Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Dec 20, 2016 – 05:06 PM EST

PDB ID	:	5MG3
EMDB ID:	:	EMD-3506
Title	:	EM fitted model of bacterial holo-translocon
Authors	:	Schaffitzel, C.; Botte, M.
Deposited on	:	2016-11-20
Resolution	:	14.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

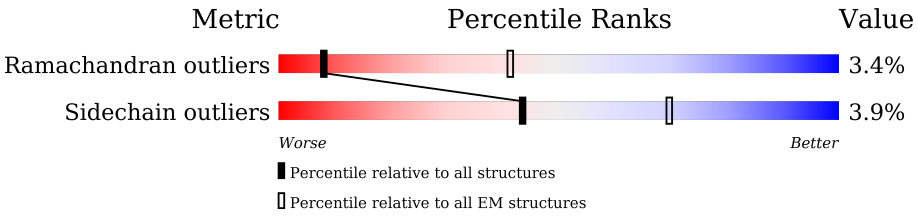
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 14.00 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)
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 <=5%

Mol	Chain	Length	Quality of chain
1	Y	458	70% 22%
2	E	140	33% 11% 54%
3	G	136	20% 76%
4	D	622	53% 11% 33%
5	F	323	68% 17% 5% 11%
6	C	559	63% 16% 19%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 26650 atoms, of which 13553 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 Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	Y	443	7004	2259	3581	566	580	18	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	-14	VAL	-	expression tag	UNP P0AGA2
Y	-13	TRP	-	expression tag	UNP P0AGA2
Y	-12	ASN	-	expression tag	UNP P0AGA2
Y	-11	CYS	-	expression tag	UNP P0AGA2
Y	-10	GLU	-	expression tag	UNP P0AGA2
Y	-9	ARG	-	expression tag	UNP P0AGA2
Y	-8	ILE	-	expression tag	UNP P0AGA2
Y	-7	THR	-	expression tag	UNP P0AGA2
Y	-6	ILE	-	expression tag	UNP P0AGA2
Y	-5	SER	-	expression tag	UNP P0AGA2
Y	-4	HIS	-	expression tag	UNP P0AGA2
Y	-3	ARG	-	expression tag	UNP P0AGA2
Y	-2	LYS	-	expression tag	UNP P0AGA2
Y	-1	GLN	-	expression tag	UNP P0AGA2
Y	0	THR	-	expression tag	UNP P0AGA2

- Molecule 2 is a protein called Protein translocase subunit SecE.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	E	65	1062	332	552	91	86	1	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	369	MET	-	initiating methionine	UNP P0AG96
E	370	HIS	-	expression tag	UNP P0AG96

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Chain	Residue	Modelled	Actual	Comment	Reference
E	371	HIS	-	expression tag	UNP P0AG96
E	372	HIS	-	expression tag	UNP P0AG96
E	373	HIS	-	expression tag	UNP P0AG96
E	374	HIS	-	expression tag	UNP P0AG96
E	375	HIS	-	expression tag	UNP P0AG96
E	376	ASP	-	expression tag	UNP P0AG96
E	377	ASP	-	expression tag	UNP P0AG96
E	378	ASP	-	expression tag	UNP P0AG96
E	379	ASP	-	expression tag	UNP P0AG96
E	380	LYS	-	expression tag	UNP P0AG96
E	381	ALA	-	expression tag	UNP P0AG96
E	382	MET	-	expression tag	UNP P0AG96
E	383	GLY	-	expression tag	UNP P0AG96

- Molecule 3 is a protein called Protein-export membrane protein SecG.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	G	32	Total	C	H	N	O	S	0	0
			480	151	244	39	44	2		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	439	VAL	-	expression tag	UNP P0AG99
G	440	GLY	-	expression tag	UNP P0AG99
G	441	THR	-	expression tag	UNP P0AG99
G	442	GLY	-	expression tag	UNP P0AG99
G	443	TRP	-	expression tag	UNP P0AG99
G	444	TYR	-	expression tag	UNP P0AG99
G	445	SER	-	expression tag	UNP P0AG99
G	446	GLY	-	expression tag	UNP P0AG99
G	447	SER	-	expression tag	UNP P0AG99
G	448	PRO	-	expression tag	UNP P0AG99
G	449	GLY	-	expression tag	UNP P0AG99
G	450	ILE	-	expression tag	UNP P0AG99
G	451	LEU	-	expression tag	UNP P0AG99
G	452	TYR	-	expression tag	UNP P0AG99
G	453	HIS	-	expression tag	UNP P0AG99
G	454	TRP	-	expression tag	UNP P0AG99
G	455	PRO	-	expression tag	UNP P0AG99
G	456	GLU	-	expression tag	UNP P0AG99
G	457	VAL	-	expression tag	UNP P0AG99

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Chain	Residue	Modelled	Actual	Comment	Reference
G	458	LEU	-	expression tag	UNP P0AG99
G	459	ARG	-	expression tag	UNP P0AG99
G	460	ILE	-	expression tag	UNP P0AG99
G	461	GLN	-	expression tag	UNP P0AG99
G	462	GLU	-	expression tag	UNP P0AG99
G	463	LEU	-	expression tag	UNP P0AG99
G	464	ILE	-	expression tag	UNP P0AG99

- Molecule 4 is a protein called Protein translocase subunit SecD.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	414	Total	C	H	N	O	S	0	0
			6419	1991	3291	545	582	10		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	MET	-	initiating methionine	UNP P0AG90
D	-5	HIS	-	expression tag	UNP P0AG90
D	-4	HIS	-	expression tag	UNP P0AG90
D	-3	HIS	-	expression tag	UNP P0AG90
D	-2	HIS	-	expression tag	UNP P0AG90
D	-1	HIS	-	expression tag	UNP P0AG90
D	0	HIS	-	expression tag	UNP P0AG90
D	1	MET	-	expression tag	UNP P0AG90
D	142	VAL	ALA	conflict	UNP P0AG90

- Molecule 5 is a protein called Protein translocase subunit SecF.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	F	289	Total	C	H	N	O	S	0	0
			4502	1434	2291	366	398	13		

- Molecule 6 is a protein called Membrane protein insertase YidC.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	C	455	Total	C	H	N	O	S	0	0
			7183	2336	3594	582	650	21		

There are 17 discrepancies between the modelled and reference sequences:

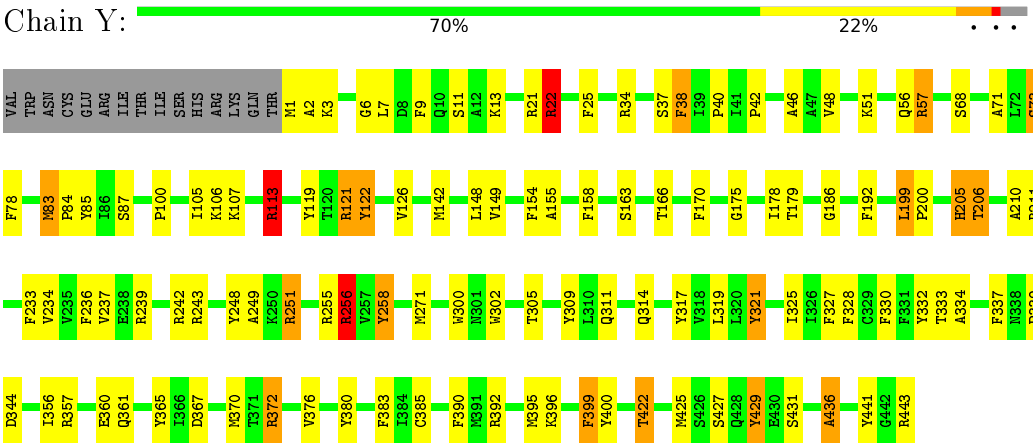
Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	MET	-	initiating methionine	UNP P25714
C	-3	ASP	-	expression tag	UNP P25714
C	-2	PRO	-	expression tag	UNP P25714
C	-1	SER	-	expression tag	UNP P25714
C	0	SER	-	expression tag	UNP P25714
C	1	ARG	-	expression tag	UNP P25714
C	228	ALA	GLU	conflict	UNP P25714
C	229	ALA	LYS	conflict	UNP P25714
C	231	ALA	GLU	conflict	UNP P25714
C	232	ALA	LYS	conflict	UNP P25714
C	234	ALA	LYS	conflict	UNP P25714
C	549	HIS	-	expression tag	UNP P25714
C	550	HIS	-	expression tag	UNP P25714
C	551	HIS	-	expression tag	UNP P25714
C	552	HIS	-	expression tag	UNP P25714
C	553	HIS	-	expression tag	UNP P25714
C	554	HIS	-	expression tag	UNP P25714

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

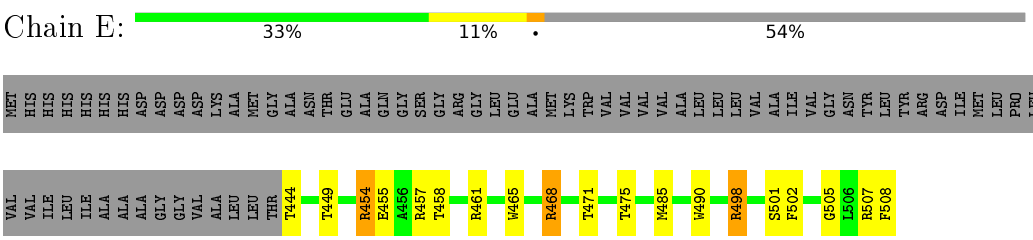
- Molecule 1: Protein translocase subunit SecY

Chain Y:



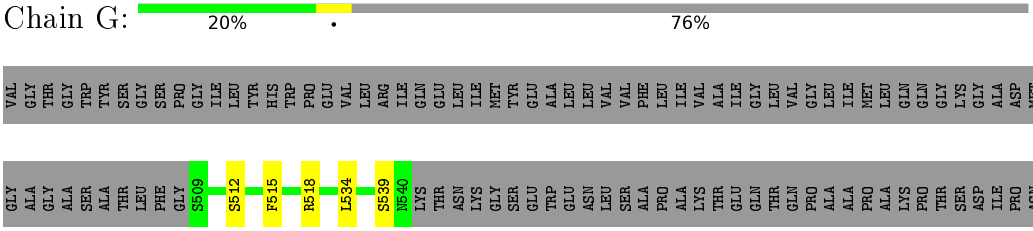
- Molecule 2: Protein translocase subunit SecE

Chain E:



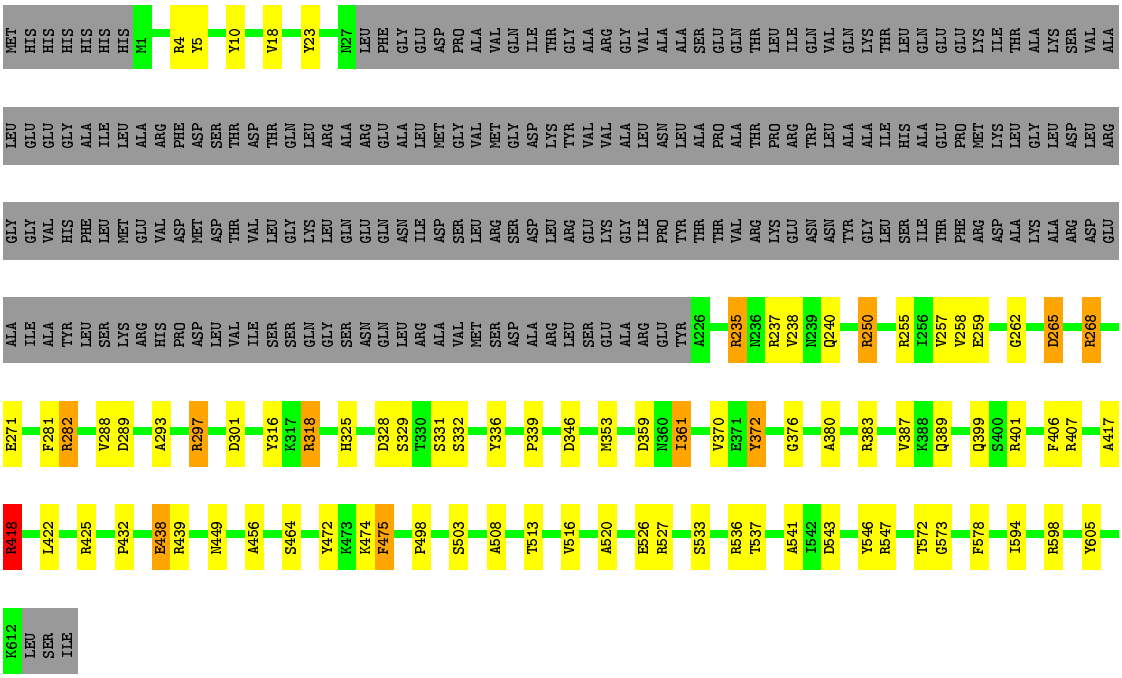
- Molecule 3: Protein-export membrane protein SecG

Chain G:



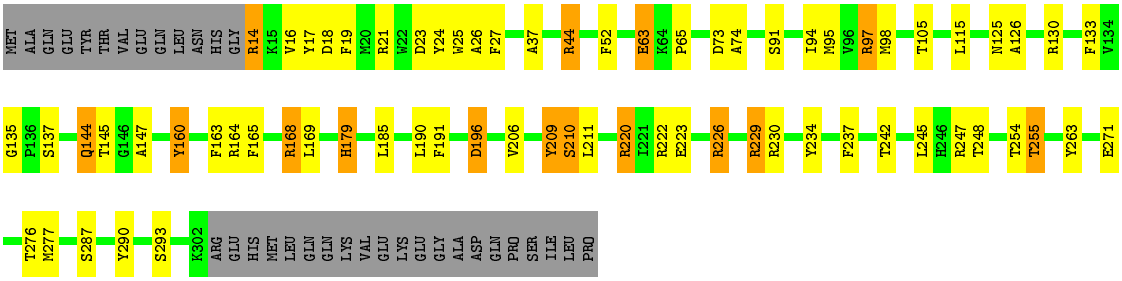
- Molecule 4: Protein translocase subunit SecD

Chain D:



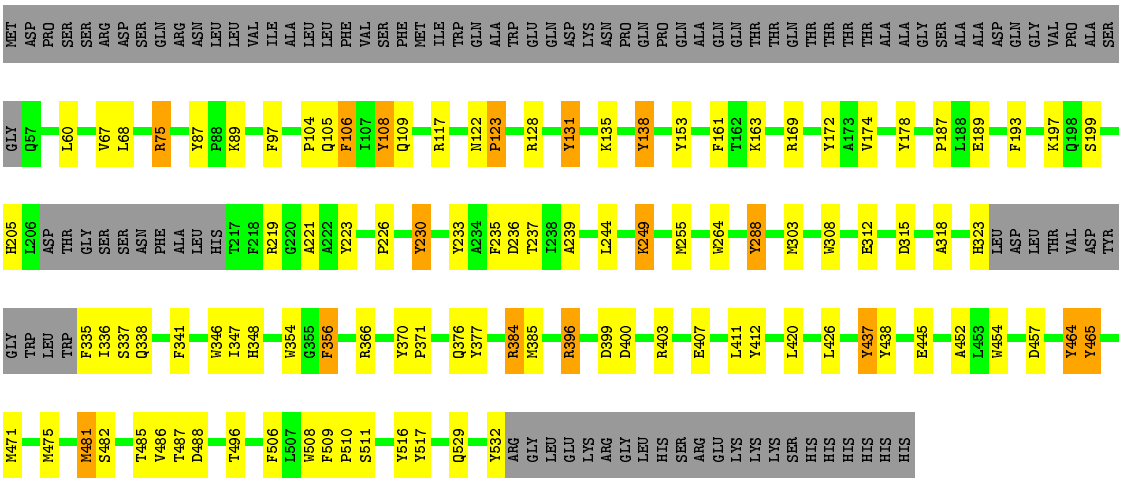
• Molecule 5: Protein translocase subunit SecF

Chain F:



• Molecule 6: Membrane protein insertase YidC

Chain C:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	53648	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	100	Depositor
Electron dose ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality

5.1 Standard geometry

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	Y	2.09	27/3501 (0.8%)	2.13	116/4744 (2.4%)
2	E	1.78	6/518 (1.2%)	2.24	19/702 (2.7%)
3	G	1.72	3/238 (1.3%)	1.91	5/320 (1.6%)
4	D	1.62	20/3163 (0.6%)	2.06	82/4288 (1.9%)
5	F	1.59	4/2250 (0.2%)	2.18	77/3049 (2.5%)
6	C	1.62	16/3683 (0.4%)	1.99	97/5013 (1.9%)
All	All	1.76	76/13353 (0.6%)	2.09	396/18116 (2.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Y	0	11
2	E	0	3
4	D	0	9
5	F	0	13
6	C	0	21
All	All	0	57

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	317	TYR	CG-CD2	35.73	1.85	1.39
1	Y	317	TYR	CG-CD1	34.43	1.83	1.39
1	Y	317	TYR	CE2-CZ	33.58	1.82	1.38
1	Y	317	TYR	CE1-CZ	33.16	1.81	1.38
1	Y	317	TYR	CD1-CE1	23.16	1.74	1.39
1	Y	317	TYR	CD2-CE2	22.28	1.72	1.39
2	E	501	SER	CA-CB	8.63	1.65	1.52
1	Y	68	SER	CA-CB	8.40	1.65	1.52
1	Y	427	SER	CA-CB	8.27	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	383	PHE	CG-CD2	8.03	1.50	1.38
1	Y	87	SER	CA-CB	7.00	1.63	1.52
1	Y	258	TYR	CG-CD2	6.79	1.48	1.39
4	D	533	SER	CA-CB	6.74	1.63	1.52
1	Y	78	PHE	CG-CD1	6.58	1.48	1.38
6	C	407	GLU	CB-CG	6.57	1.64	1.52
4	D	503	SER	CA-CB	6.53	1.62	1.52
6	C	153	TYR	CG-CD1	6.49	1.47	1.39
3	G	539	SER	CA-CB	6.43	1.62	1.52
6	C	178	TYR	CZ-OH	6.23	1.48	1.37
5	F	63	GLU	CD-OE1	6.17	1.32	1.25
6	C	323	HIS	CB-CG	6.16	1.61	1.50
4	D	5	TYR	CE2-CZ	6.14	1.46	1.38
6	C	87	TYR	CG-CD2	6.06	1.47	1.39
6	C	464	TYR	CG-CD2	6.01	1.47	1.39
2	E	505	GLY	CA-C	-5.94	1.42	1.51
2	E	465	TRP	CD2-CE2	5.92	1.48	1.41
5	F	293	SER	CA-CB	5.86	1.61	1.52
4	D	376	GLY	N-CA	5.82	1.54	1.46
4	D	257	VAL	CB-CG1	5.77	1.65	1.52
4	D	526	GLU	CG-CD	5.74	1.60	1.51
4	D	598	ARG	N-CA	5.67	1.57	1.46
3	G	515	PHE	CE2-CZ	5.64	1.48	1.37
6	C	106	PHE	CG-CD1	5.64	1.47	1.38
6	C	108	TYR	CG-CD1	5.63	1.46	1.39
1	Y	332	TYR	CE1-CZ	5.62	1.45	1.38
4	D	331	SER	CB-OG	5.60	1.49	1.42
1	Y	192	PHE	CE2-CZ	5.59	1.48	1.37
1	Y	76	SER	CA-CB	5.59	1.61	1.52
4	D	464	SER	CB-OG	5.58	1.49	1.42
2	E	507	ARG	CZ-NH1	-5.52	1.25	1.33
1	Y	328	PHE	CG-CD1	5.50	1.47	1.38
4	D	546	TYR	CG-CD1	5.49	1.46	1.39
3	G	512	SER	CA-CB	5.47	1.61	1.52
1	Y	42	PRO	N-CD	-5.44	1.40	1.47
1	Y	219	VAL	CA-CB	5.43	1.66	1.54
4	D	262	GLY	N-CA	-5.43	1.38	1.46
6	C	532	TYR	CE2-CZ	5.42	1.45	1.38
6	C	189	GLU	CD-OE1	5.40	1.31	1.25
6	C	354	TRP	C-N	5.37	1.42	1.33
4	D	361	ILE	C-N	5.34	1.42	1.33
1	Y	205	HIS	CA-CB	5.28	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Y	385	CYS	CB-SG	5.27	1.91	1.82
6	C	226	PRO	CA-C	-5.25	1.42	1.52
6	C	445	GLU	CB-CG	5.25	1.62	1.52
1	Y	148	LEU	CB-CG	5.23	1.67	1.52
4	D	598	ARG	CD-NE	5.22	1.55	1.46
1	Y	149	VAL	CA-CB	5.22	1.65	1.54
4	D	573	GLY	N-CA	-5.21	1.38	1.46
5	F	97	ARG	CA-CB	5.19	1.65	1.53
5	F	65	PRO	N-CD	-5.16	1.40	1.47
1	Y	38	PHE	CG-CD1	5.15	1.46	1.38
6	C	138	TYR	CG-CD2	5.13	1.45	1.39
4	D	259	GLU	CD-OE2	5.13	1.31	1.25
4	D	383	ARG	CD-NE	5.12	1.55	1.46
6	C	511	SER	CB-OG	5.11	1.48	1.42
4	D	329	SER	CA-CB	5.09	1.60	1.52
1	Y	385	CYS	N-CA	-5.08	1.36	1.46
1	Y	40	PRO	N-CD	5.07	1.54	1.47
1	Y	396	LYS	CA-CB	5.07	1.65	1.53
6	C	106	PHE	CE1-CZ	5.06	1.47	1.37
4	D	372	TYR	CE2-CZ	5.06	1.45	1.38
4	D	293	ALA	CA-CB	5.05	1.63	1.52
2	E	490	TRP	CZ2-CH2	5.04	1.47	1.37
4	D	238	VAL	CB-CG1	5.03	1.63	1.52
2	E	455	GLU	CD-OE2	5.03	1.31	1.25
1	Y	199	LEU	CA-C	5.02	1.66	1.52

