

Nov 20, 2022 - 07:00 am GMT

PDB ID	:	6H6E
EMDB ID	:	EMD-0149
Title	:	PTC3 holotoxin complex from Photorhabdus luminecens in prepore state
		(TcdA1, TcdB2, TccC3)
Authors	:	Gatsogiannis, C.; Merino, F.; Roderer, D.; Balchin, D.; Schubert, E.; Kuhlee,
		A.; Hayer-Hartl, M.; Raunser, S.
Deposited on	:	2018-07-27
Resolution	:	3.95 Å(reported)
Based on initial models	:	4O9X, 1VW1

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/EMValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.1. dev 43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.95 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.



Matria	Whole archive	EM structures
Metric	$(\# {\rm Entries})$	$(\# {\rm Entries})$
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for $\geq=3, 2, 1$ and 0 types of geometric quality criteria respectively. 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 $\leq=5\%$ The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain		
1		0510	· •		_
	А	2516	89%	6%	•
	-				_
1	В	2516	90%	6%	•
1	С	2516	90%	6%	·
					_
1	D	2516	89%	7%	·
1	Ε	2516	89%	6%	•
			-		
2	F	2434	81% 7%	12%	6



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 112922 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.

Mol	Chain	Residues		At	AltConf	Trace			
1	Δ	2417	Total	С	Ν	Ο	S	0	0
1	Л	2417	19161	12136	3248	3716	61	0	0
1	Р	9417	Total	С	Ν	Ο	S	0	0
I D	2417	19161	12136	3248	3716	61	0	0	
1	1 0	2417	Total	С	Ν	Ο	S	0	0
1			19161	12136	3248	3716	61	0	0
1	П	9417	Total	С	Ν	Ο	S	0	0
	2417	19161	12136	3248	3716	61	0	0	
1 1	F	9417	Total	С	Ν	Ο	S	0	0
		2411	19161	12136	3248	3716	61	0	0

• Molecule 1 is a protein called TcdA1.

• Molecule 2 is a protein called TcdB2,TccC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	2146	Total 17117	C 10722	N 3038	O 3322	S 35	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: TcdA1



• Molecule 1: TcdA1















A2404 A2404 B2428 C2458 A2513 A2513 A2005 C2005 C2005 C2005 C2005 C2005 C2005 C2005 C2005 C2005 C2018 C2065 R2085 R2085 R2085 R2085 R2085 R2085 R2145 R2145

• Molecule 2: TcdB2,TccC3





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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	89148	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	2.2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II $(4k \times 4k)$	Depositor
Maximum map value	0.124	Depositor
Minimum map value	-0.137	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	547.2, 547.2, 547.2	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.14, 1.14, 1.14	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	B	Bond lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	1.14	53/19574~(0.3%)	0.95	49/26589~(0.2%)	
1	В	1.13	47/19574~(0.2%)	0.94	56/26589~(0.2%)	
1	С	1.13	43/19574~(0.2%)	0.95	58/26589~(0.2%)	
1	D	1.12	44/19574~(0.2%)	0.96	73/26589~(0.3%)	
1	Е	1.12	40/19574~(0.2%)	0.96	63/26589~(0.2%)	
2	F	1.13	34/17538~(0.2%)	1.02	74/23909~(0.3%)	
All	All	1.13	261/115408~(0.2%)	0.96	373/156854~(0.2%)	

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	В	968	TYR	CG-CD1	-9.63	1.26	1.39
1	D	968	TYR	CG-CD1	-9.11	1.27	1.39
1	А	103	TYR	CB-CG	-8.09	1.39	1.51
1	С	103	TYR	CB-CG	-7.53	1.40	1.51
1	А	1769	TRP	CB-CG	-7.52	1.36	1.50
1	С	1769	TRP	CB-CG	-7.45	1.36	1.50
1	Е	1853	PHE	CB-CG	-7.34	1.38	1.51
1	Е	1005	GLU	CG-CD	-7.26	1.41	1.51
1	D	103	TYR	CB-CG	-7.16	1.41	1.51
2	F	135	GLU	CG-CD	-7.14	1.41	1.51
1	В	344	GLU	CD-OE2	-7.03	1.18	1.25
1	В	1154	TYR	CB-CG	-6.95	1.41	1.51
1	В	204	TYR	CG-CD1	-6.94	1.30	1.39
1	А	915	TRP	CB-CG	-6.87	1.37	1.50
2	F	1555	PHE	CB-CG	-6.83	1.39	1.51
1	D	1805	TYR	CB-CG	-6.78	1.41	1.51
1	Е	1236	CYS	CB-SG	-6.78	1.70	1.82
1	С	1168	TYR	CB-CG	-6.78	1.41	1.51
1	С	353	TYR	CB-CG	-6.74	1.41	1.51
1	А	182	TYR	CB-CG	-6.70	1.41	1.51
1	D	1042	GLU	CD-OE2	-6.64	1.18	1.25
1	С	2251	TYR	CB-CG	-6.58	1.41	1.51

