O	3:F:5:GLU:HB3	2.15	0.46
2:D:105:GLY:O	2:D:108:ILE:HG22	2.15	0.46
1:B:833:LEU:HD23	1:B:834:LYS:NZ	2.30	0.46
1:A:583:ILE:O	1:A:589:LYS:HA	2.14	0.46
3:F:98:MET:HE3	3:F:101:GLU:HB2	1.97	0.46
1:B:840:TRP:HB3	3:F:118:ARG:HG2	1.96	0.46
3:E:33:PRO:O	3:E:36:GLN:HG3	2.15	0.46
1:B:753:CYS:HA	1:B:756:MET:SD	2.56	0.46
1:B:358:SER:O	1:B:362:LEU:HD12	2.15	0.46
1:A:256:PHE:O	1:A:458:ALA:N	2.47	0.46
2:D:34:VAL:O	2:D:38:LEU:HG	2.14	0.46
2:C:75:THR:HA	2:C:78:LYS:HZ1	1.80	0.46
1:A:604:PRO:HA	1:A:657:ARG:O	2.16	0.46
1:A:762:LEU:HD11	1:A:784:LEU:HD21	1.98	0.46
2:D:40:GLN:HG3	2:D:42:PRO:HG3	1.97	0.46
1:A:583:ILE:HD11	1:A:592:TYR:HE2	1.79	0.46
3:F:106:ILE:CD1	3:F:114:ILE:HG21	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:GLU:HA	1:B:138:ILE:HB	1.97	0.46
1:B:376:ALA:HB3	1:B:420:LYS:HB2	1.98	0.46
1:B:358:SER:OG	1:B:434:LYS:NZ	2.48	0.46
2:C:51:LEU:HD13	2:C:59:MET:SD	2.56	0.46
1:B:826:GLN:HE22	3:F:155:GLY:HA3	1.81	0.46
1:B:846:LYS:O	1:B:849:PRO:HD2	2.15	0.46
2:C:69:PHE:HA	2:C:72:MET:SD	2.56	0.46
1:B:497:MET:HA	1:B:501:GLU:HB3	1.97	0.45
1:A:365:ILE:HA	1:A:378:MET:HE1	1.98	0.45
1:A:905:GLU:HA	1:A:908:ASN:ND2	2.30	0.45
1:B:218:GLY:O	1:B:222:LYS:NZ	2.50	0.45
1:B:367:PHE:CE1	1:B:378:MET:HB2	2.51	0.45
1:B:839:GLN:OE1	3:F:88:ARG:HB3	2.15	0.45
1:A:274:LYS:HG3	1:A:432:LYS:HD3	1.97	0.45
1:B:842:ARG:HB2	3:F:191:ALA:CB	2.45	0.45
1:B:792:ILE:HD12	1:B:796:ILE:HB	1.97	0.45
1:B:375:GLN:HG3	1:B:419:THR:HG22	1.99	0.45
1:A:630:ARG:NH1	1:A:662:LEU:HB2	2.31	0.45
1:B:72:LYS:HA	1:B:75:ILE:HG12	1.98	0.45
1:B:252:ILE:O	1:B:462:GLY:HA2	2.16	0.45
1:B:725:ILE:HG21	1:B:781:LEU:HD11	1.98	0.45
3:F:56:VAL:HG12	3:F:108:PHE:CZ	2.51	0.45
1:A:762:LEU:HD21	1:A:784:LEU:HD11	1.98	0.45
1:A:734:TYR:CE1	1:A:784:LEU:HB3	2.51	0.45
1:A:361:GLN:HA	1:A:364:ASN:HB2	1.99	0.45
2:D:98:GLU:H	2:D:100:ASN:ND2	2.14	0.45
1:B:497:MET:HA	1:B:501:GLU:CB	2.47	0.45
1:A:432:LYS:HE2	1:A:432:LYS:HB3	1.74	0.45
3:E:106:ILE:HA	3:E:110:MET:HB3	1.99	0.45
1:A:948:THR:O	1:A:952:ARG:HG2	2.17	0.45
1:B:669:LYS:HB2	1:B:669:LYS:HE3	1.73	0.45
1:B:690:GLU:O	1:B:691:LYS:HB3	2.16	0.45
2:D:119:MET:HB2	2:D:124:VAL:HG12	1.98	0.45
3:F:42:ARG:HH22	3:F:124:GLU:H	1.65	0.45
1:B:787:GLU:HG2	1:B:790:LEU:HD22	1.99	0.45
1:A:614:ASN:ND2	1:A:626:LYS:HA	2.32	0.45
1:A:724:ARG:HB2	1:A:773:LYS:HD3	1.98	0.45
1:A:490:GLN:NE2	1:A:494:ASN:HD21	2.15	0.45
1:B:176:THR:HG1	1:B:683:ARG:HA	1.81	0.45
1:A:823:LYS:HA	1:A:826:GLN:OE1	2.17	0.45
3:F:9:LYS:HA	3:F:12:LYS:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:TYR:HD2	1:A:663:TYR:HE2	1.65	0.45
1:B:438:LEU:HA	1:B:624:LEU:HD22	1.97	0.45
1:B:572:SER:HB3	1:B:580:GLU:O	2.17	0.45
1:B:839:GLN:HA	3:F:88:ARG:HB2	1.99	0.45
