



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:42 PM BST

PDB ID : 3J04
EMDB ID: : EMD-5257
Title : EM structure of the heavy meromyosin subfragment of Chick smooth muscle
Myosin with regulatory light chain in phosphorylated state
Authors : Baumann, B.A.J.; Taylor, D.; Huang, Z.; Tama, F.; Fagnant, P.M.; Trybus,
K.; Taylor, K.
Deposited on : 2011-02-18
Resolution : 20.00 Å(reported)

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

A user guide is available at

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

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

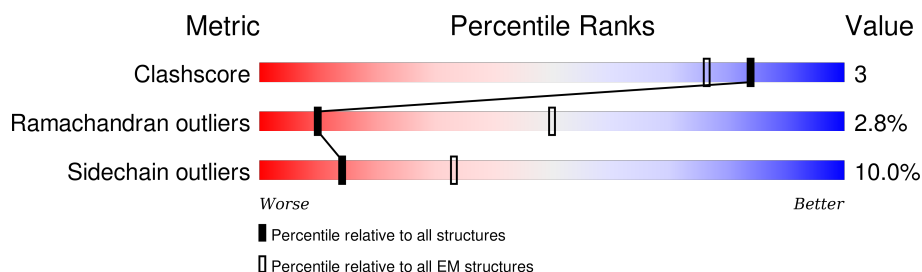
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 20.00 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 ≥ 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	909	
1	D	909	
2	B	143	
2	E	143	
3	C	148	
3	F	148	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19065 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 Myosin-11.

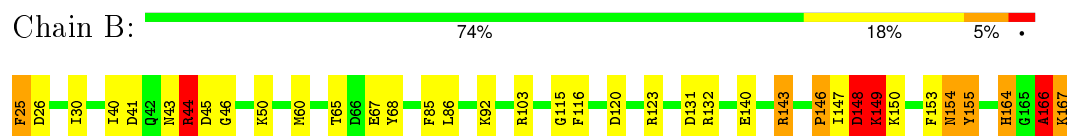
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	903	Total	C	N	O	S	0	0
			7214	4585	1228	1365	36		
1	D	903	Total	C	N	O	S	0	0
			7231	4596	1233	1366	36		

- Molecule 2 is a protein called Myosin regulatory light chain 2, smooth muscle major isoform.

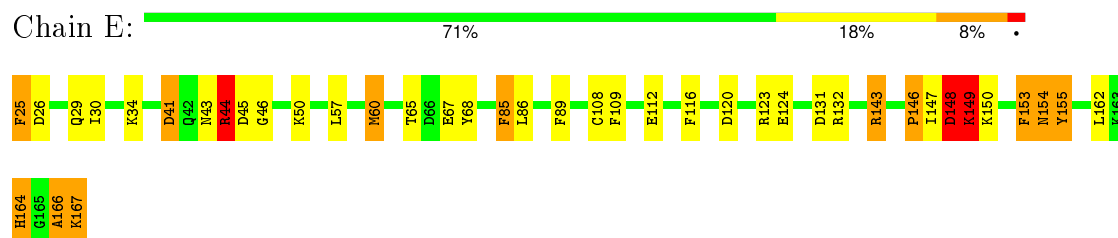
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	143	Total	C	N	O	S	0	0
			1160	727	189	234	10		
2	E	143	Total	C	N	O	S	0	0
			1160	727	189	234	10		

- Molecule 3 is a protein called Myosin light polypeptide 6.

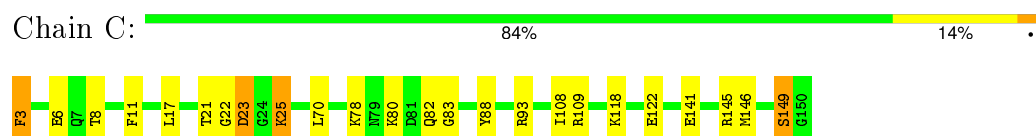
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	148	Total	C	N	O	S	0	0
			1150	716	189	234	11		
3	F	148	Total	C	N	O	S	0	0
			1150	716	189	234	11		



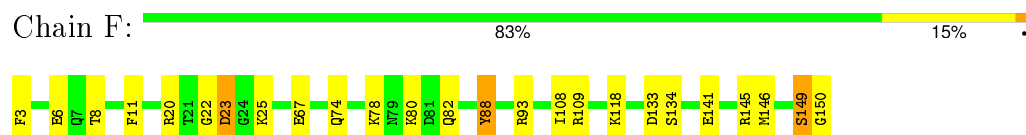
- Molecule 2: Myosin regulatory light chain 2, smooth muscle major isoform



- Molecule 3: Myosin light polypeptide 6



- Molecule 3: Myosin light polypeptide 6



4 Experimental information

Property	Value	Source
Reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	determined using ICE and corrected with CTFAPPLY	Depositor
Microscope	FEI/PHILIPS CM300FEG/T	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	4000	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	24000	Depositor
Image detector	Not provided	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.85	2/7333 (0.0%)	1.85	107/9877 (1.1%)
1	D	0.81	1/7351 (0.0%)	1.76	102/9902 (1.0%)
2	B	0.84	0/1184	1.74	22/1589 (1.4%)
2	E	0.84	0/1184	1.55	21/1589 (1.3%)
3	C	0.83	2/1163 (0.2%)	1.50	5/1559 (0.3%)
3	F	0.82	0/1163	1.30	9/1559 (0.6%)
All	All	0.83	5/19378 (0.0%)	1.74	266/26075 (1.0%)

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	46
1	D	0	48
2	B	0	11
2	E	0	13
3	C	0	5
3	F	0	5
All	All	0	128