All (261) bond length outliers are listed below:



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	264	TYR	CB-CG	-6.54	1.41	1.51
1	А	1122	TYR	CB-CG	-6.54	1.41	1.51
1	D	2297	TRP	CB-CG	-6.50	1.38	1.50
1	А	640	TRP	CB-CG	-6.49	1.38	1.50
1	Е	353	TYR	CB-CG	-6.46	1.42	1.51
2	F	2075	GLU	CD-OE1	-6.43	1.18	1.25
1	С	264	TYR	CB-CG	-6.37	1.42	1.51
1	D	204	TYR	CG-CD1	-6.36	1.30	1.39
2	F	1585	ARG	CG-CD	-6.35	1.36	1.51
1	D	1218	ASN	CB-CG	-6.34	1.36	1.51
2	F	1840	TYR	CB-CG	-6.34	1.42	1.51
1	Е	515	PHE	CB-CG	-6.32	1.40	1.51
1	Е	1769	TRP	CB-CG	-6.31	1.38	1.50
1	А	344	GLU	CD-OE2	-6.31	1.18	1.25
1	С	1660	TRP	CB-CG	-6.31	1.38	1.50
1	В	1268	TYR	CB-CG	-6.30	1.42	1.51
1	А	1268	TYR	CB-CG	-6.27	1.42	1.51
1	С	2096	PHE	CB-CG	-6.27	1.40	1.51
1	D	640	TRP	CB-CG	-6.27	1.39	1.50
1	Е	103	TYR	CB-CG	-6.26	1.42	1.51
1	А	1664	TYR	CB-CG	-6.25	1.42	1.51
1	В	103	TYR	CB-CG	-6.21	1.42	1.51
1	А	348	PHE	CB-CG	-6.18	1.40	1.51
2	F	2119	TYR	CB-CG	-6.15	1.42	1.51
1	С	1236	CYS	CB-SG	-6.15	1.71	1.82
1	С	268	PHE	CB-CG	-6.14	1.41	1.51
1	A	1805	TYR	CB-CG	-6.11	1.42	1.51
2	F	102	GLU	CD-OE2	-6.11	1.19	1.25
1	A	264	TYR	CB-CG	-6.10	1.42	1.51
1	В	1769	TRP	CB-CG	-6.09	1.39	1.50
1	Е	640	TRP	CB-CG	-6.09	1.39	1.50
1	С	1110	PHE	CB-CG	-6.09	1.41	1.51
2	F	1849	GLU	CD-OE1	-6.06	1.19	1.25
2	F	1970	GLU	CD-OE2	-6.04	1.19	1.25
1	В	2330	GLU	CD-OE2	-6.03	1.19	1.25
1	A	109	VAL	CB-CG2	-6.03	1.40	1.52
1	D	2103	TYR	CB-CG	-6.03	1.42	1.51
1	A	515	PHE	CB-CG	-6.00	1.41	1.51
1	E	2143	ASN	CB-CG	-5.99	1.37	1.51
1	D	2096	PHE	CB-CG	-5.98	1.41	1.51
1	C	1005	GLU	CD-OE1	-5.98	1.19	1.25
1	В	1816	TRP	CB-CG	-5.94	1.39	1.50