All (396) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	226	ARG	NE-CZ-NH1	28.99	134.80	120.30
4	D	297	ARG	NE-CZ-NH1	22.63	131.61	120.30
1	Y	392	ARG	NE-CZ-NH1	18.04	129.32	120.30
4	D	268	ARG	NE-CZ-NH1	17.26	128.93	120.30
5	F	168	ARG	NE-CZ-NH1	17.14	128.87	120.30
4	D	268	ARG	NE-CZ-NH2	-16.78	111.91	120.30
5	F	168	ARG	NE-CZ-NH2	-16.68	111.96	120.30
4	D	282	ARG	NE-CZ-NH1	16.08	128.34	120.30
4	D	297	ARG	NE-CZ-NH2	-15.60	112.50	120.30
5	F	247	ARG	NE-CZ-NH2	-15.48	112.56	120.30
6	C	75	ARG	NE-CZ-NH1	15.38	127.99	120.30
4	D	407	ARG	NE-CZ-NH1	15.06	127.83	120.30
6	C	384	ARG	NE-CZ-NH2	-14.76	112.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	113	ARG	NE-CZ-NH2	-14.46	113.07	120.30
2	E	502	PHE	CB-CG-CD2	13.37	130.16	120.80
4	D	418	ARG	NE-CZ-NH1	13.30	126.95	120.30
1	Y	25	PHE	CB-CG-CD1	-13.18	111.57	120.80
1	Y	121	ARG	NE-CZ-NH1	13.13	126.87	120.30
1	Y	372	ARG	NE-CZ-NH1	13.10	126.85	120.30
6	C	335	PHE	CB-CG-CD1	12.76	129.73	120.80
2	E	502	PHE	CB-CG-CD1	-12.66	111.94	120.80
1	Y	25	PHE	CB-CG-CD2	12.54	129.58	120.80
4	D	336	TYR	CB-CG-CD2	-12.54	113.47	121.00
5	F	160	TYR	CB-CG-CD1	-12.47	113.52	121.00
4	D	237	ARG	NE-CZ-NH1	12.47	126.53	120.30
1	Y	21	ARG	NE-CZ-NH1	12.40	126.50	120.30
2	E	461	ARG	NE-CZ-NH1	12.25	126.43	120.30
1	Y	256	ARG	NE-CZ-NH1	12.07	126.34	120.30
2	E	457	ARG	NE-CZ-NH2	-12.05	114.28	120.30
4	D	235	ARG	NE-CZ-NH1	12.03	126.31	120.30
5	F	222	ARG	NE-CZ-NH1	11.80	126.20	120.30
5	F	230	ARG	NE-CZ-NH2	-11.66	114.47	120.30
1	Y	34	ARG	NE-CZ-NH1	11.65	126.12	120.30
4	D	406	PHE	CB-CG-CD2	-11.61	112.67	120.80
1	Y	243	ARG	NE-CZ-NH1	11.54	126.07	120.30
6	C	131	TYR	CB-CG-CD2	-11.50	114.10	121.00
1	Y	236	PHE	CB-CG-CD2	-11.50	112.75	120.80
6	C	75	ARG	NE-CZ-NH2	-11.47	114.57	120.30
5	F	24	TYR	CB-CG-CD1	11.30	127.78	121.00
1	Y	400	TYR	CB-CG-CD1	-11.25	114.25	121.00
1	Y	243	ARG	NE-CZ-NH2	-11.22	114.69	120.30
5	F	21	ARG	NE-CZ-NH1	10.77	125.68	120.30
5	F	97	ARG	NE-CZ-NH1	10.72	125.66	120.30
6	C	403	ARG	NE-CZ-NH2	-10.71	114.95	120.30
2	E	454	ARG	NE-CZ-NH2	-10.59	115.00	120.30
1	Y	57	ARG	NE-CZ-NH2	-10.59	115.00	120.30
1	Y	170	PHE	CB-CG-CD1	-10.58	113.40	120.80
1	Y	21	ARG	NE-CZ-NH2	-10.34	115.13	120.30
5	F	18	ASP	CB-CG-OD2	10.34	127.61	118.30
1	Y	392	ARG	NE-CZ-NH2	-10.31	115.15	120.30
1	Y	390	PHE	CB-CG-CD1	-10.26	113.62	120.80
4	D	406	PHE	CB-CG-CD1	10.18	127.93	120.80
1	Y	372	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	Y	357	ARG	NE-CZ-NH2	-10.13	115.24	120.30
1	Y	383	PHE	CB-CG-CD1	10.10	127.87	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	23	TYR	CB-CG-CD2	-10.10	114.94	121.00
5	F	226	ARG	NH1-CZ-NH2	-10.07	108.32	119.40
6	C	131	TYR	CB-CG-CD1	10.01	127.00	121.00
5	F	23	ASP	CB-CG-OD1	9.99	127.29	118.30
1	Y	122	TYR	CB-CG-CD2	-9.93	115.04	121.00
1	Y	251	ARG	NE-CZ-NH1	9.84	125.22	120.30
4	D	250	ARG	NE-CZ-NH1	9.76	125.18	120.30
5	F	255	THR	CA-CB-CG2	-9.73	98.78	112.40
6	C	161	PHE	CB-CG-CD2	9.71	127.60	120.80
5	F	52	PHE	CB-CG-CD1	-9.71	114.00	120.80
1	Y	380	TYR	CB-CG-CD1	9.68	126.81	121.00
4	D	328	ASP	CB-CG-OD2	-9.66	109.60	118.30
5	F	229	ARG	NE-CZ-NH1	9.59	125.10	120.30
6	C	128	ARG	NE-CZ-NH1	9.47	125.03	120.30
2	E	485	MET	CG-SD-CE	-9.45	85.08	100.20
1	Y	365	TYR	CB-CG-CD1	-9.42	115.35	121.00
5	F	21	ARG	NE-CZ-NH2	-9.38	115.61	120.30
4	D	546	TYR	CB-CG-CD1	9.27	126.56	121.00
1	Y	327	PHE	CB-CG-CD2	9.27	127.29	120.80
4	D	598	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	Y	38	PHE	CB-CG-CD2	9.22	127.26	120.80
1	Y	330	PHE	CB-CG-CD1	-9.20	114.36	120.80
1	Y	400	TYR	CB-CG-CD2	9.11	126.46	121.00
6	C	385	MET	CG-SD-CE	-9.11	85.63	100.20
5	F	234	TYR	CB-CG-CD1	-9.08	115.55	121.00
3	G	515	PHE	CB-CG-CD2	-9.06	114.46	120.80
6	C	464	TYR	CB-CG-CD1	9.04	126.43	121.00
1	Y	34	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	Y	365	TYR	CB-CG-CD2	9.02	126.41	121.00
4	D	418	ARG	NE-CZ-NH2	-8.99	115.81	120.30
4	D	281	PHE	CB-CG-CD2	-8.97	114.52	120.80
4	D	372	TYR	CB-CG-CD2	-8.89	115.66	121.00
6	C	370	TYR	CB-CG-CD1	-8.79	115.72	121.00
5	F	14	ARG	NE-CZ-NH2	-8.78	115.91	120.30
5	F	237	PHE	CB-CG-CD2	-8.75	114.68	120.80
4	D	353	MET	CG-SD-CE	-8.72	86.24	100.20
6	C	506	PHE	CB-CG-CD1	-8.69	114.72	120.80
6	C	366	ARG	NE-CZ-NH1	8.68	124.64	120.30
6	C	341	PHE	CB-CG-CD1	8.65	126.86	120.80
2	E	507	ARG	NE-CZ-NH2	-8.64	115.98	120.30
6	C	315	ASP	CB-CG-OD2	-8.54	110.62	118.30
4	D	547	ARG	NE-CZ-NH2	8.52	124.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	383	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	Y	113	ARG	NH1-CZ-NH2	8.45	128.70	119.40
4	D	546	TYR	CB-CG-CD2	-8.39	115.97	121.00
5	F	229	ARG	NE-CZ-NH2	-8.38	116.11	120.30
6	C	233	TYR	CB-CG-CD2	8.37	126.02	121.00
1	Y	211	ARG	NE-CZ-NH1	8.33	124.46	120.30
5	F	277	MET	CG-SD-CE	-8.30	86.92	100.20
5	F	165	PHE	CB-CG-CD2	8.27	126.59	120.80
1	Y	383	PHE	CB-CG-CD2	-8.22	115.04	120.80
5	F	160	TYR	CG-CD2-CE2	-8.20	114.74	121.30
5	F	276	THR	CA-CB-CG2	-8.18	100.95	112.40
5	F	97	ARG	CD-NE-CZ	8.14	135.00	123.60
5	F	24	TYR	CB-CG-CD2	-8.13	116.12	121.00
5	F	163	PHE	CB-CG-CD1	8.11	126.48	120.80
6	C	532	TYR	CG-CD2-CE2	-8.08	114.83	121.30
1	Y	22	ARG	NE-CZ-NH2	-8.08	116.26	120.30
4	D	23	TYR	CB-CG-CD1	7.95	125.77	121.00
1	Y	340	ARG	NE-CZ-NH1	7.90	124.25	120.30
2	E	454	ARG	NE-CZ-NH1	7.88	124.24	120.30
5	F	19	PHE	CB-CG-CD1	7.82	126.28	120.80
6	C	356	PHE	CB-CG-CD1	7.82	126.27	120.80
4	D	439	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	Y	330	PHE	CB-CG-CD2	7.77	126.24	120.80
4	D	255	ARG	NE-CZ-NH1	7.75	124.18	120.30
4	D	472	TYR	CB-CG-CD1	7.73	125.64	121.00
1	Y	121	ARG	NE-CZ-NH2	-7.63	116.49	120.30
4	D	318	ARG	NE-CZ-NH2	7.62	124.11	120.30
4	D	250	ARG	NH1-CZ-NH2	-7.61	111.02	119.40
1	Y	166	THR	CA-CB-CG2	-7.61	101.74	112.40
1	Y	239	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	Y	357	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	Y	300	TRP	CB-CG-CD2	-7.59	116.73	126.60
6	C	178	TYR	CG-CD2-CE2	-7.52	115.28	121.30
5	F	247	ARG	CD-NE-CZ	-7.48	113.12	123.60
6	C	399	ASP	CB-CG-OD1	7.41	124.97	118.30
6	C	396	ARG	NE-CZ-NH2	-7.36	116.62	120.30
5	F	230	ARG	NE-CZ-NH1	7.32	123.96	120.30
4	D	383	ARG	NE-CZ-NH1	7.32	123.96	120.30
6	C	509	PHE	CB-CG-CD1	-7.32	115.68	120.80
4	D	547	ARG	NH1-CZ-NH2	-7.30	111.37	119.40
6	C	396	ARG	NE-CZ-NH1	7.29	123.94	120.30
4	D	598	ARG	NE-CZ-NH1	7.26	123.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	336	TYR	CB-CG-CD1	7.24	125.35	121.00
6	C	236	ASP	CB-CG-OD2	7.18	124.77	118.30
6	C	488	ASP	CB-CG-OD1	7.17	124.76	118.30
1	Y	78	PHE	CB-CG-CD2	7.15	125.81	120.80
6	C	366	ARG	NH1-CZ-NH2	-7.15	111.54	119.40
4	D	328	ASP	CB-CG-OD1	7.12	124.71	118.30
1	Y	192	PHE	CB-CG-CD1	7.08	125.76	120.80
1	Y	158	PHE	CB-CG-CD1	-7.08	115.84	120.80
6	C	230	TYR	CB-CG-CD2	-7.06	116.77	121.00
6	C	356	PHE	CB-CG-CD2	-7.04	115.87	120.80
5	F	105	THR	CA-CB-CG2	7.03	122.24	112.40
6	C	516	TYR	CB-CG-CD2	-7.02	116.79	121.00
4	D	380	ALA	N-CA-CB	-7.02	100.27	110.10
4	D	250	ARG	NE-CZ-NH2	6.99	123.79	120.30
5	F	196	ASP	CB-CG-OD2	6.99	124.59	118.30
6	C	308	TRP	CE3-CZ3-CH2	-6.96	113.54	121.20
6	C	452	ALA	CB-CA-C	-6.95	99.67	110.10
4	D	255	ARG	NH1-CZ-NH2	-6.94	111.77	119.40
6	C	128	ARG	NE-CZ-NH2	-6.93	116.84	120.30
6	C	315	ASP	CB-CG-OD1	6.89	124.50	118.30
1	Y	210	ALA	N-CA-CB	-6.89	100.45	110.10
5	F	226	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	Y	1	MET	CG-SD-CE	-6.83	89.27	100.20
4	D	475	PHE	CB-CG-CD1	-6.83	116.02	120.80
5	F	164	ARG	NE-CZ-NH2	6.79	123.69	120.30
6	C	288	TYR	CB-CG-CD1	-6.79	116.93	121.00
4	D	605	TYR	CB-CG-CD1	-6.78	116.93	121.00
5	F	220	ARG	NE-CZ-NH1	6.78	123.69	120.30
4	D	547	ARG	NE-CZ-NH1	6.76	123.68	120.30
2	E	498	ARG	NE-CZ-NH2	6.74	123.67	120.30
4	D	255	ARG	NE-CZ-NH2	6.68	123.64	120.30
4	D	237	ARG	NE-CZ-NH2	-6.67	116.97	120.30
5	F	191	PHE	CB-CG-CD2	-6.66	116.14	120.80
2	E	461	ARG	NE-CZ-NH2	-6.66	116.97	120.30
5	F	97	ARG	NE-CZ-NH2	-6.64	116.98	120.30
6	C	138	TYR	CZ-CE2-CD2	6.61	125.74	119.80
5	F	44	ARG	NE-CZ-NH2	6.59	123.60	120.30
6	C	233	TYR	CB-CG-CD1	-6.56	117.06	121.00
4	D	541	ALA	N-CA-CB	-6.56	100.91	110.10
6	C	68	LEU	CB-CG-CD1	-6.56	99.85	111.00
4	D	265	ASP	CB-CG-OD1	6.56	124.20	118.30
5	F	263	TYR	CB-CG-CD2	6.50	124.90	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	4	ARG	NE-CZ-NH1	6.50	123.55	120.30
5	F	210	SER	N-CA-CB	6.50	120.25	110.50
6	C	346	TRP	CG-CD1-NE1	6.48	116.58	110.10
1	Y	255	ARG	NE-CZ-NH2	6.41	123.51	120.30
6	C	341	PHE	CB-CG-CD2	-6.41	116.31	120.80
4	D	407	ARG	NH1-CZ-NH2	-6.40	112.36	119.40
1	Y	239	ARG	NE-CZ-NH2	-6.39	117.10	120.30
4	D	543	ASP	CB-CG-OD2	-6.38	112.56	118.30
6	C	438	TYR	CB-CG-CD2	-6.37	117.18	121.00
5	F	95	MET	CG-SD-CE	-6.32	90.08	100.20
6	C	346	TRP	CD1-NE1-CE2	-6.31	103.33	109.00
1	Y	78	PHE	CB-CG-CD1	-6.29	116.40	120.80
3	G	518	ARG	NE-CZ-NH2	-6.28	117.16	120.30
3	G	518	ARG	CD-NE-CZ	6.28	132.39	123.60