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	SER	C-O	-13.16	0.98	1.23
1	D	2	SER	C-O	-12.97	0.98	1.23
1	A	2	SER	N-CA	-6.24	1.33	1.46
3	C	23	ASP	C-N	5.38	1.42	1.33
3	C	83	GLY	C-N	-5.18	1.22	1.34

All (266) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	719	GLN	O-C-N	-53.98	31.43	123.20
1	D	837	ASN	O-C-N	-48.98	44.33	122.70
1	A	822	MET	O-C-N	-40.25	58.30	122.70
1	A	42	HIS	O-C-N	-36.58	61.01	123.20
1	D	841	TRP	O-C-N	-36.19	64.80	122.70
1	A	794	ASP	O-C-N	-36.11	64.92	122.70
1	D	793	THR	O-C-N	-32.07	71.39	122.70
1	A	796	ILE	CA-C-O	-32.00	52.90	120.10
3	C	149	SER	O-C-N	-31.91	68.95	123.20
1	A	205	LYS	O-C-N	29.14	169.33	122.70
1	D	205	LYS	O-C-N	28.72	168.65	122.70
2	B	166	ALA	O-C-N	-28.28	77.45	122.70
1	D	723	ASN	O-C-N	-27.71	78.36	122.70
1	A	206	ASP	O-C-N	-27.40	78.86	122.70
1	D	206	ASP	O-C-N	-26.15	80.86	122.70
1	A	786	GLU	O-C-N	25.52	163.53	122.70
1	A	796	ILE	O-C-N	-25.08	82.58	122.70
1	D	720	GLY	O-C-N	24.18	161.38	122.70
1	A	785	GLU	O-C-N	23.22	159.86	122.70
1	D	822	MET	O-C-N	-23.17	85.63	122.70
1	A	782	ALA	O-C-N	-22.96	85.96	122.70
1	A	784	LEU	O-C-N	-22.72	86.34	122.70
1	D	820	THR	O-C-N	22.43	158.59	122.70
1	D	839	GLN	O-C-N	-22.40	86.85	122.70
1	D	817	GLN	O-C-N	22.35	158.45	122.70
1	A	794	ASP	CA-C-N	22.05	165.72	117.20
1	D	837	ASN	CA-C-O	-21.94	74.03	120.10
1	D	723	ASN	C-N-CA	-21.80	67.19	121.70
1	A	205	LYS	CA-C-N	-21.13	70.71	117.20
1	A	42	HIS	C-N-CA	20.92	166.22	122.30
1	D	205	LYS	CA-C-N	-20.79	71.46	117.20
3	C	149	SER	CA-C-N	20.58	157.35	116.20
1	D	790	LEU	O-C-N	20.39	155.32	122.70
1	D	720	GLY	CA-C-N	-20.32	72.48	117.20
2	B	153	PHE	O-C-N	19.56	153.99	122.70
1	D	717	CYS	O-C-N	-19.35	91.74	122.70
1	A	785	GLU	CA-C-O	-19.07	80.06	120.10
2	E	153	PHE	O-C-N	19.00	153.10	122.70
1	A	786	GLU	CA-C-N	-18.72	76.01	117.20
1	A	817	GLN	O-C-N	-18.68	92.81	122.70
1	D	820	THR	CA-C-N	-18.21	77.13	117.20
1	D	819	LEU	O-C-N	-17.98	93.93	122.70
1	D	822	MET	CA-C-O	17.85	157.59	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	819	LEU	C-N-CA	16.85	163.82	121.70
1	D	817	GLN	CA-C-N	-16.16	81.66	117.20
1	A	823	LYS	C-N-CA	-15.99	81.72	121.70
2	B	166	ALA	CA-C-N	15.75	151.85	117.20
3	F	149	SER	O-C-N	-15.47	96.91	123.20
1	A	787	GLU	O-C-N	-15.34	98.16	122.70
1	A	783	HIS	C-N-CA	15.26	159.85	121.70
1	A	458	ALA	O-C-N	-15.22	98.34	122.70
1	D	790	LEU	CA-C-N	-15.14	83.89	117.20
1	D	458	ALA	O-C-N	-14.89	98.88	122.70
1	A	42	HIS	CA-C-O	-14.41	89.84	120.10
2	E	154	ASN	O-C-N	-14.03	100.26	122.70
2	B	153	PHE	CA-C-N	-13.87	86.68	117.20
2	E	153	PHE	CA-C-N	-13.53	87.44	117.20
2	B	154	ASN	O-C-N	-13.44	101.20	122.70
1	A	782	ALA	CA-C-N	13.42	146.73	117.20
1	A	821	ALA	C-N-CA	-13.30	88.46	121.70
1	A	42	HIS	N-CA-C	-13.27	75.18	111.00
1	D	822	MET	C-N-CA	13.25	154.82	121.70
1	A	783	HIS	O-C-N	13.04	143.56	122.70
1	D	2	SER	O-C-N	-13.03	101.85	122.70
1	D	797	ILE	C-N-CA	-12.90	89.45	121.70
1	A	719	GLN	N-CA-C	12.79	145.53	111.00
1	D	819	LEU	CA-C-O	12.77	146.91	120.10
1	A	787	GLU	C-N-CA	12.59	153.18	121.70
1	D	821	ALA	O-C-N	-12.54	102.64	122.70
1	A	817	GLN	C-N-CA	12.46	152.85	121.70
1	A	822	MET	C-N-CA	-12.44	90.61	121.70
1	D	724	ARG	N-CA-C	-11.81	79.11	111.00
1	D	837	ASN	N-CA-C	-11.81	79.12	111.00
1	D	723	ASN	CA-C-O	-11.69	95.55	120.10
1	D	717	CYS	C-N-CA	11.64	150.80	121.70
1	A	852	GLN	O-C-N	11.40	140.94	122.70
1	D	841	TRP	CA-C-N	11.25	141.96	117.20
1	A	783	HIS	CA-C-O	-11.06	96.87	120.10
1	A	505	TYR	CB-CG-CD2	-11.06	114.36	121.00
3	F	150	GLY	CA-C-O	-11.00	100.80	120.60
1	A	818	GLN	C-N-CA	-10.86	94.56	121.70
1	A	823	LYS	CA-C-N	-10.85	93.33	117.20
1	D	797	ILE	CA-C-O	-10.56	97.93	120.10
1	A	796	ILE	C-N-CA	-10.52	95.41	121.70