1:B:120:PHE:CD1	1:B:497:MET:HG2	2.51	0.45
1:A:603:ASP:HB2	1:A:659:VAL:HA	1.99	0.45
1:B:167:ASP:HB2	1:B:773:LYS:HE2	1.99	0.45
3:E:6:LYS:HZ1	3:E:34:PRO:HG3	1.82	0.45
1:B:430:LEU:HD11	1:B:613:LEU:CD1	2.47	0.45
1:B:488:LYS:O	1:B:492:LEU:N	2.50	0.45
1:B:764:PRO:HA	1:B:767:TYR:CE2	2.50	0.45
2:D:9:ALA:HA	2:D:12:LYS:HD2	1.99	0.45
1:B:732:GLN:HB3	2:D:94:VAL:CA	2.41	0.44
1:B:510:ILE:HG21	1:B:775:PHE:CE1	2.51	0.44
1:B:250:LYS:HD2	1:B:267:ILE:HG23	1.98	0.44
1:B:144:LYS:HB3	1:B:149:MET:HG3	1.98	0.44
2:C:119:MET:HB3	2:C:123:GLU:HB2	1.99	0.44
1:B:687:PRO:HB2	1:B:696:LEU:HA	1.99	0.44
1:A:607:ASP:HA	1:A:610:THR:HB	1.98	0.44
1:B:393:ILE:HD11	1:B:398:PHE:CD1	2.47	0.44
1:B:817:GLN:HG3	3:F:134:LEU:HB3	2.00	0.44
1:A:506:GLN:OE1	1:A:514:PHE:HB2	2.17	0.44
1:B:505:TYR:HB3	1:B:510:ILE:HG12	1.97	0.44
1:A:42:HIS:HB2	1:A:44:PHE:O	2.17	0.44
1:A:711:LEU:HD22	1:A:711:LEU:H	1.81	0.44
3:F:54:HIS:CB	3:F:57:GLN:HB2	2.44	0.44
1:A:159:THR:O	1:A:163:SER:HB2	2.17	0.44
1:B:141:TYR:CD2	1:B:149:MET:SD	3.10	0.44
1:B:139:ASP:HA	1:B:142:LYS:HB2	2.00	0.44
1:B:556:VAL:O	1:B:560:ILE:HG12	2.18	0.44
1:B:36:TRP:CD1	1:B:78:MET:HA	2.53	0.44
1:B:199:SER:CB	1:B:221:GLU:HG2	2.48	0.44
1:A:285:ARG:HD2	1:A:321:VAL:O	2.17	0.44
1:B:753:CYS:HA	1:B:756:MET:HG2	1.99	0.44
2:D:101:GLY:HA2	2:D:140:TYR:HE2	1.81	0.44
1:B:573:LYS:HD2	1:B:573:LYS:H	1.83	0.44
3:F:59:PHE:N	3:F:59:PHE:CD2	2.84	0.44
1:A:429:ALA:HB2	1:A:603:ASP:HA	2.00	0.44
3:F:12:LYS:O	3:F:15:LYS:HB2	2.17	0.44
1:B:270:TYR:O	1:B:440:ARG:NH2	2.51	0.44
3:E:158:PHE:HB3	3:E:162:GLU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:PHE:HD2	1:B:683:ARG:HG3	1.82	0.44
3:E:5:GLU:HG3	3:E:6:LYS:N	2.33	0.44
1:A:254:ILE:O	1:A:460:PHE:HA	2.17	0.44
1:B:859:GLU:O	1:B:863:MET:N	2.51	0.44
1:A:477:PHE:HB3	1:A:600:LYS:HD3	1.99	0.44
1:A:265:ALA:O	1:A:450:LEU:HB3	2.17	0.44
1:B:158:ASP:HB2	1:B:193:TYR:OH	2.17	0.44
1:A:357:SER:O	1:A:361:GLN:HB2	2.17	0.44
3:E:11:LYS:HB2	3:F:77:ASN:CB	2.47	0.44
1:A:605:LEU:HD23	1:A:630:ARG:HH12	1.82	0.44
1:A:825:ILE:HG13	3:E:131:ALA:HB1	2.00	0.44
1:B:86:VAL:HG13	1:B:88:ASP:O	2.18	0.44
2:C:34:VAL:O	2:C:38:LEU:HG	2.18	0.44
1:B:108:TYR:HD2	1:B:696:LEU:HD12	1.82	0.44
3:F:79:ILE:HG22	3:F:99:VAL:HA	1.99	0.43
1:B:732:GLN:CA	2:D:94:VAL:HA	2.48	0.43
1:B:795:VAL:O	1:B:799:PHE:N	2.51	0.43
1:B:15:VAL:O	1:B:17:LYS:HG3	2.18	0.43
1:B:391:MET:HB3	1:B:393:ILE:HG23	2.01	0.43
1:B:842:ARG:HB2	3:F:191:ALA:HB3	2.00	0.43
1:B:840:TRP:HA	3:F:195:GLY:HA3	2.00	0.43
1:B:497:MET:O	1:B:716:ILE:HG12	2.18	0.43
1:B:115:THR:O	1:B:121:CYS:HA	2.19	0.43
3:F:130:ASN:HB3	3:F:134:LEU:HG	2.00	0.43
1:B:145:LYS:NZ	1:B:789:ASP:OD2	2.52	0.43