6	C	481	MET	N-CA-CB	6.26	121.86	110.60
1	Y	258	TYR	N-CA-CB	6.24	121.84	110.60
5	F	14	ARG	NE-CZ-NH1	6.23	123.42	120.30
6	C	475	MET	CG-SD-CE	-6.22	90.25	100.20
4	D	328	ASP	N-CA-CB	6.21	121.78	110.60
5	F	206	VAL	CG1-CB-CG2	6.21	120.83	110.90
1	Y	170	PHE	CB-CG-CD2	6.20	125.14	120.80
5	F	25	TRP	CD1-CG-CD2	6.18	111.25	106.30
6	C	384	ARG	NH1-CZ-NH2	6.18	126.20	119.40
2	E	465	TRP	CB-CG-CD1	-6.16	119.00	127.00
2	E	468	ARG	CD-NE-CZ	6.15	132.22	123.60
4	D	547	ARG	O-C-N	-6.15	112.74	123.20
6	C	454	TRP	CA-CB-CG	6.14	125.37	113.70
1	Y	199	LEU	N-CA-CB	6.12	122.64	110.40
5	F	25	TRP	CD1-NE1-CE2	6.12	114.50	109.00
5	F	160	TYR	CD1-CG-CD2	6.09	124.60	117.90
6	C	516	TYR	CG-CD2-CE2	-6.08	116.44	121.30
1	Y	249	ALA	N-CA-CB	6.08	118.61	110.10
1	Y	309	TYR	CB-CG-CD1	-6.07	117.36	121.00
4	D	301	ASP	CB-CG-OD1	6.07	123.76	118.30
5	F	163	PHE	CB-CG-CD2	-6.07	116.55	120.80
5	F	242	THR	CA-CB-CG2	-6.06	103.92	112.40
6	C	532	TYR	CB-CG-CD1	-6.04	117.38	121.00
4	D	235	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	Y	73	SER	N-CA-CB	6.02	119.53	110.50
6	C	488	ASP	CB-CG-OD2	-6.00	112.91	118.30
6	C	197	LYS	N-CA-CB	5.97	121.35	110.60
4	D	359	ASP	N-CA-CB	-5.94	99.90	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	11	SER	N-CA-CB	5.94	119.41	110.50
5	F	190	LEU	CB-CG-CD1	5.94	121.09	111.00
4	D	425	ARG	NE-CZ-NH2	-5.93	117.34	120.30
6	C	161	PHE	CB-CG-CD1	-5.93	116.65	120.80
6	C	109	GLN	O-C-N	-5.91	113.25	122.70
5	F	234	TYR	CZ-CE2-CD2	-5.91	114.49	119.80
1	Y	367	ASP	CB-CG-OD2	5.88	123.59	118.30
6	C	471	MET	CA-CB-CG	5.88	123.30	113.30
3	G	515	PHE	CB-CG-CD1	5.87	124.91	120.80
1	Y	441	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	Y	242	ARG	NE-CZ-NH1	5.86	123.23	120.30
6	C	117	ARG	NE-CZ-NH2	5.86	123.23	120.30
6	C	486	VAL	O-C-N	-5.85	113.34	122.70
1	Y	376	VAL	CG1-CB-CG2	5.83	120.23	110.90
4	D	18	VAL	CA-CB-CG2	-5.83	102.16	110.90
5	F	169	LEU	CB-CA-C	-5.82	99.14	110.20
6	C	482	SER	N-CA-CB	5.82	119.22	110.50
1	Y	200	PRO	N-CA-CB	5.81	110.27	103.30
1	Y	425	MET	CG-SD-CE	-5.79	90.93	100.20
4	D	359	ASP	CB-CG-OD2	-5.79	113.09	118.30
4	D	318	ARG	N-CA-CB	5.79	121.02	110.60
1	Y	163	SER	N-CA-CB	5.78	119.17	110.50
1	Y	429	TYR	CG-CD2-CE2	5.78	125.92	121.30
2	E	498	ARG	NH1-CZ-NH2	-5.77	113.06	119.40
2	E	508	PHE	CB-CG-CD1	5.77	124.84	120.80
4	D	572	THR	CA-CB-CG2	-5.76	104.34	112.40
6	C	346	TRP	CD1-CG-CD2	-5.75	101.70	106.30
4	D	406	PHE	CB-CA-C	5.75	121.89	110.40
6	C	264	TRP	NE1-CE2-CD2	5.74	113.04	107.30
4	D	516	VAL	CG1-CB-CG2	-5.74	101.72	110.90
1	Y	233	PHE	CD1-CE1-CZ	5.73	126.98	120.10
5	F	147	ALA	CB-CA-C	5.73	118.69	110.10
1	Y	85	TYR	CB-CG-CD2	5.72	124.43	121.00
4	D	407	ARG	CG-CD-NE	-5.71	99.81	111.80
1	Y	119	TYR	CZ-CE2-CD2	-5.70	114.67	119.80
1	Y	311	GLN	N-CA-CB	-5.70	100.35	110.60
6	C	318	ALA	N-CA-CB	-5.69	102.13	110.10
1	Y	337	PHE	CB-CG-CD2	5.69	124.78	120.80
6	C	239	ALA	C-N-CA	5.67	135.89	121.70
5	F	115	LEU	CB-CG-CD1	-5.66	101.38	111.00
4	D	547	ARG	CA-C-N	5.66	127.51	116.20
6	C	153	TYR	CG-CD1-CE1	-5.63	116.80	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	256	ARG	CG-CD-NE	-5.62	100.00	111.80
1	Y	399	PHE	CB-CG-CD2	-5.62	116.87	120.80
6	C	199	SER	CA-C-O	5.61	131.88	120.10
5	F	145	THR	CA-CB-CG2	-5.60	104.56	112.40
6	C	288	TYR	CG-CD1-CE1	-5.59	116.83	121.30
5	F	126	ALA	CB-CA-C	-5.57	101.75	110.10
1	Y	321	TYR	CB-CG-CD1	5.57	124.34	121.00
1	Y	233	PHE	CG-CD1-CE1	-5.56	114.68	120.80
5	F	196	ASP	CB-CG-OD1	-5.55	113.30	118.30
1	Y	431	SER	N-CA-CB	5.53	118.79	110.50
1	Y	158	PHE	CB-CG-CD2	5.53	124.67	120.80
5	F	94	ILE	O-C-N	-5.52	113.87	122.70
5	F	185	LEU	CB-CG-CD1	5.51	120.37	111.00
5	F	223	GLU	OE1-CD-OE2	-5.51	116.69	123.30
6	C	249	LYS	N-CA-CB	5.50	120.51	110.60
4	D	422	LEU	CB-CA-C	5.49	120.64	110.20
6	C	308	TRP	CG-CD2-CE3	-5.49	128.96	133.90
2	E	498	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	Y	68	SER	N-CA-CB	5.48	118.72	110.50
4	D	282	ARG	NH1-CZ-NH2	-5.48	113.38	119.40
1	Y	248	TYR	CG-CD1-CE1	-5.47	116.92	121.30
5	F	271	GLU	O-C-N	-5.46	113.91	123.20
6	C	465	TYR	CG-CD2-CE2	-5.46	116.93	121.30
6	C	308	TRP	CA-CB-CG	5.45	124.06	113.70
1	Y	300	TRP	CD1-CG-CD2	5.45	110.66	106.30
5	F	25	TRP	CG-CD1-NE1	-5.45	104.65	110.10
1	Y	400	TYR	N-CA-CB	5.44	120.40	110.60
1	Y	256	ARG	NH1-CZ-NH2	-5.44	113.42	119.40
6	C	230	TYR	CD1-CE1-CZ	-5.43	114.91	119.80
5	F	37	ALA	N-CA-CB	-5.43	102.50	110.10
5	F	222	ARG	NH1-CZ-NH2	-5.43	113.43	119.40
1	Y	40	PRO	O-C-N	-5.42	114.03	122.70
1	Y	390	PHE	CB-CG-CD2	5.41	124.59	120.80
6	C	122	ASN	CB-CG-OD1	5.40	132.39	121.60
4	D	456	ALA	CB-CA-C	-5.39	102.01	110.10
6	C	346	TRP	CD2-CE2-CZ2	-5.38	115.84	122.30
5	F	137	SER	N-CA-CB	5.38	118.57	110.50
4	D	536	ARG	CD-NE-CZ	5.38	131.13	123.60
6	C	135	LYS	CB-CA-C	5.37	121.15	110.40
4	D	271	GLU	OE1-CD-OE2	5.37	129.75	123.30
6	C	465	TYR	CB-CG-CD1	-5.37	117.78	121.00
6	C	366	ARG	NE-CZ-NH2	5.37	122.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	412	TYR	CB-CG-CD1	5.37	124.22	121.00
1	Y	344	ASP	O-C-N	-5.36	114.12	122.70
4	D	573	GLY	O-C-N	-5.36	114.12	122.70
6	C	174	VAL	CA-CB-CG2	-5.35	102.87	110.90
6	C	509	PHE	CB-CG-CD2	5.35	124.55	120.80
1	Y	321	TYR	CA-CB-CG	5.35	123.56	113.40
4	D	438	GLU	C-N-CA	5.34	135.06	121.70
5	F	209	TYR	CB-CG-CD2	-5.34	117.80	121.00
6	C	464	TYR	N-CA-CB	5.34	120.22	110.60
5	F	247	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	Y	255	ARG	NH1-CZ-NH2	-5.33	113.53	119.40
1	Y	436	ALA	O-C-N	-5.33	114.17	122.70
4	D	513	THR	N-CA-CB	5.33	120.44	110.30
5	F	26	ALA	N-CA-CB	5.33	117.57	110.10
6	C	108	TYR	CB-CG-CD2	5.33	124.20	121.00
1	Y	192	PHE	CB-CG-CD2	-5.33	117.07	120.80
1	Y	443	ARG	NE-CZ-NH1	-5.32	117.64	120.30
4	D	425	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	Y	83	MET	CG-SD-CE	-5.31	91.70	100.20
3	G	534	LEU	CB-CG-CD2	5.31	120.03	111.00
6	C	123	PRO	N-CA-CB	-5.31	96.76	102.60
6	C	338	GLN	CA-C-N	5.31	131.96	117.10
2	E	457	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	Y	333	THR	C-N-CA	5.30	134.96	121.70
1	Y	367	ASP	CB-CG-OD1	-5.29	113.54	118.30
5	F	144	GLN	CB-CG-CD	5.28	125.34	111.60
4	D	370	VAL	CA-CB-CG1	-5.28	102.98	110.90
6	C	153	TYR	CD1-CE1-CZ	5.28	124.55	119.80
6	C	255	MET	CG-SD-CE	5.27	108.63	100.20
6	C	346	TRP	CH2-CZ2-CE2	5.27	122.67	117.40
2	E	485	MET	N-CA-CB	5.26	120.07	110.60
4	D	289	ASP	CB-CG-OD1	5.26	123.03	118.30
6	C	221	ALA	N-CA-CB	-5.26	102.74	110.10
6	C	370	TYR	CG-CD2-CE2	-5.26	117.09	121.30
1	Y	107	LYS	N-CA-CB	5.25	120.06	110.60
1	Y	319	LEU	O-C-N	-5.25	114.30	122.70
6	C	68	LEU	CB-CG-CD2	5.25	119.92	111.00
6	C	437	TYR	O-C-N	-5.24	114.32	122.70
1	Y	175	GLY	O-C-N	-5.24	114.32	122.70
1	Y	37	SER	N-CA-CB	5.22	118.34	110.50
1	Y	57	ARG	NE-CZ-NH1	5.22	122.91	120.30
4	D	456	ALA	N-CA-CB	5.22	117.41	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	508	TRP	CH2-CZ2-CE2	5.21	122.61	117.40
1	Y	325	ILE	CG1-CB-CG2	-5.20	99.95	111.40
1	Y	271	MET	CG-SD-CE	-5.20	91.88	100.20
6	C	60	LEU	CB-CG-CD2	5.19	119.82	111.00
1	Y	38	PHE	CB-CG-CD1	-5.19	117.17	120.80
6	C	178	TYR	CD1-CG-CD2	5.19	123.60	117.90
6	C	336	ILE	C-N-CA	5.18	134.65	121.70
5	F	27	PHE	CB-CG-CD1	5.17	124.42	120.80
5	F	248	THR	CA-CB-CG2	5.16	119.63	112.40
5	F	165	PHE	CB-CG-CD1	-5.15	117.19	120.80
5	F	17	TYR	CB-CG-CD1	-5.15	117.91	121.00
1	Y	339	PRO	O-C-N	-5.14	114.48	122.70
5	F	73	ASP	CB-CA-C	5.13	120.66	110.40
5	F	226	ARG	CG-CD-NE	-5.13	101.03	111.80
1	Y	429	TYR	CB-CG-CD1	5.11	124.06	121.00
6	C	106	PHE	CG-CD2-CE2	5.10	126.41	120.80
6	C	235	PHE	CB-CG-CD2	5.10	124.37	120.80
1	Y	258	TYR	CZ-CE2-CD2	5.09	124.39	119.80
4	D	527	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	Y	84	PRO	N-CA-CB	5.08	109.40	103.30
1	Y	155	ALA	N-CA-CB	5.07	117.20	110.10
1	Y	186	GLY	O-C-N	-5.07	114.59	122.70
1	Y	422	THR	OG1-CB-CG2	-5.07	98.34	110.00
4	D	508	ALA	N-CA-CB	-5.07	103.01	110.10
5	F	52	PHE	CB-CG-CD2	5.07	124.35	120.80
1	Y	327	PHE	CB-CG-CD1	-5.07	117.25	120.80
4	D	594	ILE	CA-CB-CG1	5.07	120.62	111.00
6	C	237	THR	N-CA-CB	5.06	119.92	110.30
6	C	264	TRP	CG-CD2-CE3	-5.06	129.34	133.90
4	D	422	LEU	CB-CG-CD1	5.06	119.60	111.00
1	Y	429	TYR	CG-CD1-CE1	-5.06	117.25	121.30
1	Y	311	GLN	CB-CA-C	5.05	120.51	110.40
6	C	193	PHE	CG-CD2-CE2	5.05	126.36	120.80
1	Y	380	TYR	CB-CG-CD2	-5.05	117.97	121.00
2	E	471	THR	O-C-N	-5.05	114.63	122.70
6	C	163	LYS	N-CA-CB	-5.05	101.52	110.60
2	E	444	THR	CA-CB-OG1	5.04	119.59	109.00
4	D	332	SER	N-CA-C	-5.04	97.38	111.00
4	D	401	ARG	NE-CZ-NH2	5.04	122.82	120.30
4	D	520	ALA	CB-CA-C	-5.03	102.56	110.10
1	Y	2	ALA	CB-CA-C	-5.02	102.56	110.10
1	Y	395	MET	CG-SD-CE	-5.02	92.17	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	443	ARG	CD-NE-CZ	5.02	130.62	123.60
4	D	449	ASN	CB-CG-OD1	-5.01	111.58	121.60
5	F	74	ALA	N-CA-CB	-5.01	103.08	110.10
1	Y	234	VAL	CA-CB-CG2	-5.01	103.39	110.90
1	Y	211	ARG	NH1-CZ-NH2	-5.01	113.89	119.40