1	A	822	MET	CA-C-O	-10.47	98.11	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	852	GLN	CA-C-N	-10.29	94.57	117.20
1	A	718	ARG	O-C-N	-10.27	106.27	122.70
1	A	799	PHE	C-N-CA	-10.27	96.03	121.70
1	A	505	TYR	CB-CG-CD1	10.23	127.14	121.00
1	A	785	GLU	C-N-CA	10.17	147.12	121.70
1	D	793	THR	CA-C-O	-9.87	99.37	120.10
1	A	818	GLN	O-C-N	9.71	138.24	122.70
1	A	821	ALA	O-C-N	-9.69	107.19	122.70
1	D	839	GLN	N-CA-C	9.63	136.99	111.00
1	A	787	GLU	CA-C-O	9.53	140.12	120.10
1	A	784	LEU	CA-C-N	9.40	137.89	117.20
2	E	149	LYS	N-CA-C	9.39	136.36	111.00
2	B	149	LYS	N-CA-C	9.36	136.27	111.00
1	D	821	ALA	C-N-CA	9.21	144.74	121.70
1	D	505	TYR	CB-CG-CD2	-9.16	115.51	121.00
1	D	717	CYS	CA-C-O	8.95	138.88	120.10
1	D	276	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	D	505	TYR	CB-CG-CD1	8.85	126.31	121.00
1	A	816	GLN	O-C-N	-8.73	108.74	122.70
1	D	450	LEU	O-C-N	-8.62	108.91	122.70
2	E	166	ALA	O-C-N	-8.59	108.95	122.70
2	B	143	ARG	NE-CZ-NH2	8.58	124.59	120.30
1	A	799	PHE	N-CA-C	-8.57	87.86	111.00
2	E	143	ARG	NE-CZ-NH2	8.48	124.54	120.30
1	A	276	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	D	839	GLN	CB-CA-C	-8.39	93.62	110.40
2	B	155	TYR	CB-CG-CD2	-8.36	115.98	121.00
2	B	123	ARG	NE-CZ-NH2	8.28	124.44	120.30
1	D	162	ARG	NE-CZ-NH1	8.21	124.40	120.30
2	E	149	LYS	CB-CA-C	-8.20	94.00	110.40
2	E	123	ARG	NE-CZ-NH2	8.20	124.40	120.30
2	B	149	LYS	CB-CA-C	-8.17	94.06	110.40
1	A	822	MET	N-CA-C	-8.16	88.96	111.00
2	E	155	TYR	CB-CG-CD2	-8.02	116.19	121.00
1	A	852	GLN	C-N-CA	8.01	141.74	121.70
2	B	155	TYR	CB-CG-CD1	7.99	125.79	121.00
2	E	155	TYR	CB-CG-CD1	7.98	125.79	121.00
1	D	722	PRO	O-C-N	-7.81	110.20	122.70
1	D	809	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	A	371	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	107	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	A	719	GLN	CA-C-O	-7.58	104.18	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	162	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	A	799	PHE	O-C-N	7.56	134.80	122.70
2	B	85	PHE	CB-CG-CD1	7.54	126.08	120.80
1	D	818	GLN	C-N-CA	7.42	140.25	121.70
1	A	809	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	D	734	TYR	CB-CG-CD1	7.39	125.43	121.00
1	D	107	ARG	NE-CZ-NH1	7.38	123.99	120.30
2	E	153	PHE	C-N-CA	7.38	140.15	121.70
1	A	450	LEU	O-C-N	-7.37	110.90	122.70
1	D	791	LYS	CA-C-O	-7.26	104.84	120.10
1	D	344	PHE	CB-CG-CD1	7.20	125.84	120.80
3	F	93	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	D	797	ILE	CA-C-N	7.12	132.85	117.20
1	D	371	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	D	302	ARG	NE-CZ-NH1	7.03	123.81	120.30
2	B	85	PHE	CB-CG-CD2	-7.00	115.90	120.80
1	D	445	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	A	823	LYS	O-C-N	6.98	133.86	122.70
1	D	733	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	A	821	ALA	CA-C-N	-6.94	101.92	117.20
1	A	791	LYS	O-C-N	-6.94	111.60	122.70
1	D	818	GLN	O-C-N	-6.86	111.72	122.70
1	A	344	PHE	CB-CG-CD1	6.84	125.59	120.80
1	D	823	LYS	O-C-N	-6.84	111.76	122.70
2	B	67	GLU	N-CA-CB	-6.83	98.30	110.60
2	E	60	MET	CG-SD-CE	-6.75	89.39	100.20
1	A	484	TYR	CB-CG-CD2	-6.73	116.96	121.00
1	D	844	PHE	CB-CG-CD1	6.70	125.49	120.80
1	A	817	GLN	CA-C-O	6.68	134.13	120.10
3	F	149	SER	CA-C-N	6.67	129.53	116.20
3	C	88	TYR	CB-CG-CD1	6.66	124.99	121.00
2	B	153	PHE	C-N-CA	6.66	138.34	121.70
1	A	302	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	445	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	D	302	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	302	ARG	NE-CZ-NH1	6.51	123.56	120.30
2	E	120	ASP	CB-CA-C	6.51	123.42	110.40
3	F	23	ASP	CB-CA-C	6.51	123.42	110.40
1	D	290	PHE	CB-CG-CD1	6.50	125.35	120.80