1:A:275:SER:HA	1:A:432:LYS:HZ3	1.84	0.43
1:B:785:GLU:CD	1:B:788:ARG:HH21	2.22	0.43
2:D:35:MET:HG2	2:D:73:MET:SD	2.57	0.43
1:A:162:ARG:CZ	1:A:162:ARG:HA	2.49	0.43
1:A:375:GLN:HA	1:A:419:THR:HA	1.99	0.43
1:B:225:LEU:O	1:B:229:PRO:HD2	2.18	0.43
1:B:153:ILE:HD11	1:B:173:ILE:HG21	2.00	0.43
2:D:103:VAL:HG12	2:D:138:ILE:HB	2.00	0.43
1:B:776:PHE:HB2	1:B:781:LEU:HB2	1.99	0.43
3:F:130:ASN:O	3:F:134:LEU:HG	2.18	0.43
1:B:351:SER:O	1:B:354:ARG:HG2	2.19	0.43
1:A:842:ARG:HB3	3:E:194:GLU:HB3	2.01	0.43
1:A:805:GLY:O	1:A:809:ARG:HG2	2.18	0.43
2:D:21:THR:HA	3:F:154:TRP:HZ2	1.82	0.43
1:B:860:MET:O	1:B:864:LYS:HG2	2.18	0.43
1:A:429:ALA:O	1:A:433:ALA:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:GLU:HA	1:A:530:ARG:HB2	1.99	0.43
3:E:33:PRO:HA	3:E:34:PRO:HD3	1.81	0.43
1:A:663:TYR:O	1:A:667:LEU:HB2	2.18	0.43
1:B:842:ARG:HD2	3:F:193:GLU:HB2	2.00	0.43
1:A:725:ILE:O	1:A:774:ILE:N	2.52	0.43
1:A:470:GLU:HG2	1:A:482:ILE:HG21	2.00	0.43
1:A:387:VAL:HG22	1:A:434:LYS:HD2	1.99	0.43
1:B:292:TYR:HB3	1:B:332:PHE:HB2	2.00	0.43
1:A:311:ASN:N	1:A:311:ASN:HD22	2.15	0.43
3:E:37:LYS:HD2	3:F:89:LEU:HD22	2.00	0.43
1:A:856:ARG:HH22	1:B:856:ARG:HB3	1.82	0.43
1:B:114:TYR:CD2	1:B:123:VAL:HG22	2.53	0.43
1:A:420:LYS:HB3	1:A:421:GLU:OE2	2.18	0.43
3:F:12:LYS:HE2	3:F:105:PRO:O	2.19	0.43
1:B:502:GLN:OE1	1:B:514:PHE:HA	2.19	0.43
2:D:101:GLY:HA2	2:D:140:TYR:CE2	2.54	0.43
2:D:102:THR:HB	2:D:137:CYS:HB3	2.00	0.43
1:A:746:PHE:HE1	1:B:303:ASN:HA	1.83	0.43
1:B:814:LYS:HE3	1:B:814:LYS:O	2.19	0.43
1:A:854:ALA:O	1:A:858:LYS:HG3	2.18	0.43
1:B:6:LEU:HB2	1:B:11:LYS:HG3	2.00	0.43
3:E:62:ALA:HB1	3:E:66:ILE:HD13	2.01	0.43
1:B:14:PHE:CD2	1:B:150:PRO:HG3	2.54	0.43
1:A:540:LEU:HD22	1:A:558:LYS:HD3	2.00	0.43
1:B:758:LYS:NZ	1:B:761:GLU:O	2.52	0.43
1:B:407:ILE:O	1:B:408:LYS:NZ	2.52	0.43
1:B:839:GLN:O	3:F:195:GLY:HA3	2.19	0.42
1:A:540:LEU:HD21	1:A:562:GLU:HG3	2.00	0.42
3:F:33:PRO:HA	3:F:34:PRO:HD2	1.87	0.42
1:B:171:GLN:O	1:B:461:LEU:HA	2.19	0.42
1:A:908:ASN:O	1:A:911:ASP:HB2	2.19	0.42
1:A:554:SER:HA	1:A:557:GLU:HG2	2.00	0.42
1:B:255:ASN:HA	1:B:460:PHE:HA	2.01	0.42
3:F:171:PRO:HB2	3:F:178:ILE:HG22	2.01	0.42
1:B:339:MET:SD	1:B:349:GLN:HG2	2.60	0.42
1:A:720:GLY:O	1:A:777:ARG:NH1	2.53	0.42
1:B:381:ASN:O	1:B:385:GLN:N	2.51	0.42
1:B:145:LYS:CB	1:B:782:ALA:HB1	2.50	0.42
1:A:367:PHE:HE1	1:A:378:MET:SD	2.43	0.42
1:A:758:LYS:NZ	1:A:762:LEU:O	2.51	0.42
1:B:220:LEU:O	1:B:223:GLN:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:LYS:HG2	1:B:593:ASN:ND2	2.33	0.42
1:B:11:LYS:NZ	1:B:16:ASP:OD2	2.52	0.42
1:B:163:SER:OG	1:B:724:ARG:HG3	2.20	0.42
3:E:2:GLY:HA2	3:F:92:GLU:HG2	2.00	0.42
1:A:603:ASP:HB2	1:A:659:VAL:CA	2.50	0.42
