



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:39 PM BST

PDB ID : 3IZP
Title : Conformation of EF-G during translocation
Authors : Li, W.; Trabuco, L.G.; Schulten, K.; Frank, J.
Deposited on : 2010-11-15
Resolution : unknown (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

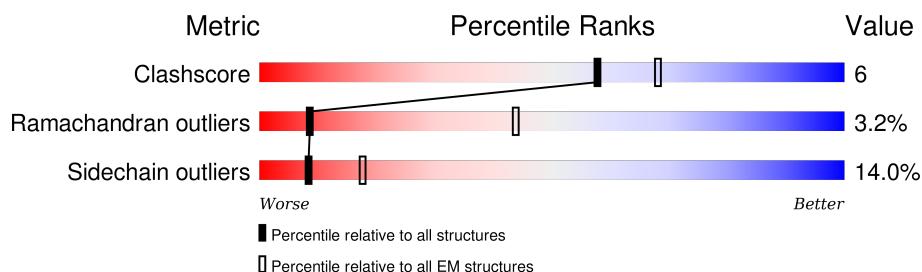
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY


The reported resolution of this entry is unknown.

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	E	688	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 5382 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 Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	688	5382	3416	920	1025	21	0	0

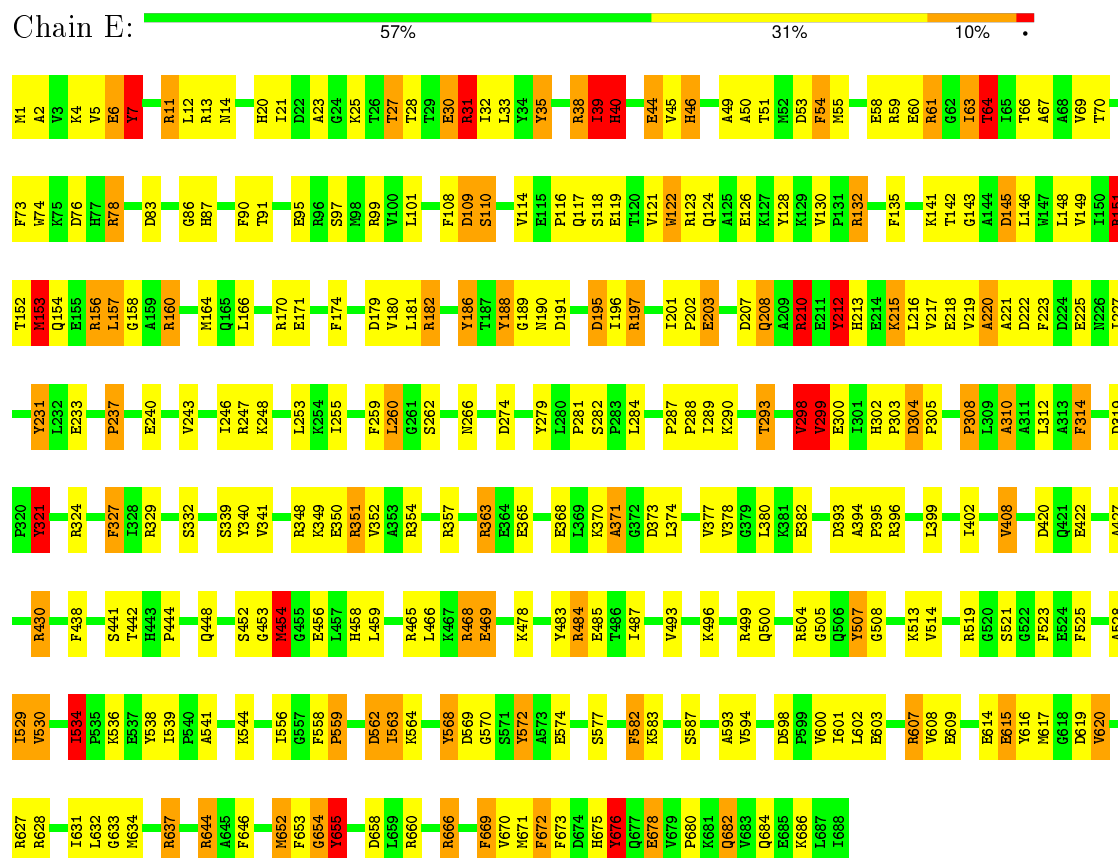
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	573	ALA	HIS	CONFLICT	UNP P13551