1	A	791	LYS	CA-C-O	6.49	133.72	120.10
1	D	724	ARG	O-C-N	-6.42	112.42	122.70
2	B	116	PHE	CB-CG-CD1	-6.42	116.31	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	PHE	CB-CG-CD2	-6.39	116.33	120.80
1	D	838	TRP	O-C-N	-6.38	112.48	122.70
2	E	67	GLU	N-CA-CB	-6.37	99.13	110.60
3	C	88	TYR	CB-CG-CD2	-6.35	117.19	121.00
1	A	818	GLN	CA-C-N	-6.28	103.38	117.20
1	D	733	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	D	869	ARG	CD-NE-CZ	-6.27	114.82	123.60
1	A	795	VAL	O-C-N	-6.24	112.71	122.70
1	A	42	HIS	CB-CA-C	6.21	122.83	110.40
1	D	721	PHE	CA-C-O	-6.17	107.15	120.10
2	B	164	HIS	N-CA-CB	6.15	121.67	110.60
1	A	279	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	D	344	PHE	CB-CG-CD2	-6.12	116.51	120.80
2	E	164	HIS	N-CA-CB	6.12	121.61	110.60
1	A	816	GLN	CA-C-N	-6.12	103.74	117.20
2	B	116	PHE	CB-CG-CD2	6.06	125.04	120.80
1	D	820	THR	C-N-CA	6.06	136.84	121.70
2	E	41	ASP	N-CA-CB	-6.04	99.73	110.60
1	D	796	ILE	O-C-N	-6.02	113.07	122.70
1	A	206	ASP	C-N-CA	5.93	136.54	121.70
1	A	315	PHE	CB-CG-CD1	5.93	124.95	120.80
1	D	484	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	A	777	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	D	794	ASP	O-C-N	-5.90	113.26	122.70
1	D	799	PHE	O-C-N	-5.89	113.27	122.70
2	E	85	PHE	CB-CG-CD1	5.89	124.92	120.80
1	A	784	LEU	C-N-CA	5.88	136.40	121.70
3	F	20	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	E	116	PHE	CB-CG-CD2	5.85	124.89	120.80
1	D	290	PHE	CB-CG-CD2	-5.84	116.71	120.80
1	A	290	PHE	CB-CG-CD1	5.82	124.88	120.80
1	D	817	GLN	C-N-CA	5.82	136.25	121.70
1	D	253	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	2	SER	O-C-N	-5.80	113.42	122.70
1	D	154	TYR	CB-CG-CD1	5.79	124.47	121.00
1	A	107	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	811	ALA	O-C-N	-5.79	113.44	122.70
1	D	822	MET	N-CA-C	-5.78	95.40	111.00
1	D	804	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	A	822	MET	CA-C-N	-5.76	104.54	117.20
1	A	105	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	A	717	CYS	O-C-N	-5.68	113.61	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	790	LEU	C-N-CA	5.68	135.89	121.70
1	D	837	ASN	CB-CA-C	5.67	121.74	110.40
1	D	724	ARG	CB-CA-C	5.67	121.74	110.40
1	D	844	PHE	CB-CG-CD2	-5.67	116.83	120.80
1	D	315	PHE	CB-CG-CD1	5.63	124.74	120.80
1	A	776	PHE	CB-CG-CD1	5.63	124.74	120.80
1	A	315	PHE	CB-CG-CD2	-5.60	116.88	120.80
2	E	116	PHE	CB-CG-CD1	-5.60	116.88	120.80
1	D	285	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	D	247	ARG	NE-CZ-NH1	5.58	123.09	120.30
3	F	6	GLU	N-CA-CB	-5.58	100.55	110.60
1	D	206	ASP	C-N-CA	5.57	135.63	121.70
1	D	721	PHE	CA-C-N	5.54	132.60	117.10
1	A	797	ILE	CB-CA-C	-5.53	100.55	111.60
1	A	791	LYS	C-N-CA	5.51	135.49	121.70
1	D	89	MET	CG-SD-CE	-5.49	91.41	100.20
1	D	734	TYR	CB-CG-CD2	-5.49	117.71	121.00
2	B	148	ASP	C-N-CA	5.48	135.40	121.70
1	D	253	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	507	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	D	279	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	823	LYS	N-CA-C	5.44	125.69	111.00
1	A	804	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	354	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	247	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	162	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	A	285	ARG	NE-CZ-NH1	5.39	122.99	120.30
2	E	148	ASP	C-N-CA	5.37	135.13	121.70
1	A	89	MET	CG-SD-CE	-5.36	91.62	100.20
2	B	103	ARG	NE-CZ-NH1	-5.35	117.63	120.30
1	D	440	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	484	TYR	CB-CG-CD1	5.34	124.20	121.00
1	A	801	ALA	N-CA-CB	5.33	117.56	110.10
1	A	811	ALA	C-N-CA	5.32	135.00	121.70