3:F:12:LYS:HA	3:F:15:LYS:HG3	2.02	0.42
3:F:9:LYS:O	3:F:10:LYS:NZ	2.51	0.42
1:A:547:PHE:HB3	1:A:550:ALA:CB	2.48	0.42
1:A:361:GLN:HG3	1:A:364:ASN:HB2	2.01	0.42
1:B:973:ALA:O	1:B:974:LYS:NZ	2.49	0.42
3:E:30:ALA:HA	3:E:37:LYS:HG2	2.02	0.42
1:A:437:ARG:HD2	1:A:440:ARG:HD2	2.01	0.42
2:D:140:TYR:HA	2:D:143:LEU:HB3	2.01	0.42
1:A:251:PHE:O	1:A:267:ILE:HA	2.19	0.42
1:A:844:PHE:HB2	3:E:190:GLY:O	2.20	0.42
3:F:118:ARG:NH2	3:F:186:ILE:O	2.53	0.42
1:B:683:ARG:NH2	1:B:708:ASN:OD1	2.52	0.42
2:D:95:PHE:CD2	2:D:108:ILE:HG12	2.55	0.42
2:D:120:THR:O	2:D:124:VAL:HG13	2.20	0.42
1:A:183:LYS:HZ1	1:A:468:GLY:HA3	1.85	0.42
1:B:788:ARG:O	1:B:792:ILE:HG12	2.20	0.42
1:A:486:ASN:HB3	1:A:586:TYR:OH	2.19	0.42
1:B:387:VAL:HG12	1:B:391:MET:SD	2.60	0.42
3:F:76:LYS:HA	3:F:102:ALA:O	2.20	0.42
1:A:923:LYS:NZ	1:A:927:GLU:OE1	2.52	0.42
1:A:444:THR:HG21	1:A:620:PHE:O	2.20	0.42
3:F:17:ALA:O	3:F:20:GLU:HB2	2.20	0.42
1:B:15:VAL:HG22	1:B:87:GLU:HG2	2.02	0.42
1:A:541:LEU:HD11	1:A:598:LEU:HA	2.01	0.42
1:B:711:LEU:O	1:B:714:ILE:HB	2.19	0.42
1:B:189:LYS:HD3	1:B:189:LYS:HA	1.86	0.42
1:A:731:ARG:HH11	1:B:385:GLN:NE2	2.18	0.42
1:B:728:GLN:OE1	1:B:749:GLY:HA3	2.20	0.42
1:B:736:ILE:HG13	1:B:739:ALA:HB2	2.02	0.42
3:E:5:GLU:HG3	3:E:6:LYS:H	1.85	0.42
1:B:853:SER:HB3	3:F:54:HIS:O	2.19	0.42
2:D:48:MET:SD	2:D:54:PRO:HD2	2.60	0.42
1:B:344:PHE:O	1:B:349:GLN:NE2	2.53	0.42
1:B:89:MET:HB3	1:B:714:ILE:HG12	2.02	0.42
1:B:234:PHE:CE1	1:B:289:ILE:HG12	2.55	0.42
3:E:41:GLN:NE2	3:F:87:GLY:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:37:LYS:HD2	3:F:89:LEU:CD2	2.50	0.41
1:A:427:ILE:HA	1:A:427:ILE:HD12	1.94	0.41
1:A:601:ASN:C	1:A:659:VAL:HG23	2.40	0.41
3:E:60:LYS:NZ	3:E:60:LYS:HB2	2.35	0.41
2:D:83:GLY:HA3	2:D:88:TYR:CE2	2.44	0.41
1:B:678:ASN:HA	1:B:679:PRO:HD2	1.86	0.41
1:A:576:LYS:HD2	1:A:577:ASP:N	2.35	0.41
1:B:834:LYS:HD2	1:B:834:LYS:H	1.84	0.41
1:B:741:ALA:O	1:B:743:PRO:HD3	2.20	0.41
1:B:398:PHE:O	1:B:402:ILE:HB	2.20	0.41
1:B:842:ARG:HG3	3:F:193:GLU:HB2	2.01	0.41
1:B:255:ASN:HD22	1:B:264:GLY:HA3	1.86	0.41
1:A:846:LYS:HZ3	3:E:193:GLU:CD	2.23	0.41
1:A:397:ASP:HA	1:A:400:ARG:NH1	2.35	0.41
2:D:46:GLU:O	2:D:49:LYS:HB3	2.21	0.41
3:E:15:LYS:HB2	3:F:69:ASP:OD2	2.20	0.41
1:B:175:CYS:HB2	1:B:183:LYS:HG3	2.02	0.41
1:A:273:GLU:CA	1:A:478:GLU:HG2	2.34	0.41
1:B:398:PHE:HA	1:B:609:VAL:HG23	2.02	0.41
1:B:100:VAL:HG21	1:B:711:LEU:HD13	2.02	0.41
1:A:916:CYS:SG	1:B:916:CYS:SG	3.17	0.41
1:A:280:GLN:HB2	1:A:317:SER:OG	2.21	0.41
1:B:716:ILE:O	1:B:719:GLN:HG2	2.20	0.41
1:A:425:PHE:CD2	1:A:599:THR:HB	2.55	0.41
1:B:732:GLN:HB3	2:D:94:VAL:C	2.40	0.41
1:B:725:ILE:O	1:B:774:ILE:HG22	2.21	0.41
1:B:776:PHE:CD1	1:B:781:LEU:HA	2.55	0.41