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: Elongation factor G



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	50000	Depositor
Image detector	Kodak SO163 film	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	E	1.61	24/5482 (0.4%)	2.15	188/7421 (2.5%)

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	E	0	51

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	676	TYR	CB-CG	-8.54	1.38	1.51
1	E	237	PRO	N-CD	-7.66	1.37	1.47
1	E	35	TYR	CB-CG	-7.27	1.40	1.51
1	E	465	ARG	CD-NE	6.62	1.57	1.46
1	E	6	GLU	CG-CD	-6.41	1.42	1.51
1	E	572	TYR	CE1-CZ	6.33	1.46	1.38
1	E	616	TYR	CD1-CE1	6.30	1.48	1.39
1	E	123	ARG	CD-NE	6.23	1.57	1.46
1	E	672	PHE	CG-CD2	5.85	1.47	1.38
1	E	203	GLU	CG-CD	-5.72	1.43	1.51
1	E	600	VAL	N-CA	-5.70	1.34	1.46
1	E	484	ARG	CD-NE	5.55	1.55	1.46
1	E	240	GLU	CB-CG	5.48	1.62	1.52
1	E	504	ARG	NE-CZ	5.46	1.40	1.33
1	E	441	SER	CA-CB	5.44	1.61	1.52
1	E	559	PRO	N-CD	-5.27	1.40	1.47
1	E	225	GLU	CG-CD	5.17	1.59	1.51
1	E	469	GLU	N-CA	-5.16	1.36	1.46
1	E	614	GLU	CG-CD	5.15	1.59	1.51
1	E	568	TYR	CE2-CZ	5.12	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	243	VAL	CA-CB	-5.10	1.44	1.54
1	E	122	TRP	CD2-CE2	5.06	1.47	1.41
1	E	676	TYR	CE2-CZ	5.02	1.45	1.38
1	E	110	SER	CA-CB	5.01	1.60	1.52