1	D	354	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	D	105	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	D	869	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	D	503	GLU	CB-CA-C	-5.23	99.94	110.40
1	A	154	TYR	CB-CG-CD1	5.21	124.13	121.00
1	D	315	PHE	CB-CG-CD2	-5.19	117.17	120.80
1	A	290	PHE	CB-CG-CD2	-5.19	117.17	120.80
1	D	107	ARG	NE-CZ-NH2	-5.18	117.71	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	6	GLU	N-CA-CB	-5.17	101.30	110.60
3	F	11	PHE	CB-CG-CD1	5.15	124.41	120.80
1	A	823	LYS	CB-CA-C	-5.14	100.13	110.40
2	E	85	PHE	CB-CG-CD2	-5.11	117.23	120.80
2	B	120	ASP	CB-CA-C	5.08	120.57	110.40
1	A	797	ILE	O-C-N	-5.07	114.59	122.70
1	D	2	SER	CA-C-O	5.07	130.74	120.10
1	A	715	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	507	ARG	NE-CZ-NH2	-5.06	117.77	120.30
3	F	88	TYR	CB-CG-CD2	-5.06	117.96	121.00
2	B	44	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	A	823	LYS	CA-C-O	-5.03	109.53	120.10
1	A	530	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (128) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	ARG	Sidechain
1	A	127	TYR	Sidechain
1	A	168	ARG	Sidechain
1	A	206	ASP	Mainchain,Peptide
1	A	212	GLY	Peptide
1	A	270	TYR	Sidechain
1	A	276	ARG	Sidechain
1	A	285	ARG	Sidechain
1	A	288	HIS	Mainchain
1	A	41	LYS	Mainchain
1	A	42	HIS	Mainchain,Peptide
1	A	450	LEU	Mainchain
1	A	458	ALA	Mainchain
1	A	657	ARG	Sidechain
1	A	718	ARG	Mainchain,Peptide
1	A	719	GLN	Mainchain
1	A	724	ARG	Mainchain
1	A	768	ARG	Sidechain
1	A	782	ALA	Mainchain,Peptide
1	A	783	HIS	Peptide
1	A	784	LEU	Mainchain,Peptide
1	A	785	GLU	Peptide
1	A	787	GLU	Mainchain
1	A	790	LEU	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	793	THR	Mainchain
1	A	794	ASP	Mainchain,Peptide
1	A	795	VAL	Mainchain,Peptide
1	A	796	ILE	Mainchain,Peptide
1	A	800	GLN	Peptide
1	A	816	GLN	Mainchain
1	A	817	GLN	Mainchain
1	A	821	ALA	Mainchain
1	A	822	MET	Mainchain
1	A	823	LYS	Mainchain
1	A	836	ARG	Sidechain
1	A	852	GLN	Peptide
1	A	855	ARG	Sidechain
1	A	869	ARG	Sidechain
2	B	131	ASP	Peptide
2	B	146	PRO	Peptide
2	B	147	ILE	Peptide
2	B	148	ASP	Mainchain,Peptide
2	B	154	ASN	Mainchain
2	B	166	ALA	Mainchain,Peptide
2	B	40	ILE	Peptide
2	B	44	ARG	Peptide
2	B	68	TYR	Sidechain
3	C	109	ARG	Sidechain
3	C	145	ARG	Sidechain
3	C	149	SER	Mainchain,Peptide
3	C	93	ARG	Sidechain
1	D	107	ARG	Sidechain
1	D	127	TYR	Sidechain
1	D	162	ARG	Sidechain
1	D	168	ARG	Sidechain
1	D	206	ASP	Mainchain,Peptide
1	D	212	GLY	Peptide
1	D	270	TYR	Sidechain
1	D	276	ARG	Sidechain
1	D	285	ARG	Sidechain
1	D	288	HIS	Mainchain
1	D	450	LEU	Mainchain
1	D	458	ALA	Mainchain
1	D	657	ARG	Sidechain
1	D	717	CYS	Mainchain,Peptide
1	D	719	GLN	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	720	GLY	Peptide
1	D	722	PRO	Mainchain
1	D	723	ASN	Mainchain
1	D	724	ARG	Mainchain
1	D	731	ARG	Sidechain
1	D	734	TYR	Sidechain
1	D	768	ARG	Sidechain
1	D	788	ARG	Peptide
1	D	791	LYS	Mainchain
1	D	793	THR	Mainchain
1	D	794	ASP	Mainchain
1	D	796	ILE	Mainchain
1	D	797	ILE	Mainchain
1	D	799	PHE	Mainchain,Peptide
1	D	815	ARG	Sidechain
1	D	821	ALA	Mainchain,Peptide
1	D	822	MET	Peptide
1	D	823	LYS	Mainchain
1	D	827	ARG	Sidechain
1	D	833	LEU	Peptide
1	D	834	LYS	Peptide
1	D	836	ARG	Sidechain
1	D	837	ASN	Mainchain
1	D	839	GLN	Mainchain
1	D	840	TRP	Peptide
1	D	841	TRP	Mainchain,Peptide
1	D	855	ARG	Sidechain
1	D	869	ARG	Sidechain
2	E	109	PHE	Sidechain
2	E	131	ASP	Peptide
2	E	146	PRO	Peptide
2	E	147	ILE	Peptide
2	E	148	ASP	Mainchain,Peptide
2	E	153	PHE	Peptide
2	E	154	ASN	Mainchain
2	E	166	ALA	Mainchain,Peptide
2	E	44	ARG	Sidechain,Peptide
2	E	68	TYR	Sidechain
3	F	109	ARG	Sidechain
3	F	145	ARG	Sidechain
3	F	149	SER	Mainchain,Peptide
3	F	88	TYR	Sidechain