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	C	108	TYR	Sidechain
6	C	131	TYR	Sidechain
6	C	138	TYR	Sidechain
6	C	169	ARG	Sidechain
6	C	172	TYR	Sidechain
6	C	205	HIS	Mainchain
6	C	219	ARG	Sidechain
6	C	223	TYR	Sidechain
6	C	230	TYR	Sidechain
6	C	288	TYR	Sidechain
6	C	356	PHE	Sidechain
6	C	377	TYR	Sidechain
6	C	384	ARG	Sidechain
6	C	396	ARG	Sidechain
6	C	437	TYR	Sidechain
6	C	464	TYR	Sidechain
6	C	465	TYR	Sidechain
6	C	496	THR	Mainchain
6	C	517	TYR	Sidechain
6	C	75	ARG	Sidechain
6	C	97	PHE	Sidechain
4	D	10	TYR	Sidechain
4	D	250	ARG	Sidechain
4	D	268	ARG	Sidechain
4	D	282	ARG	Sidechain
4	D	316	TYR	Sidechain
4	D	372	TYR	Sidechain
4	D	387	VAL	Peptide
4	D	418	ARG	Sidechain
4	D	578	PHE	Sidechain
2	E	454	ARG	Sidechain
2	E	468	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	E	498	ARG	Sidechain
5	F	130	ARG	Sidechain
5	F	133	PHE	Sidechain
5	F	135	GLY	Peptide
5	F	160	TYR	Sidechain
5	F	168	ARG	Sidechain
5	F	179	HIS	Sidechain
5	F	209	TYR	Sidechain,Peptide
5	F	226	ARG	Sidechain
5	F	229	ARG	Sidechain
5	F	287	SER	Peptide
5	F	290	TYR	Sidechain
5	F	44	ARG	Sidechain
1	Y	113	ARG	Sidechain
1	Y	122	TYR	Sidechain
1	Y	154	PHE	Sidechain
1	Y	206	THR	Peptide
1	Y	22	ARG	Sidechain
1	Y	256	ARG	Sidechain
1	Y	372	ARG	Sidechain
1	Y	38	PHE	Sidechain
1	Y	399	PHE	Sidechain
1	Y	429	TYR	Sidechain
1	Y	7	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Y	3423	3581	3583	0	0
2	E	510	552	551	0	0
3	G	236	244	243	0	0
4	D	3128	3291	3292	0	0
5	F	2211	2291	2290	0	0
6	C	3589	3594	3591	0	0
All	All	13097	13553	13550	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	Y	441/458 (96%)	367 (83%)	50 (11%)	24 (5%)	2 29
2	E	63/140 (45%)	57 (90%)	5 (8%)	1 (2%)	12 56
3	G	30/136 (22%)	29 (97%)	1 (3%)	0	100 100
4	D	410/622 (66%)	373 (91%)	25 (6%)	12 (3%)	6 43
5	F	287/323 (89%)	257 (90%)	24 (8%)	6 (2%)	9 50
6	C	449/559 (80%)	395 (88%)	40 (9%)	14 (3%)	5 42
All	All	1680/2238 (75%)	1478 (88%)	145 (9%)	57 (3%)	8 40