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	7	TYR	CB-CG-CD1	26.43	136.86	121.00
1	E	132	ARG	NE-CZ-NH1	18.60	129.60	120.30
1	E	7	TYR	CB-CG-CD2	-17.29	110.62	121.00
1	E	348	ARG	NE-CZ-NH1	15.16	127.88	120.30
1	E	132	ARG	NE-CZ-NH2	-14.89	112.86	120.30
1	E	568	TYR	CB-CG-CD2	-14.80	112.12	121.00
1	E	61	ARG	NE-CZ-NH2	14.33	127.47	120.30
1	E	538	TYR	CB-CG-CD1	14.24	129.54	121.00
1	E	538	TYR	CB-CG-CD2	-13.73	112.76	121.00
1	E	363	ARG	NE-CZ-NH1	13.14	126.87	120.30
1	E	644	ARG	NE-CZ-NH2	-12.96	113.82	120.30
1	E	396	ARG	NE-CZ-NH2	-12.70	113.95	120.30
1	E	660	ARG	NE-CZ-NH1	12.17	126.39	120.30
1	E	637	ARG	NE-CZ-NH1	11.92	126.26	120.30
1	E	13	ARG	NE-CZ-NH1	11.18	125.89	120.30
1	E	210	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	E	655	TYR	CB-CG-CD2	10.48	127.29	121.00
1	E	182	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	E	31	ARG	NE-CZ-NH2	-10.37	115.12	120.30
1	E	644	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	E	519	ARG	NE-CZ-NH1	10.15	125.38	120.30
1	E	558	PHE	CB-CG-CD2	10.06	127.84	120.80
1	E	607	ARG	NE-CZ-NH2	-9.90	115.35	120.30
1	E	156	ARG	NE-CZ-NH1	9.67	125.14	120.30
1	E	628	ARG	NE-CZ-NH1	9.47	125.04	120.30
1	E	170	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	E	231	TYR	CB-CG-CD1	9.39	126.64	121.00
1	E	7	TYR	CG-CD2-CE2	9.36	128.78	121.30
1	E	59	ARG	NE-CZ-NH2	-9.33	115.63	120.30
1	E	197	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	E	655	TYR	CB-CG-CD1	-9.23	115.46	121.00
1	E	38	ARG	NE-CZ-NH1	-9.01	115.80	120.30
1	E	634	MET	CG-SD-CE	-8.90	85.97	100.20
1	E	31	ARG	NE-CZ-NH1	8.87	124.74	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	499	ARG	NE-CZ-NH2	-8.64	115.98	120.30
1	E	188	TYR	CG-CD2-CE2	-8.50	114.50	121.30
1	E	523	PHE	CB-CG-CD2	-8.49	114.86	120.80
1	E	304	ASP	CB-CG-OD1	8.47	125.92	118.30
1	E	499	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	E	454	MET	CG-SD-CE	8.40	113.65	100.20
1	E	363	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	E	666	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	E	669	PHE	CB-CG-CD2	8.36	126.65	120.80
1	E	430	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	E	314	PHE	CB-CG-CD2	8.23	126.56	120.80
1	E	182	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	E	465	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	E	188	TYR	CB-CG-CD2	-7.93	116.24	121.00
1	E	197	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	E	427	ALA	CB-CA-C	-7.75	98.48	110.10
1	E	151	ARG	NE-CZ-NH1	-7.74	116.43	120.30
1	E	13	ARG	NH1-CZ-NH2	-7.61	111.03	119.40
1	E	152	THR	N-CA-CB	7.56	124.67	110.30
1	E	523	PHE	CB-CG-CD1	7.49	126.04	120.80
1	E	348	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	E	180	VAL	CA-CB-CG1	-7.43	99.75	110.90
1	E	259	PHE	CB-CG-CD1	7.42	125.99	120.80
1	E	7	TYR	CZ-CE2-CD2	-7.34	113.19	119.80
1	E	627	ARG	CG-CD-NE	-7.30	96.47	111.80
1	E	660	ARG	NE-CZ-NH2	-7.27	116.67	120.30
1	E	153	MET	CG-SD-CE	-7.25	88.60	100.20
1	E	262	SER	N-CA-CB	7.25	121.37	110.50
1	E	123	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	E	652	MET	CG-SD-CE	-7.17	88.73	100.20
1	E	247	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	E	135	PHE	CB-CG-CD2	7.14	125.80	120.80
1	E	90	PHE	CB-CG-CD1	-7.03	115.88	120.80
1	E	126	GLU	N-CA-CB	7.02	123.23	110.60
1	E	122	TRP	CA-CB-CG	6.94	126.89	113.70
1	E	504	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	E	354	ARG	NE-CZ-NH1	-6.84	116.88	120.30
1	E	483	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	E	40	HIS	CA-CB-CG	6.82	125.19	113.60
1	E	223	PHE	CB-CG-CD2	6.76	125.53	120.80
1	E	354	ARG	NE-CZ-NH2	6.69	123.64	120.30
1	E	658	ASP	CB-CG-OD1	-6.68	112.29	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	525	PHE	CB-CG-CD1	6.64	125.45	120.80
1	E	231	TYR	CG-CD2-CE2	6.59	126.57	121.30
1	E	186	TYR	CG-CD2-CE2	-6.50	116.10	121.30
1	E	370	LYS	N-CA-CB	-6.50	98.90	110.60
1	E	615	GLU	CB-CA-C	6.49	123.38	110.40
1	E	2	ALA	N-CA-CB	6.45	119.12	110.10
1	E	259	PHE	CB-CG-CD2	-6.43	116.30	120.80
1	E	61	ARG	NH1-CZ-NH2	-6.42	112.34	119.40
1	E	378	VAL	CA-CB-CG1	6.41	120.51	110.90
1	E	340	TYR	CB-CG-CD1	-6.39	117.17	121.00
1	E	135	PHE	CB-CG-CD1	-6.38	116.33	120.80
1	E	627	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	E	654	GLY	O-C-N	-6.32	112.58	122.70
1	E	371	ALA	CB-CA-C	-6.30	100.65	110.10
1	E	157	LEU	CB-CG-CD2	6.27	121.66	111.00