1:A:428:GLU:HB2	1:A:432:LYS:CE	2.46	0.41
3:E:147:LEU:HD12	3:E:177:LEU:HD23	2.01	0.41
1:B:727:PHE:CZ	1:B:750:LYS:HA	2.55	0.41
1:B:86:VAL:HG22	1:B:87:GLU:H	1.83	0.41
1:A:339:MET:HB3	1:A:344:PHE:HD1	1.85	0.41
1:A:733:ARG:HG2	1:A:788:ARG:HD3	2.01	0.41
1:B:409:VAL:HB	1:B:414:VAL:HG21	2.02	0.41
3:F:31:PRO:HG2	3:F:36:GLN:NE2	2.36	0.41
3:F:91:THR:OG1	3:F:93:GLN:HB3	2.20	0.41
1:A:199:SER:HB2	1:A:221:GLU:OE2	2.20	0.41
1:A:241:LYS:NZ	1:A:471:ILE:O	2.51	0.41
1:A:477:PHE:CZ	1:A:481:CYS:SG	3.13	0.41
1:A:602:MET:O	1:A:658:THR:HA	2.20	0.41
1:A:825:ILE:CG1	3:E:131:ALA:HB1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:609:VAL:O	1:B:612:LEU:HB3	2.20	0.41
1:B:141:TYR:HD1	1:B:193:TYR:OH	2.04	0.41
3:F:68:GLN:HB2	3:F:78:ASP:OD2	2.21	0.41
1:B:115:THR:N	1:B:122:VAL:O	2.54	0.41
1:B:685:ILE:HD12	1:B:704:GLN:HB3	2.01	0.41
1:B:393:ILE:HD13	1:B:613:LEU:HG	2.03	0.41
1:B:188:LYS:HA	1:B:191:ILE:HB	2.03	0.41
1:A:744:LYS:HA	1:B:303:ASN:OD1	2.20	0.41
1:B:97:GLU:CD	1:B:706:ARG:HH21	2.24	0.41
1:B:618:ASP:HB3	1:B:621:VAL:HG23	2.01	0.41
1:B:348:GLU:O	1:B:352:ILE:HG13	2.21	0.41
1:B:442:ILE:HA	1:B:442:ILE:HD13	1.93	0.41
3:F:74:ILE:HG23	3:F:78:ASP:HB3	2.02	0.41
1:B:49:ILE:HG23	1:B:57:VAL:CG1	2.49	0.41
1:A:611:SER:O	1:A:615:GLN:NE2	2.53	0.41
1:A:602:MET:HG3	1:A:604:PRO:HD3	2.02	0.41
1:A:491:GLN:HE22	1:A:520:ASP:HA	1.85	0.41
1:B:17:LYS:HE3	1:B:87:GLU:HG3	2.01	0.41
1:B:800:GLN:HE21	2:D:119:MET:HG2	1.84	0.41
1:B:174:LEU:HD21	1:B:674:LEU:HD22	2.03	0.41
1:B:734:TYR:CE2	1:B:788:ARG:HD3	2.56	0.41
1:B:6:LEU:HB3	1:B:10:GLU:HB3	2.02	0.41
1:B:738:ALA:HB2	1:B:759:ALA:CB	2.51	0.41
1:A:832:TYR:HE1	1:A:836:ARG:NH1	2.18	0.41
3:F:27:ALA:O	3:F:29:PRO:HD3	2.20	0.41
1:A:173:ILE:O	1:A:463:ILE:HA	2.21	0.41
3:E:129:VAL:HA	3:E:183:PHE:CD2	2.56	0.41
1:A:238:LYS:HD3	1:A:285:ARG:HD3	2.02	0.41
1:A:721:PHE:CB	1:A:775:PHE:HB3	2.51	0.41
3:E:43:SER:HA	3:F:193:GLU:O	2.20	0.41
1:A:804:ARG:NH2	2:C:119:MET:SD	2.94	0.41
1:A:769:ILE:HD13	1:A:774:ILE:HG12	2.03	0.41
1:B:493:PHE:HD2	1:B:494:ASN:ND2	2.19	0.41
3:F:16:LYS:N	3:F:100:ALA:O	2.53	0.41
1:A:563:GLN:OE1	1:A:566:HIS:HD2	2.04	0.41
1:B:731:ARG:NH1	1:B:749:GLY:HA2	2.36	0.40
3:E:6:LYS:O	3:E:10:LYS:NZ	2.51	0.40
1:B:399:THR:HA	1:B:402:ILE:HG22	2.02	0.40
1:B:361:GLN:NE2	1:B:364:ASN:ND2	2.69	0.40
1:A:772:SER:OG	1:A:773:LYS:HE3	2.21	0.40
1:A:603:ASP:HB2	1:A:659:VAL:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:736:ILE:HG23	1:B:794:ASP:OD1	2.21	0.40
1:B:800:GLN:NE2	2:D:119:MET:HG2	2.35	0.40
1:B:251:PHE:O	1:B:267:ILE:HA	2.21	0.40
2:C:53:ASN:N	2:C:54:PRO:HD3	2.35	0.40
3:E:141:LYS:NZ	3:E:173:ASP:O	2.51	0.40
3:F:16:LYS:H	3:F:100:ALA:HB1	1.85	0.40