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	48	VAL
1	Y	71	ALA
1	Y	113	ARG
1	Y	199	LEU
1	Y	305	THR
1	Y	341	GLU
4	D	318	ARG
4	D	389	GLN
4	D	537	THR
5	F	196	ASP
5	F	210	SER
6	C	337	SER
1	Y	57	ARG
1	Y	73	SER

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Mol	Chain	Res	Type
1	Y	258	TYR
2	E	449	THR
4	D	240	GLN
4	D	258	VAL
4	D	265	ASP
4	D	399	GLN
4	D	475	PHE
5	F	125	ASN
5	F	211	LEU
6	C	312	GLU
6	C	348	HIS
6	C	411	LEU
6	C	426	LEU
1	Y	22	ARG
1	Y	105	ILE
1	Y	205	HIS
1	Y	206	THR
1	Y	334	ALA
1	Y	343	ALA
1	Y	360	GLU
4	D	325	HIS
4	D	346	ASP
6	C	244	LEU
6	C	347	ILE
6	C	457	ASP
1	Y	46	ALA
1	Y	314	GLN
1	Y	436	ALA
4	D	417	ALA
5	F	16	VAL
5	F	91	SER
6	C	106	PHE
6	C	481	MET
1	Y	142	MET
1	Y	251	ARG
6	C	485	THR
6	C	105	GLN
6	C	420	LEU
4	D	288	VAL
1	Y	100	PRO
1	Y	356	ILE
6	C	371	PRO