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	2277	GLU	CD-OE2	-5.93	1.19	1.25
2	F	1746	GLU	CD-OE1	-5.93	1.19	1.25
1	Е	268	PHE	CB-CG	-5.92	1.41	1.51
1	В	204	TYR	CB-CG	-5.91	1.42	1.51
1	Е	92	TYR	CB-CG	-5.90	1.42	1.51
2	F	1425	TYR	CB-CG	-5.89	1.42	1.51
1	D	1664	TYR	CB-CG	-5.84	1.42	1.51
1	В	264	TYR	CB-CG	-5.84	1.42	1.51
1	Е	1800	TRP	NE1-CE2	-5.84	1.29	1.37
1	В	1005	GLU	CD-OE1	-5.82	1.19	1.25
1	А	1168	TYR	CB-CG	-5.82	1.43	1.51
2	F	26	GLU	CD-OE2	-5.81	1.19	1.25
1	В	1634	GLU	CD-OE1	-5.80	1.19	1.25
1	С	589	TYR	CG-CD2	-5.80	1.31	1.39
1	D	1149	CYS	CB-SG	-5.80	1.72	1.81
1	А	1634	GLU	CD-OE1	-5.80	1.19	1.25
1	D	1236	CYS	CB-SG	-5.79	1.72	1.81
1	D	2240	PHE	CB-CG	-5.78	1.41	1.51
1	D	1470	TYR	CB-CG	-5.76	1.43	1.51
1	Е	705	GLU	CD-OE2	-5.75	1.19	1.25
1	D	1168	TYR	CB-CG	-5.73	1.43	1.51
1	D	2017	TRP	CB-CG	-5.72	1.40	1.50
1	Е	1634	GLU	CD-OE2	-5.71	1.19	1.25
1	С	2147	PHE	CG-CD2	-5.70	1.30	1.38
1	В	640	TRP	CB-CG	-5.69	1.40	1.50
1	С	483	TYR	CB-CG	-5.68	1.43	1.51
2	F	198	GLU	CD-OE1	-5.68	1.19	1.25
1	С	344	GLU	CD-OE2	-5.67	1.19	1.25
1	А	2513	TYR	CB-CG	-5.67	1.43	1.51
1	В	2283	GLU	CD-OE1	-5.66	1.19	1.25
2	F	1128	TYR	CE1-CZ	-5.66	1.31	1.38
2	F	1446	TRP	CZ3-CH2	-5.66	1.31	1.40
1	В	353	TYR	CB-CG	-5.65	1.43	1.51
1	В	705	GLU	CD-OE2	-5.65	1.19	1.25
1	В	1847	HIS	CB-CG	-5.64	1.39	1.50
2	F	55	PHE	CB-CG	-5.63	1.41	1.51
1	С	738	TYR	CB-CG	-5.63	1.43	1.51
2	F	367	GLU	CD-OE1	-5.63	1.19	1.25
2	F	190	GLU	CD-OE2	-5.62	1.19	1.25
1	Е	1005	GLU	CD-OE1	-5.62	1.19	1.25
1	С	2393	PHE	CB-CG	-5.61	1.41	1.51
1	D	659	TYR	CB-CG	-5.61	1.43	1.51



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	136	TYR	CB-CG	-5.60	1.43	1.51
1	С	1283	SER	CB-OG	-5.59	1.34	1.42
2	F	1437	GLU	CG-CD	-5.58	1.43	1.51
1	Е	1768	PHE	CB-CG	-5.58	1.41	1.51
1	D	1634	GLU	CD-OE2	-5.58	1.19	1.25
1	А	377	GLU	CD-OE1	-5.55	1.19	1.25
1	С	2330	GLU	CD-OE1	-5.54	1.19	1.25
1	А	1310	TYR	CB-CG	-5.52	1.43	1.51
1	Е	2400	GLU	CD-OE1	-5.52	1.19	1.25
1	В	1002	GLU	CD-OE2	-5.52	1.19	1.25
1	В	483	TYR	CB-CG	-5.51	1.43	1.51
1	А	429	GLU	CD-OE2	-5.50	1.19	1.25
1	Е	348	PHE	CB-CG	-5.50	1.42	1.51
1	Е	1139	ASN	CB-CG	-5.50	1.38	1.51
1	А	2159	GLU	CD-OE1	-5.49	1.19	1.25
1	С	705	GLU	CD-OE2	-5.49	1.19	1.25
2	F	1162	VAL	CB-CG1	-5.49	1.41	1.52
1	Е	1721	TRP	CB-CG	-5.48	1.40	1.50
1	С	1634	GLU	CD-OE2	-5.47	1.19	1.25
1	В	328	TYR	CB-CG	-5.46	1.43	1.51
1	D	1039	TYR	CB-CG	-5.46	1.43	1.51
1	D	1555	PHE	CB-CG	-5.46	1.42	1.51
2	F	771	TRP	CB-CG	-5.46	1.40	1.50
1	Е	344	GLU	CD-OE2	-5.46	1.19	1.25
2	F	779	ARG	CZ-NH1	-5.46	1.25	1.33
1	С	1168	TYR	CG-CD1	-5.45	1.32	1.39
1	E	1634	GLU	CD-OE1	-5.43	1.19	1.25
1	A	1567	TYR	CB-CG	-5.42	1.43	1.51
1	В	2240	PHE	CB-CG	-5.42	1.42	1.51
1	С	2147	PHE	CB-CG	-5.42	1.42	1.51
1	D	2308	GLU	CD-OE1	-5.41	1.19	1.25
1	D	141	ARG	CG-CD	-5.40	1.38	1.51
1	D	2143	ASN	CB-CG	-5.40	1.38	1.51
1	D	915	TRP	CB-CG	-5.40	1.40	1.50
1	С	2297	TRP	CB-CG	-5.40	1.40	1.50
1	A	137	TYR	CB-CG	-5.39	1.43	1.51
2	F	1746	GLU	CD-OE2	-5.39	1.19	1.25
1	E	810	TRP	CB-CG	-5.38	1.40	1.50
1	A	1430	TYR	CB-CG	-5.38	1.43	1.51
1	В	1109	TYR	CB-CG	-5.38	1.43	1.51
1	В	1536	GLU	CD-OE2	-5.38	1.19	1.25
1	В	2318	GLU	CD-OE2	-5.38	1.19	1.25