1:A:52:GLU:OE1	1:A:72:LYS:NZ	2.53	0.40
3:F:195:GLY:HA2	3:F:196:ALA:O	2.21	0.40
1:B:33:LYS:O	1:B:48:SER:HA	2.21	0.40
3:F:42:ARG:NH2	3:F:120:ALA:O	2.54	0.40
1:B:141:TYR:HA	1:B:149:MET:SD	2.60	0.40
1:B:218:GLY:O	1:B:222:LYS:HB2	2.21	0.40
1:A:58:THR:HG22	1:A:69:THR:OG1	2.21	0.40
3:F:146:THR:O	3:F:149:ARG:NH1	2.54	0.40
1:B:55:ASP:O	1:B:71:SER:HA	2.22	0.40
1:B:400:ARG:HH21	1:B:400:ARG:HD3	1.71	0.40
1:A:690:GLU:HB3	1:A:692:ARG:HG3	2.03	0.40
3:F:74:ILE:CG2	3:F:106:ILE:HD12	2.51	0.40
1:B:251:PHE:CE2	1:B:674:LEU:HD21	2.57	0.40
1:B:866:GLU:CD	1:B:869:ARG:HH21	2.25	0.40
1:B:176:THR:O	1:B:684:CYS:HB2	2.22	0.40
1:A:491:GLN:HG2	1:A:522:GLN:CD	2.42	0.40
1:A:348:GLU:O	1:A:352:ILE:HG13	2.21	0.40
3:F:76:LYS:HG3	3:F:103:PRO:HA	2.02	0.40
2:D:31:CYS:HB2	2:D:64:LEU:HD11	2.02	0.40
1:B:663:TYR:O	1:B:667:LEU:N	2.53	0.40
3:F:142:CYS:HB3	3:F:147:LEU:HD21	2.02	0.40
1:B:530:ARG:HH11	1:B:530:ARG:HD2	1.74	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	930/974 (96%)	739 (80%)	154 (17%)	37 (4%)	4	35
1	B	932/974 (96%)	764 (82%)	127 (14%)	41 (4%)	3	33
2	C	146/151 (97%)	127 (87%)	12 (8%)	7 (5%)	3	32
2	D	146/151 (97%)	122 (84%)	18 (12%)	6 (4%)	3	35
3	E	194/196 (99%)	159 (82%)	23 (12%)	12 (6%)	2	26
3	F	194/196 (99%)	118 (61%)	52 (27%)	24 (12%)	0	8
All	All	2542/2642 (96%)	2029 (80%)	386 (15%)	127 (5%)	5	31

All (127) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	181	ALA
1	A	224	LEU
1	A	429	ALA
1	A	533	ASN
1	A	795	VAL
1	A	848	LYS
1	B	16	ASP
1	B	257	ASP
1	B	369	LYS
1	B	407	ILE
1	B	469	PHE
1	B	533	ASN
1	B	735	GLU
1	B	743	PRO
1	B	793	THR
1	B	794	ASP
1	B	837	ASN
1	B	848	LYS
1	B	853	SER
1	B	856	ARG
2	C	100	ASN
2	D	94	VAL
2	D	97	LYS
2	D	116	GLY
2	D	121	GLU
3	E	29	PRO
3	F	11	LYS
3	F	14	LYS
3	F	53	GLN

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Mol	Chain	Res	Type
3	F	54	HIS
3	F	110	MET
3	F	120	ALA
3	F	123	ASP
3	F	125	GLU
3	F	188	THR
1	A	32	LYS
1	A	134	SER
1	A	288	HIS
1	A	371	ARG
1	A	508	GLU
1	A	564	GLY
1	A	605	LEU
1	A	670	LEU
1	A	780	VAL
1	A	846	LYS
1	A	860	MET
1	B	77	LYS
1	B	184	THR
1	B	346	GLU
1	B	393	ILE
1	B	511	GLU
1	B	733	ARG
1	B	762	LEU
1	B	813	ALA
1	B	819	LEU
1	B	836	ARG
1	B	854	ALA
2	C	6	GLU
2	C	57	ASP
2	C	77	ALA
3	E	47	VAL
3	E	49	ALA
3	E	55	GLN
3	E	178	ILE
3	F	15	LYS
3	F	70	LYS
3	F	121	GLY
1	A	257	ASP
1	A	374	ASP
1	A	426	ALA
1	A	574	GLN

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Mol	Chain	Res	Type
1	A	852	GLN
1	B	565	ASN
1	B	572	SER
1	B	817	GLN
1	B	839	GLN
2	D	57	ASP
3	E	188	THR
3	E	194	GLU
3	F	3	ASP
3	F	17	ALA
3	F	29	PRO
3	F	190	GLY
1	A	151	PRO
1	A	603	ASP
1	A	632	VAL
1	A	717	CYS
1	A	854	ALA
1	B	151	PRO
1	B	564	GLY
1	B	567	ALA