1	E	179	ASP	CB-CG-OD2	6.24	123.92	118.30
1	E	598	ASP	CB-CG-OD1	6.24	123.92	118.30
1	E	514	VAL	CA-CB-CG2	-6.23	101.55	110.90
1	E	210	ARG	NH1-CZ-NH2	6.21	126.24	119.40
1	E	38	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	E	357	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	E	619	ASP	CB-CG-OD1	6.17	123.85	118.30
1	E	615	GLU	OE1-CD-OE2	-6.12	115.95	123.30
1	E	673	PHE	CB-CG-CD2	-6.11	116.53	120.80
1	E	669	PHE	CB-CG-CD1	-6.10	116.53	120.80
1	E	513	LYS	N-CA-CB	6.10	121.58	110.60
1	E	314	PHE	CB-CG-CD1	-6.08	116.54	120.80
1	E	78	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	E	530	VAL	CA-CB-CG1	6.06	119.99	110.90
1	E	310	ALA	CB-CA-C	6.06	119.19	110.10
1	E	90	PHE	CB-CG-CD2	6.06	125.04	120.80
1	E	507	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	E	408	VAL	O-C-N	-6.04	113.03	122.70
1	E	160	ARG	CD-NE-CZ	-5.96	115.26	123.60
1	E	218	GLU	OE1-CD-OE2	-5.94	116.17	123.30
1	E	221	ALA	CB-CA-C	5.92	118.98	110.10
1	E	293	THR	CA-CB-CG2	-5.90	104.14	112.40
1	E	46	HIS	CA-CB-CG	-5.89	103.59	113.60
1	E	562	ASP	CB-CG-OD2	5.89	123.60	118.30
1	E	30	GLU	O-C-N	-5.77	113.47	122.70
1	E	78	ARG	NE-CZ-NH2	5.77	123.18	120.30
1	E	182	ARG	CD-NE-CZ	5.75	131.64	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	568	TYR	CG-CD1-CE1	-5.73	116.72	121.30
1	E	658	ASP	CB-CG-OD2	5.71	123.44	118.30
1	E	628	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	E	109	ASP	CB-CG-OD2	5.66	123.39	118.30
1	E	321	TYR	CB-CG-CD1	5.65	124.39	121.00
1	E	351	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	E	186	TYR	CD1-CE1-CZ	-5.60	114.76	119.80
1	E	672	PHE	CB-CG-CD1	5.58	124.71	120.80
1	E	521	SER	CB-CA-C	-5.57	99.52	110.10
1	E	393	ASP	CB-CG-OD1	-5.57	113.29	118.30
1	E	54	PHE	CB-CG-CD1	-5.55	116.91	120.80
1	E	14	ASN	CA-CB-CG	-5.55	101.19	113.40
1	E	616	TYR	CG-CD1-CE1	-5.55	116.86	121.30
1	E	186	TYR	CG-CD1-CE1	5.54	125.73	121.30
1	E	13	ARG	NE-CZ-NH2	5.53	123.06	120.30
1	E	299	VAL	CB-CA-C	5.53	121.90	111.40
1	E	164	MET	N-CA-CB	-5.52	100.66	110.60
1	E	454	MET	CA-CB-CG	-5.51	103.92	113.30
1	E	485	GLU	CG-CD-OE2	5.51	129.33	118.30
1	E	243	VAL	CA-CB-CG1	5.49	119.13	110.90
1	E	617	MET	CG-SD-CE	-5.49	91.42	100.20
1	E	145	ASP	CB-CG-OD2	5.47	123.22	118.30
1	E	27	THR	OG1-CB-CG2	-5.43	97.51	110.00
1	E	587	SER	N-CA-CB	5.42	118.63	110.50
1	E	69	VAL	CA-CB-CG2	-5.42	102.77	110.90
1	E	212	TYR	CA-CB-CG	-5.41	103.13	113.40
1	E	577	SER	N-CA-CB	5.40	118.60	110.50
1	E	609	GLU	C-N-CA	5.40	135.19	121.70
1	E	682	GLN	CB-CA-C	5.39	121.19	110.40
1	E	207	ASP	O-C-N	-5.39	114.07	122.70
1	E	70	THR	CA-C-N	5.37	129.01	117.20
1	E	220	ALA	CB-CA-C	-5.36	102.06	110.10
1	E	465	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	E	670	VAL	CA-CB-CG1	-5.35	102.87	110.90
1	E	569	ASP	CB-CG-OD2	5.34	123.11	118.30
1	E	324	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	E	7	TYR	CD1-CG-CD2	-5.32	112.05	117.90
1	E	54	PHE	CB-CA-C	5.31	121.03	110.40
1	E	212	TYR	CB-CG-CD1	-5.31	117.81	121.00
1	E	321	TYR	N-CA-CB	5.30	120.14	110.60
1	E	678	GLU	C-N-CA	5.30	134.95	121.70
1	E	95	GLU	CB-CA-C	-5.30	99.80	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	327	PHE	CB-CG-CD1	5.29	124.50	120.80
1	E	21	ILE	CA-CB-CG2	-5.29	100.33	110.90
1	E	507	TYR	CA-CB-CG	5.28	123.43	113.40
1	E	123	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	E	673	PHE	CZ-CE2-CD2	5.25	126.41	120.10
1	E	534	ILE	CA-CB-CG1	5.23	120.94	111.00
1	E	191	ASP	O-C-N	5.23	131.07	122.70
1	E	607	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	E	33	LEU	CB-CG-CD2	5.21	119.86	111.00
1	E	216	LEU	CB-CA-C	5.21	120.11	110.20
1	E	149	VAL	O-C-N	-5.20	114.37	122.70
1	E	653	PHE	CB-CG-CD1	5.19	124.44	120.80
1	E	49	ALA	CB-CA-C	-5.16	102.37	110.10
1	E	215	LYS	N-CA-CB	5.15	119.87	110.60
1	E	188	TYR	CZ-CE2-CD2	5.15	124.43	119.80
1	E	620	VAL	CB-CA-C	5.14	121.17	111.40
1	E	675	HIS	CB-CA-C	-5.14	100.13	110.40
1	E	373	ASP	CA-CB-CG	5.12	124.67	113.40
1	E	248	LYS	C-N-CA	5.12	133.05	122.30
1	E	686	LYS	N-CA-CB	5.10	119.79	110.60
1	E	44	GLU	CB-CA-C	-5.08	100.24	110.40
1	E	123	ARG	CG-CD-NE	-5.07	101.15	111.80
1	E	217	VAL	CA-CB-CG2	-5.04	103.34	110.90
1	E	233	GLU	OE1-CD-OE2	-5.03	117.27	123.30
1	E	627	ARG	NH1-CZ-NH2	5.03	124.93	119.40
1	E	212	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	E	627	ARG	NE-CZ-NH1	-5.01	117.79	120.30
1	E	284	LEU	CB-CG-CD1	-5.00	102.49	111.00