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	7214	0	7236	14	0
1	D	7231	0	7262	11	0
2	B	1160	0	1076	31	0
2	E	1160	0	1076	34	0
3	C	1150	0	1116	16	0
3	F	1150	0	1114	3	0
All	All	19065	0	18880	107	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 3.

All (107) 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)
2:E:25:PHE:CE2	2:E:86:LEU:HD11	1.15	1.63
3:C:3:PHE:CZ	3:C:70:LEU:HD11	1.15	1.61
2:E:25:PHE:CZ	2:E:30:ILE:HD11	1.34	1.60
2:B:25:PHE:CZ	2:B:30:ILE:HD11	1.29	1.59
2:E:25:PHE:CZ	2:E:86:LEU:HD11	1.36	1.59
2:B:25:PHE:HE2	2:B:86:LEU:CD1	1.09	1.58
2:E:25:PHE:CE2	2:E:86:LEU:CD1	1.84	1.55
2:B:25:PHE:CE2	2:B:86:LEU:CD1	1.80	1.54
2:B:25:PHE:CZ	2:B:86:LEU:HD11	1.43	1.51
2:B:25:PHE:CE2	2:B:86:LEU:HD11	1.01	1.50
2:E:25:PHE:HE2	2:E:86:LEU:CD1	1.17	1.50
3:C:3:PHE:HZ	3:C:70:LEU:CD1	1.20	1.50
2:B:25:PHE:CE1	2:B:30:ILE:HD11	1.53	1.42
2:B:25:PHE:CZ	2:B:30:ILE:CD1	2.06	1.36
2:E:25:PHE:CZ	2:E:30:ILE:CD1	2.13	1.29
2:E:25:PHE:CE1	2:E:30:ILE:HD11	1.67	1.28
2:E:167:LYS:NZ	2:E:167:LYS:HA	1.49	1.26
2:B:167:LYS:NZ	2:B:167:LYS:HA	1.58	1.18
2:E:167:LYS:HZ3	2:E:167:LYS:CA	1.55	1.17
2:B:167:LYS:CA	2:B:167:LYS:HZ2	1.61	1.12
3:C:3:PHE:CZ	3:C:70:LEU:CD1	2.06	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:VAL:O	1:A:783:HIS:O	1.71	1.09
2:B:167:LYS:CA	2:B:167:LYS:NZ	2.24	0.97
2:E:25:PHE:HE2	2:E:86:LEU:HD12	1.28	0.95
2:E:167:LYS:CA	2:E:167:LYS:NZ	2.17	0.95
2:B:25:PHE:HE2	2:B:86:LEU:HD12	1.31	0.95
3:C:3:PHE:CD2	3:C:11:PHE:HE2	1.85	0.95
2:E:167:LYS:C	2:E:167:LYS:HZ2	1.68	0.94
2:B:167:LYS:HZ2	2:B:167:LYS:HA	0.77	0.94
2:B:167:LYS:C	2:B:167:LYS:HZ1	1.73	0.91
1:D:2:SER:OG	1:D:18:ASN:OD1	1.90	0.90
2:E:25:PHE:CE2	2:E:86:LEU:HD12	2.05	0.86
2:B:167:LYS:NZ	2:B:167:LYS:C	2.30	0.86
2:E:25:PHE:CZ	2:E:86:LEU:CD1	2.30	0.85
2:B:25:PHE:HE2	2:B:86:LEU:HD13	1.38	0.85
2:B:25:PHE:CZ	2:B:86:LEU:CD1	2.34	0.85
2:E:167:LYS:C	2:E:167:LYS:NZ	2.31	0.84
2:E:25:PHE:HE2	2:E:86:LEU:HD13	1.40	0.82
2:B:25:PHE:CE1	2:B:30:ILE:CD1	2.44	0.82
2:E:25:PHE:HZ	2:E:30:ILE:HD11	1.35	0.81
2:B:25:PHE:HZ	2:B:30:ILE:HD11	1.42	0.81
2:B:25:PHE:HZ	2:B:86:LEU:HD21	1.46	0.79
3:C:3:PHE:CD2	3:C:11:PHE:CE2	2.71	0.78
2:E:25:PHE:CE1	2:E:30:ILE:CD1	2.54	0.77
2:E:167:LYS:HZ3	2:E:167:LYS:HA	0.67	0.77
2:B:25:PHE:CZ	2:B:30:ILE:HD13	2.17	0.76
2:E:25:PHE:CE2	2:E:86:LEU:HD13	2.16	0.75
3:C:3:PHE:CE1	3:C:8:THR:OG1	2.42	0.72
1:D:845:THR:HG22	2:E:167:LYS:HE2	1.70	0.72
2:E:25:PHE:CZ	2:E:30:ILE:HD13	2.23	0.71
3:C:3:PHE:CE2	3:C:11:PHE:CE2	2.79	0.71
1:D:2:SER:HG	1:D:18:ASN:CG	1.94	0.70
2:B:25:PHE:CE2	2:B:86:LEU:HD13	2.16	0.67
2:E:25:PHE:HZ	2:E:86:LEU:HD11	1.42	0.67
2:E:25:PHE:HD2	2:E:89:PHE:HE2	1.44	0.64
3:C:3:PHE:CE1	3:C:70:LEU:HD11	2.15	0.64
1:D:2:SER:CB	1:D:18:ASN:OD1	2.46	0.63
2:B:25:PHE:CE2	2:B:86:LEU:HD12	2.10	0.63
3:C:3:PHE:CD1	3:C:8:THR:OG1	2.51	0.62
1:A:39:SER:HB3	1:A:42:HIS:O	1.99	0.61
1:A:2:SER:HB2	1:A:18:ASN:OD1	1.99	0.61
3:C:3:PHE:HD1	3:C:3:PHE:O	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:PHE:CE2	2:B:30:ILE:HD13	2.37	0.60
2:B:25:PHE:CE2	2:B:30:ILE:CD1	2.78	0.60
2:B:25:PHE:HZ	2:B:86:LEU:CD2	2.15	0.60
3:C:3:PHE:CE2	3:C:11:PHE:CD2	2.89	0.59
3:C:3:PHE:CE2	3:C:11:PHE:HE2	2.16	0.59
2:B:25:PHE:CZ	2:B:86:LEU:HD21	2.34	0.59
2:E:25:PHE:HZ	2:E:86:LEU:HD21	1.67	0.59
1:D:845:THR:CG2	2:E:167:LYS:HE2	2.34	0.58
3:C:3:PHE:CE2	3:C:70:LEU:CD1	2.83	0.57
2:E:25:PHE:O	2:E:25:PHE:HD1	1.89	0.56
1:A:447:ASN:O	1:A:451:ASP:OD2	2.24	0.56
2:B:25:PHE:HD1	2:B:25:PHE:O	1.89	0.55
3:F:3:PHE:HD1	3:F:8:THR:HG1	1.54	0.55
3:C:3:PHE:HD2	3:C:11:PHE:HE2	1.46	0.55
1:A:883:GLU:OE1	1:A:887:LYS:NZ	2.40	0.55
2:E:25:PHE:CE2	2:E:30:ILE:CD1	2.86	0.54
2:E:25:PHE:HD2	2:E:89:PHE:CE2	2.24	0.52
1:A:876:LYS:NZ	1:A:880:GLU:OE2	2.38	0.52
1:A:40:GLU:CD	1:A:41:LYS:HZ2	2.13	0.51
1:D:40:GLU:CD	1:D:41:LYS:HZ2	2.13	0.51
1:A:883:GLU:OE2	1:A:887:LYS:NZ	2.40	0.51
2:E:25:PHE:CE2	2:E:30:ILE:HD13	2.46	0.51
1:A:780:VAL:O	1:A:783:HIS:C	2.47	0.50
1:A:876:LYS:NZ	1:A:880:GLU:OE1	2.46	0.46
3:F:3:PHE:N	3:F:3:PHE:CD2	2.84	0.46
1:D:2:SER:HB2	1:D:18:ASN:OD1	2.14	0.45
1:A:800:GLN:H	1:A:802:GLN:H	1.63	0.45
2:B:25:PHE:HZ	2:B:30:ILE:CD1	2.04	0.43
1:D:421:GLU:H	1:D:421:GLU:CD	2.22	0.43
1:D:838:TRP:CD2	1:D:841:TRP:HB2	2.53	0.43
2:B:25:PHE:C	2:B:25:PHE:CD1	2.92	0.43
3:C:3:PHE:N	3:C:3:PHE:CD1	2.84	0.42
2:E:25:PHE:C	2:E:25:PHE:CD1	2.93	0.42
1:A:421:GLU:CD	1:A:421:GLU:H	2.22	0.42
1:A:865:GLU:OE1	1:A:869:ARG:NH2	2.53	0.42
1:D:789:ASP:HA	1:D:792:ILE:HG22	2.02	0.42
2:B:25:PHE:CZ	2:B:86:LEU:CD2	3.01	0.41
2:E:41:ASP:OD2	2:E:44:ARG:HA	2.20	0.41
3:C:23:ASP:OD2	3:C:25:LYS:NZ	2.50	0.41
1:A:801:ALA:HA	1:A:804:ARG:HB2	2.02	0.41
2:B:25:PHE:CE1	2:B:30:ILE:CG1	3.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:3:PHE:CD2	3:F:74:GLN:HG2	2.56	0.41
2:E:57:LEU:HD12	2:E:60:MET:HE2	2.01	0.41
2:E:25:PHE:CD2	2:E:89:PHE:HE2	2.31	0.41
1:D:102:HIS:O	1:D:106:GLU:HG2	2.21	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	899/909 (99%)	807 (90%)	69 (8%)	23 (3%)	7	45
1	D	899/909 (99%)	808 (90%)	65 (7%)	26 (3%)	6	43
2	B	141/143 (99%)	123 (87%)	11 (8%)	7 (5%)	3	31
2	E	141/143 (99%)	123 (87%)	12 (8%)	6 (4%)	3	34
3	C	146/148 (99%)	135 (92%)	9 (6%)	2 (1%)	14	58
3	F	146/148 (99%)	135 (92%)	8 (6%)	3 (2%)	9	50
All	All	2372/2400 (99%)	2131 (90%)	174 (7%)	67 (3%)	10	44