1	B	579	THR
2	D	6	GLU
3	F	82	THR
3	F	195	GLY
1	A	92	LEU
1	A	93	THR
1	A	132	ILE
1	A	469	PHE
1	A	546	TRP
1	A	565	ASN
1	B	362	LEU
1	B	531	PRO
3	E	44	GLY
3	E	141	LYS
3	F	12	LYS
3	F	13	SER
3	F	72	GLY
3	F	95	LEU
1	B	379	PRO
1	B	629	ASP
1	B	722	PRO
1	B	725	ILE

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Mol	Chain	Res	Type
2	C	39	GLY
2	C	94	VAL
3	E	105	PRO
1	A	743	PRO
2	C	76	ILE
3	F	44	GLY
3	F	105	PRO
1	A	393	ILE
1	A	413	VAL
3	E	87	GLY
1	B	132	ILE
3	E	140	GLY
1	B	764	PRO

### 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	828/859 (96%)	741 (90%)	87 (10%)	8	36
1	B	829/859 (96%)	720 (87%)	109 (13%)	5	28
2	C	127/130 (98%)	118 (93%)	9 (7%)	18	55
2	D	127/130 (98%)	113 (89%)	14 (11%)	8	34
3	E	162/162 (100%)	146 (90%)	16 (10%)	10	39
3	F	162/162 (100%)	137 (85%)	25 (15%)	3	22
All	All	2235/2302 (97%)	1975 (88%)	260 (12%)	11	32

All (260) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	SER
1	A	26	GLN
1	A	42	HIS
1	A	51	GLU
1	A	55	ASP

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Mol	Chain	Res	Type
1	A	79	ASN
1	A	96	ASN
1	A	110	SER
1	A	146	ARG
1	A	147	HIS
1	A	162	ARG
1	A	163	SER
1	A	178	GLU
1	A	211	GLN
1	A	214	SER
1	A	222	LYS
1	A	228	ASN
1	A	247	ARG
1	A	259	THR
1	A	266	ASN
1	A	278	ILE
1	A	279	ARG
1	A	280	GLN
1	A	286	THR
1	A	302	ARG
1	A	311	ASN
1	A	312	ASN
1	A	314	THR
1	A	329	ASP
1	A	342	MET
1	A	357	SER
1	A	366	VAL
1	A	375	GLN
1	A	388	CYS
1	A	389	HIS
1	A	396	THR
1	A	408	LYS
1	A	412	ASP
1	A	420	LYS
1	A	425	PHE
1	A	430	LEU
1	A	434	LYS
1	A	435	PHE
1	A	451	ASP
1	A	488	LYS
1	A	495	HIS
1	A	506	GLN

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Mol	Chain	Res	Type
1	A	513	ASN
1	A	522	GLN
1	A	526	GLU
1	A	543	GLU
1	A	547	PHE
1	A	565	ASN
1	A	566	HIS
1	A	568	LYS
1	A	573	LYS
1	A	576	LYS
1	A	577	ASP
1	A	579	THR
1	A	586	TYR
1	A	597	TRP
1	A	603	ASP
1	A	615	GLN
1	A	623	ASP
1	A	624	LEU
1	A	657	ARG
1	A	662	LEU
1	A	699	HIS
1	A	707	CYS
1	A	711	LEU
1	A	715	ARG
1	A	727	PHE
1	A	730	PHE
1	A	748	ASP
1	A	751	GLN
1	A	778	THR
1	A	796	ILE
1	A	833	LEU
1	A	837	ASN
1	A	843	LEU
1	A	856	ARG
1	A	865	GLU
1	A	867	PHE
1	A	869	ARG
1	A	882	LYS
1	A	932	GLU
1	A	956	ASP
1	B	3	GLN
1	B	8	ASP

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Mol	Chain	Res	Type
1	B	14	PHE
1	B	16	ASP
1	B	21	ASN
1	B	26	GLN
1	B	33	LYS
1	B	51	GLU
1	B	52	GLU
1	B	77	LYS
1	B	79	ASN
1	B	103	ASN
1	B	109	PHE
1	B	139	ASP
1	B	150	PRO
1	B	162	ARG
1	B	200	SER
1	B	201	HIS
1	B	222	LYS
1	B	228	ASN
1	B	245	SER
1	B	247	ARG
1	B	266	ASN
1	B	278	ILE
1	B	280	GLN
1	B	286	THR
1	B	302	ARG
1	B	303	ASN
1	B	304	ASP
1	B	311	ASN
1	B	314	THR
1	B	326	GLN
1	B	329	ASP
1	B	347	GLU
1	B	369	LYS
1	B	370	GLU