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	С	1364	TYR	CB-CG	-5.37	1.43	1.51
1	А	1951	GLN	CG-CD	-5.37	1.38	1.51
2	F	339	GLU	CD-OE2	-5.36	1.19	1.25
1	С	1664	TYR	CG-CD2	-5.35	1.32	1.39
1	D	937	PHE	CB-CG	-5.35	1.42	1.51
2	F	1527	TYR	CB-CG	-5.34	1.43	1.51
1	В	1430	TYR	CB-CG	-5.34	1.43	1.51
1	D	1131	PHE	CB-CG	-5.34	1.42	1.51
1	В	1634	GLU	CD-OE2	-5.33	1.19	1.25
1	А	488	TYR	CB-CG	-5.33	1.43	1.51
1	Е	1847	HIS	CB-CG	-5.33	1.40	1.50
1	А	1139	ASN	CB-CG	-5.32	1.38	1.51
1	В	2446	GLU	CD-OE2	-5.32	1.19	1.25
1	А	2096	PHE	CB-CG	-5.31	1.42	1.51
1	В	1145	HIS	CB-CG	-5.31	1.40	1.50
1	В	515	PHE	CB-CG	-5.30	1.42	1.51
1	А	205	GLU	CD-OE1	-5.30	1.19	1.25
1	Ε	1960	TRP	NE1-CE2	-5.29	1.30	1.37
1	С	2446	GLU	CD-OE2	-5.28	1.19	1.25
1	D	730	PHE	CB-CG	-5.28	1.42	1.51
1	С	996	TYR	CB-CG	-5.28	1.43	1.51
1	Е	434	TYR	CB-CG	-5.28	1.43	1.51
1	D	2513	TYR	CB-CG	-5.28	1.43	1.51
1	В	2308	GLU	CD-OE1	-5.27	1.19	1.25
1	А	1560	GLU	CG-CD	-5.27	1.44	1.51
1	С	1352	TYR	CB-CG	-5.26	1.43	1.51
1	В	563	PHE	CB-CG	-5.26	1.42	1.51
1	D	842	ASP	CB-CG	-5.26	1.40	1.51
1	А	1800	TRP	CZ3-CH2	-5.26	1.31	1.40
1	А	1328	TYR	CB-CG	-5.25	1.43	1.51
1	В	1021	TRP	CB-CG	-5.24	1.40	1.50
1	С	1005	GLU	CD-OE2	-5.24	1.19	1.25
1	Ε	1149	CYS	CB-SG	-5.24	1.73	1.81
1	В	988	GLU	CD-OE1	-5.23	1.19	1.25
2	F	781	PHE	CB-CG	-5.23	1.42	1.51
1	C	1724	HIS	CB-CG	-5.22	1.40	1.50
1	В	$15\overline{60}$	GLU	CD-OE1	-5.22	1.20	1.25
1	D	779	PHE	CB-CG	-5.22	1.42	1.51
1	A	1816	TRP	CB-CG	$-5.2\overline{2}$	1.40	1.50
1	E	1109	TYR	CB-CG	-5.21	1.43	1.51
1	D	1005	GLU	CD-OE1	-5.21	1.20	1.25
1	C	1139	ASN	CB-CG	-5.20	1.39	1.51