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	533	ASN
1	A	564	GLY
1	A	679	PRO
1	A	724	ARG
1	A	785	GLU
1	A	786	GLU
1	A	801	ALA
1	A	823	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	852	GLN
2	B	149	LYS
2	B	164	HIS
1	D	168	ARG
1	D	533	ASN
1	D	564	GLY
1	D	679	PRO
1	D	724	ARG
1	D	790	LEU
1	D	793	THR
1	D	794	ASP
1	D	819	LEU
1	D	823	LYS
1	D	824	VAL
1	D	834	LYS
1	D	837	ASN
1	D	839	GLN
2	E	108	CYS
2	E	149	LYS
2	E	164	HIS
3	F	118	LYS
1	A	168	ARG
1	A	205	LYS
1	A	572	SER
1	A	796	ILE
3	C	118	LYS
1	D	205	LYS
1	D	572	SER
1	D	795	VAL
1	D	835	LEU
1	D	838	TRP
1	A	29	TRP
1	A	206	ASP
1	A	783	HIS
2	B	46	GLY
2	B	166	ALA
1	D	29	TRP
1	D	206	ASP
2	E	46	GLY
3	F	22	GLY
1	A	235	GLY
1	A	531	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	235	GLY
1	A	718	ARG
1	A	784	LEU
2	B	45	ASP
1	D	325	ALA
1	D	531	PRO
1	D	579	THR
3	F	133	ASP
1	A	325	ALA
1	A	579	THR
1	A	797	ILE
2	B	115	GLY
3	C	22	GLY
1	D	796	ILE
2	E	45	ASP
2	B	146	PRO
2	E	146	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	779/801 (97%)	707 (91%)	72 (9%)	11	43
1	D	782/801 (98%)	704 (90%)	78 (10%)	9	38
2	B	125/125 (100%)	108 (86%)	17 (14%)	5	27
2	E	125/125 (100%)	106 (85%)	19 (15%)	3	22
3	C	125/127 (98%)	114 (91%)	11 (9%)	12	45
3	F	125/127 (98%)	115 (92%)	10 (8%)	15	50
All	All	2061/2106 (98%)	1854 (90%)	207 (10%)	14	38