1	B	371	ARG
1	B	372	ASN
1	B	382	THR
1	B	394	ASN
1	B	396	THR
1	B	399	THR
1	B	402	ILE
1	B	408	LYS

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Mol	Chain	Res	Type
1	B	411	ARG
1	B	412	ASP
1	B	445	ARG
1	B	476	SER
1	B	484	TYR
1	B	494	ASN
1	B	497	MET
1	B	503	GLU
1	B	511	GLU
1	B	513	ASN
1	B	515	ILE
1	B	538	LEU
1	B	543	GLU
1	B	553	THR
1	B	565	ASN
1	B	568	LYS
1	B	570	GLN
1	B	573	LYS
1	B	576	LYS
1	B	577	ASP
1	B	579	THR
1	B	603	ASP
1	B	665	GLU
1	B	675	ARG
1	B	682	VAL
1	B	686	ILE
1	B	691	LYS
1	B	703	GLU
1	B	711	LEU
1	B	716	ILE
1	B	719	GLN
1	B	724	ARG
1	B	728	GLN
1	B	730	PHE
1	B	731	ARG
1	B	733	ARG
1	B	744	LYS
1	B	751	GLN
1	B	760	LEU
1	B	761	GLU
1	B	764	PRO
1	B	778	THR

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Mol	Chain	Res	Type
1	B	781	LEU
1	B	812	PHE
1	B	814	LYS
1	B	828	ASN
1	B	833	LEU
1	B	834	LYS
1	B	836	ARG
1	B	839	GLN
1	B	843	LEU
1	B	844	PHE
1	B	849	PRO
1	B	852	GLN
1	B	853	SER
1	B	856	ARG
1	B	862	SER
1	B	886	GLU
1	B	907	ASP
1	B	911	ASP
1	B	932	GLU
1	B	939	ASP
1	B	959	SER
1	B	960	GLU
1	B	974	LYS
2	C	25	LYS
2	C	50	VAL
2	C	60	ASN
2	C	67	GLU
2	C	73	MET
2	C	78	LYS
2	C	80	LYS
2	C	82	GLN
2	C	134	SER
2	D	25	LYS
2	D	60	ASN
2	D	73	MET
2	D	78	LYS
2	D	80	LYS
2	D	82	GLN
2	D	90	GLU
2	D	96	ASP
2	D	102	THR
2	D	103	VAL

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Mol	Chain	Res	Type
2	D	108	ILE
2	D	110	HIS
2	D	121	GLU
2	D	132	GLU
3	E	4	ASP
3	E	16	LYS
3	E	29	PRO
3	E	37	LYS
3	E	41	GLN
3	E	51	PHE
3	E	55	GLN
3	E	71	ASP
3	E	108	PHE
3	E	115	PHE
3	E	123	ASP
3	E	126	ASP
3	E	135	PHE
3	E	145	GLU
3	E	173	ASP
3	E	187	LEU
3	F	10	LYS
3	F	29	PRO
3	F	33	PRO
3	F	42	ARG
3	F	48	PHE
3	F	50	MET
3	F	61	GLU
3	F	67	ASP
3	F	69	ASP
3	F	70	LYS
3	F	77	ASN
3	F	84	ASP
3	F	85	SER
3	F	86	LEU
3	F	88	ARG
3	F	89	LEU
3	F	90	CYS
3	F	95	LEU
3	F	110	MET
3	F	118	ARG
3	F	124	GLU
3	F	145	GLU

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Mol	Chain	Res	Type
3	F	165	GLN
3	F	187	LEU
3	F	193	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	223	GLN
1	A	311	ASN
1	A	312	ASN
1	A	375	GLN
1	A	494	ASN
1	A	565	ASN
1	A	566	HIS
1	A	614	ASN
1	A	615	GLN
1	A	678	ASN
1	A	680	ASN
1	A	728	GLN
1	A	852	GLN
1	A	908	ASN
1	A	922	ASN
1	B	26	GLN
1	B	186	ASN
1	B	223	GLN
1	B	311	ASN
1	B	326	GLN
1	B	361	GLN
1	B	364	ASN
1	B	372	ASN
1	B	385	GLN
1	B	389	HIS
1	B	494	ASN
1	B	593	ASN
1	B	608	ASN
1	B	614	ASN
1	B	751	GLN
1	B	800	GLN
1	B	818	GLN
1	B	852	GLN
1	B	899	GLN

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Mol	Chain	Res	Type
2	C	7	GLN
2	C	100	ASN
2	D	16	GLN
2	D	74	GLN
2	D	100	ASN
2	D	135	ASN
3	E	57	GLN
3	F	36	GLN
3	F	46	ASN
3	F	93	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.