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	108	PHE	Sidechain,Peptide
1	E	11	ARG	Sidechain
1	E	128	TYR	Sidechain
1	E	130	VAL	Peptide
1	E	132	ARG	Sidechain
1	E	151	ARG	Sidechain
1	E	158	GLY	Peptide
1	E	160	ARG	Sidechain,Peptide
1	E	174	PHE	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	E	182	ARG	Sidechain
1	E	212	TYR	Sidechain
1	E	279	TYR	Sidechain
1	E	28	THR	Peptide
1	E	287	PRO	Peptide
1	E	298	VAL	Peptide
1	E	31	ARG	Sidechain
1	E	319	ASP	Peptide
1	E	321	TYR	Sidechain
1	E	329	ARG	Sidechain
1	E	351	ARG	Sidechain
1	E	363	ARG	Peptide
1	E	38	ARG	Sidechain
1	E	39	ILE	Peptide
1	E	394	ALA	Peptide
1	E	430	ARG	Sidechain
1	E	442	THR	Peptide
1	E	45	VAL	Peptide
1	E	453	GLY	Peptide
1	E	468	ARG	Sidechain
1	E	478	LYS	Peptide
1	E	50	ALA	Peptide
1	E	528	ALA	Peptide
1	E	534	ILE	Peptide
1	E	568	TYR	Sidechain
1	E	572	TYR	Sidechain
1	E	60	GLU	Peptide
1	E	607	ARG	Sidechain
1	E	61	ARG	Sidechain
1	E	637	ARG	Sidechain
1	E	652	MET	Peptide
1	E	654	GLY	Peptide
1	E	655	TYR	Sidechain,Peptide
1	E	666	ARG	Sidechain
1	E	676	TYR	Sidechain
1	E	7	TYR	Sidechain
1	E	78	ARG	Sidechain
1	E	91	THR	Mainchain
1	E	99	ARG	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	E	5382	0	5445	66	0
All	All	5382	0	5445	66	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 6.