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	26	GLN
1	A	29	TRP
1	A	33	LYS
1	A	40	GLU
1	A	53	LYS
1	A	56	GLU
1	A	58	THR
1	A	66	LYS
1	A	72	LYS
1	A	91	GLU
1	A	106	GLU
1	A	162	ARG
1	A	163	SER
1	A	167	ASP
1	A	178	GLU
1	A	204	LYS
1	A	210	THR
1	A	226	GLN
1	A	247	ARG
1	A	257	ASP
1	A	274	LYS
1	A	302	ARG
1	A	331	MET
1	A	334	GLU
1	A	345	THR
1	A	346	GLU
1	A	347	GLU
1	A	370	GLU
1	A	371	ARG
1	A	396	THR
1	A	397	ASP
1	A	412	ASP
1	A	420	LYS
1	A	445	ARG
1	A	466	ILE
1	A	489	LEU
1	A	497	MET
1	A	506	GLN
1	A	513	ASN
1	A	522	GLN
1	A	561	GLN
1	A	568	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	573	LYS
1	A	576	LYS
1	A	577	ASP
1	A	579	THR
1	A	593	ASN
1	A	603	ASP
1	A	608	ASN
1	A	619	LYS
1	A	630	ARG
1	A	637	MET
1	A	639	LYS
1	A	650	LYS
1	A	653	LYS
1	A	655	MET
1	A	686	ILE
1	A	723	ASN
1	A	735	GLU
1	A	744	LYS
1	A	776	PHE
1	A	789	ASP
1	A	790	LEU
1	A	815	ARG
1	A	819	LEU
1	A	828	ASN
1	A	840	TRP
1	A	865	GLU
1	A	870	THR
1	A	871	LYS
1	A	882	LYS
2	B	25	PHE
2	B	26	ASP
2	B	41	ASP
2	B	43	ASN
2	B	44	ARG
2	B	50	LYS
2	B	60	MET
2	B	65	THR
2	B	92	LYS
2	B	132	ARG
2	B	140	GLU
2	B	143	ARG
2	B	148	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	149	LYS
2	B	150	LYS
2	B	155	TYR
2	B	167	LYS
3	C	3	PHE
3	C	17	LEU
3	C	21	THR
3	C	25	LYS
3	C	78	LYS
3	C	80	LYS
3	C	82	GLN
3	C	108	ILE
3	C	122	GLU
3	C	141	GLU
3	C	146	MET
1	D	8	ASP
1	D	9	ASP
1	D	26	GLN
1	D	29	TRP
1	D	33	LYS
1	D	40	GLU
1	D	53	LYS
1	D	56	GLU
1	D	66	LYS
1	D	72	LYS
1	D	91	GLU
1	D	106	GLU
1	D	167	ASP
1	D	178	GLU
1	D	204	LYS
1	D	207	THR
1	D	210	THR
1	D	226	GLN
1	D	247	ARG
1	D	257	ASP
1	D	274	LYS
1	D	302	ARG
1	D	331	MET
1	D	334	GLU
1	D	345	THR
1	D	346	GLU
1	D	347	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	370	GLU
1	D	371	ARG
1	D	396	THR
1	D	397	ASP
1	D	412	ASP
1	D	420	LYS
1	D	445	ARG
1	D	466	ILE
1	D	489	LEU
1	D	497	MET
1	D	506	GLN
1	D	522	GLN
1	D	561	GLN
1	D	568	LYS
1	D	573	LYS
1	D	576	LYS
1	D	577	ASP
1	D	579	THR
1	D	593	ASN
1	D	603	ASP
1	D	608	ASN
1	D	619	LYS
1	D	630	ARG
1	D	637	MET
1	D	639	LYS
1	D	650	LYS
1	D	653	LYS
1	D	655	MET
1	D	686	ILE
1	D	703	GLU
1	D	718	ARG
1	D	719	GLN
1	D	734	TYR
1	D	735	GLU
1	D	744	LYS
1	D	763	ASP
1	D	768	ARG
1	D	784	LEU
1	D	787	GLU
1	D	791	LYS
1	D	794	ASP
1	D	807	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	819	LEU
1	D	822	MET
1	D	823	LYS
1	D	833	LEU
1	D	870	THR
1	D	872	GLU
1	D	881	LEU
1	D	882	LYS
1	D	905	GLU
2	E	25	PHE
2	E	26	ASP
2	E	29	GLN
2	E	34	LYS
2	E	43	ASN
2	E	44	ARG
2	E	50	LYS
2	E	65	THR
2	E	85	PHE
2	E	112	GLU
2	E	124	GLU
2	E	132	ARG
2	E	143	ARG
2	E	148	ASP
2	E	149	LYS
2	E	150	LYS
2	E	155	TYR
2	E	162	LEU
2	E	167	LYS
3	F	23	ASP
3	F	25	LYS
3	F	67	GLU
3	F	78	LYS
3	F	80	LYS
3	F	82	GLN
3	F	108	ILE
3	F	134	SER
3	F	141	GLU
3	F	146	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	GLN
1	A	506	GLN
1	A	522	GLN
1	A	533	ASN
1	A	751	GLN
3	C	16	GLN
1	D	223	GLN
1	D	522	GLN
1	D	533	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](#)

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.