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Mol	Chain	Res	Type
1	Y	6	GLY

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	Y	359/374 (96%)	338 (94%)	21 (6%)	25 61
2	E	54/110 (49%)	52 (96%)	2 (4%)	41 73
3	G	27/106 (26%)	27 (100%)	0	100 100
4	D	337/509 (66%)	328 (97%)	9 (3%)	52 79
5	F	237/267 (89%)	227 (96%)	10 (4%)	36 70
6	C	387/475 (82%)	375 (97%)	12 (3%)	47 77
All	All	1401/1841 (76%)	1347 (96%)	54 (4%)	43 72

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	3	LYS
1	Y	9	PHE
1	Y	13	LYS
1	Y	51	LYS
1	Y	56	GLN
1	Y	74	ARG
1	Y	83	MET
1	Y	106	LYS
1	Y	121	ARG
1	Y	126	VAL
1	Y	178	ILE
1	Y	179	THR
1	Y	216	HIS
1	Y	237	VAL
1	Y	256	ARG
1	Y	302	TRP
1	Y	321	TYR

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Mol	Chain	Res	Type
1	Y	340	ARG
1	Y	361	GLN
1	Y	370	MET
1	Y	422	THR
2	E	458	THR
2	E	475	THR
4	D	235	ARG
4	D	297	ARG
4	D	339	PRO
4	D	361	ILE
4	D	418	ARG
4	D	432	PRO
4	D	438	GLU
4	D	474	LYS
4	D	498	PRO
5	F	14	ARG
5	F	63	GLU
5	F	97	ARG
5	F	98	MET
5	F	144	GLN
5	F	179	HIS
5	F	220	ARG
5	F	245	LEU
5	F	254	THR
5	F	255	THR
6	C	67	VAL
6	C	89	LYS
6	C	104	PRO
6	C	123	PRO
6	C	187	PRO
6	C	249	LYS
6	C	303	MET
6	C	376	GLN
6	C	400	ASP
6	C	487	THR
6	C	510	PRO
6	C	529	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.