All (66) 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:E:23:ALA:H	1:E:109:ASP:HB2	1.62	0.65
1:E:487:ILE:HG22	1:E:563:ILE:HG22	1.79	0.64
1:E:210:ARG:HA	1:E:213:HIS:CD2	2.34	0.62
1:E:534:ILE:HG23	1:E:570:GLY:HA3	1.83	0.61
1:E:454:MET:H	1:E:458:HIS:CG	2.20	0.59
1:E:227:ILE:HG23	1:E:237:PRO:HG2	1.85	0.58
1:E:493:VAL:CG2	1:E:593:ALA:HB2	2.33	0.58
1:E:4:LYS:HA	1:E:7:TYR:CD1	2.39	0.56
1:E:143:GLY:H	1:E:171:GLU:CD	2.10	0.55
1:E:302:HIS:H	1:E:332:SER:CB	2.20	0.54
1:E:166:LEU:HD11	1:E:208:GLN:HB3	1.90	0.53
1:E:487:ILE:HD12	1:E:594:VAL:HA	1.91	0.52
1:E:377:VAL:HG21	1:E:380:LEU:HD13	1.92	0.51
1:E:339:SER:H	1:E:352:VAL:HG13	1.75	0.51
1:E:632:LEU:HB2	1:E:644:ARG:HB2	1.93	0.51
1:E:58:GLU:HG2	1:E:64:THR:HA	1.91	0.50
1:E:631:ILE:HG22	1:E:633:GLY:H	1.76	0.49
1:E:508:GLY:HA2	1:E:582:PHE:CD1	2.48	0.49
1:E:350:GLU:HB3	1:E:380:LEU:HD23	1.94	0.48
1:E:46:HIS:CE1	1:E:55:MET:HB2	2.48	0.48
1:E:97:SER:HB3	1:E:101:LEU:HD23	1.96	0.48
1:E:293:THR:CG2	1:E:299:VAL:HG21	2.44	0.48
1:E:487:ILE:CG2	1:E:563:ILE:HG22	2.44	0.47
1:E:220:ALA:HB1	1:E:227:ILE:HD13	1.97	0.47
1:E:119:GLU:HA	1:E:122:TRP:CD1	2.50	0.46
1:E:145:ASP:HB3	1:E:148:LEU:HD23	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39:ILE:O	1:E:40:HIS:HB2	2.15	0.46
1:E:454:MET:H	1:E:458:HIS:CD2	2.33	0.46
1:E:377:VAL:HG21	1:E:380:LEU:CD1	2.46	0.46
1:E:541:ALA:HB1	1:E:583:LYS:HB2	1.98	0.46
1:E:556:ILE:HG23	1:E:601:ILE:HD11	1.97	0.45
1:E:602:LEU:HA	1:E:678:GLU:HA	1.98	0.45
1:E:536:LYS:HA	1:E:539:ILE:HG12	1.98	0.45
1:E:151:ARG:HA	1:E:154:GLN:HE21	1.82	0.45
1:E:201:ILE:HG22	1:E:202:PRO:O	2.17	0.45
1:E:602:LEU:HB3	1:E:676:TYR:HB3	1.99	0.44
1:E:74:TRP:HE1	1:E:274:ASP:CG	2.21	0.44
1:E:210:ARG:HA	1:E:213:HIS:HD2	1.81	0.44
1:E:1:MET:HB2	1:E:6:GLU:HB3	2.00	0.44
1:E:260:LEU:HD13	1:E:260:LEU:N	2.33	0.44
1:E:493:VAL:HG21	1:E:593:ALA:HB2	1.99	0.43
1:E:44:GLU:HG2	1:E:67:ALA:H	1.83	0.43
1:E:534:ILE:HG22	1:E:582:PHE:HE2	1.83	0.43
1:E:227:ILE:HG23	1:E:237:PRO:CG	2.48	0.42
1:E:53:ASP:HB3	1:E:54:PHE:CE1	2.54	0.42
1:E:114:VAL:HG23	1:E:118:SER:HB3	2.00	0.42
1:E:310:ALA:HB1	1:E:399:LEU:HD11	2.02	0.42
1:E:290:LYS:CG	1:E:298:VAL:HG22	2.48	0.42
1:E:227:ILE:HG23	1:E:237:PRO:CB	2.48	0.42
1:E:219:VAL:O	1:E:222:ASP:HB3	2.19	0.42
1:E:671:MET:HG2	1:E:672:PHE:N	2.35	0.41
1:E:493:VAL:HG22	1:E:593:ALA:HB2	2.01	0.41
1:E:302:HIS:O	1:E:332:SER:HB2	2.20	0.41
1:E:35:TYR:CD1	1:E:266:ASN:HA	2.55	0.41
1:E:487:ILE:CD1	1:E:594:VAL:HA	2.49	0.41
1:E:20:HIS:O	1:E:63:ILE:HD13	2.20	0.41
1:E:305:PRO:HG3	1:E:371:ALA:H	1.86	0.41
1:E:299:VAL:CG2	1:E:395:PRO:HB2	2.51	0.41
1:E:290:LYS:HA	1:E:290:LYS:HD2	1.94	0.41
1:E:188:TYR:HA	1:E:195:ASP:O	2.20	0.41
1:E:500:GLN:HA	1:E:505:GLY:HA2	2.03	0.41
1:E:118:SER:HA	1:E:121:VAL:HG22	2.03	0.40
1:E:341:VAL:O	1:E:349:LYS:HA	2.21	0.40
1:E:116:PRO:O	1:E:119:GLU:HB3	2.22	0.40
1:E:119:GLU:HB2	1:E:156:ARG:HH21	1.87	0.40
1:E:153:MET:SD	1:E:153:MET:C	3.00	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	E	686/688 (100%)	611 (89%)	53 (8%)	22 (3%)	5 5

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	63	ILE
1	E	190	ASN
1	E	304	ASP
1	E	321	TYR
1	E	40	HIS
1	E	66	THR
1	E	110	SER
1	E	142	THR
1	E	189	GLY
1	E	408	VAL
1	E	529	ILE
1	E	530	VAL
1	E	562	ASP
1	E	64	THR
1	E	83	ASP
1	E	308	PRO
1	E	402	ILE
1	E	288	PRO
1	E	195	ASP
1	E	86	GLY
1	E	281	PRO
1	E	39	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	E	579/579 (100%)	498 (86%)	81 (14%)	4 4

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	5	VAL
1	E	7	TYR
1	E	11	ARG
1	E	12	LEU
1	E	25	LYS
1	E	27	THR
1	E	30	GLU
1	E	31	ARG
1	E	32	ILE
1	E	51	THR
1	E	64	THR
1	E	73	PHE
1	E	76	ASP
1	E	87	HIS
1	E	117	GLN
1	E	124	GLN
1	E	141	LYS
1	E	146	LEU
1	E	153	MET
1	E	157	LEU
1	E	181	LEU
1	E	186	TYR
1	E	196	ILE
1	E	197	ARG
1	E	203	GLU
1	E	208	GLN
1	E	210	ARG
1	E	212	TYR
1	E	215	LYS
1	E	231	TYR
1	E	246	ILE
1	E	253	LEU
1	E	255	ILE
1	E	260	LEU
1	E	282	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	289	ILE
1	E	298	VAL
1	E	299	VAL
1	E	300	GLU
1	E	303	PRO
1	E	308	PRO
1	E	312	LEU
1	E	314	PHE
1	E	327	PHE
1	E	365	GLU
1	E	368	GLU
1	E	374	LEU
1	E	382	GLU
1	E	420	ASP
1	E	422	GLU
1	E	438	PHE
1	E	444	PRO
1	E	448	GLN
1	E	452	SER
1	E	454	MET
1	E	456	GLU
1	E	459	LEU
1	E	466	LEU
1	E	468	ARG
1	E	469	GLU
1	E	484	ARG
1	E	496	LYS
1	E	507	TYR
1	E	529	ILE
1	E	534	ILE
1	E	544	LYS
1	E	559	PRO
1	E	563	ILE
1	E	564	LYS
1	E	574	GLU
1	E	582	PHE
1	E	603	GLU
1	E	608	VAL
1	E	615	GLU
1	E	620	VAL
1	E	646	PHE
1	E	655	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	669	PHE
1	E	680	PRO
1	E	682	GLN
1	E	684	GLN

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

Mol	Chain	Res	Type
1	E	20	HIS
1	E	77	HIS
1	E	87	HIS
1	E	154	GLN
1	E	302	HIS
1	E	443	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.