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Е	2183	GLU	CD-OE2	-5.19	1.20	1.25
1	В	390	GLU	CD-OE2	-5.19	1.20	1.25
1	D	2019	PHE	CB-CG	-5.18	1.42	1.51
1	Е	1954	GLU	CD-OE2	-5.17	1.20	1.25
1	В	1136	PHE	CB-CG	-5.17	1.42	1.51
1	С	1168	TYR	CD1-CE1	-5.16	1.31	1.39
1	С	2308	GLU	CD-OE1	-5.16	1.20	1.25
1	А	1810	GLN	CG-CD	-5.16	1.39	1.51
1	А	2193	GLU	CD-OE1	-5.16	1.20	1.25
1	В	2280	TYR	CE2-CZ	-5.16	1.31	1.38
1	Ε	1567	TYR	CB-CG	-5.16	1.44	1.51
1	А	1634	GLU	CD-OE2	-5.15	1.20	1.25
1	Е	390	GLU	CD-OE2	-5.15	1.20	1.25
1	А	1435	GLU	CG-CD	-5.15	1.44	1.51
1	Ε	382	GLU	CD-OE1	-5.15	1.20	1.25
1	А	2163	TYR	CB-CG	-5.14	1.44	1.51
1	Ε	2103	TYR	CB-CG	-5.14	1.44	1.51
1	А	937	PHE	CB-CG	-5.14	1.42	1.51
1	В	205	GLU	CD-OE1	-5.14	1.20	1.25
1	D	2183	GLU	CD-OE2	-5.13	1.20	1.25
1	Ε	996	TYR	CB-CG	-5.13	1.44	1.51
2	F	1437	GLU	CD-OE2	-5.13	1.20	1.25
1	С	1634	GLU	CD-OE1	-5.13	1.20	1.25
2	F	130	TYR	CB-CG	-5.12	1.44	1.51
2	F	256	TRP	CD2-CE3	-5.12	1.32	1.40
2	F	2078	TYR	CB-CG	-5.12	1.44	1.51
1	Ε	750	GLU	CD-OE1	-5.11	1.20	1.25
1	С	1268	TYR	CB-CG	-5.11	1.44	1.51
1	С	1960	TRP	NE1-CE2	-5.11	1.30	1.37
1	В	1664	TYR	CB-CG	-5.11	1.44	1.51
1	D	1268	TYR	CB-CG	-5.10	1.44	1.51
1	D	2251	TYR	CB-CG	-5.10	1.44	1.51
1	D	705	GLU	CD-OE2	-5.10	1.20	1.25
1	Ε	1021	TRP	CB-CG	-5.10	1.41	1.50
1	С	515	PHE	CB-CG	-5.10	1.42	1.51
1	D	2175	GLU	CD-OE1	-5.09	1.20	1.25
1	Ε	2202	GLU	CD-OE2	-5.08	1.20	1.25
2	F	355	GLU	CD-OE1	-5.08	1.20	1.25
2	F	625	TYR	CG-CD2	-5.08	1.32	1.39
1	Е	280	GLU	CD-OE2	-5.08	1.20	1.25
1	В	2473	GLU	CG-CD	-5.08	1.44	1.51
1	С	1141	TRP	CB-CG	-5.07	1.41	1.50



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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	705	GLU	CD-OE2	-5.07	1.20	1.25
1	А	916	GLU	CD-OE2	-5.07	1.20	1.25
1	А	2183	GLU	CD-OE2	-5.06	1.20	1.25
1	В	2272	ARG	CG-CD	-5.06	1.39	1.51
1	А	1322	TYR	CG-CD2	-5.06	1.32	1.39
1	А	2050	GLU	CD-OE2	-5.06	1.20	1.25
1	В	488	TYR	CB-CG	-5.06	1.44	1.51
1	В	1805	TYR	CB-CG	-5.05	1.44	1.51
2	F	464	TRP	CD2-CE3	-5.05	1.32	1.40
1	А	1205	TYR	CB-CG	-5.05	1.44	1.51
1	С	382	GLU	CD-OE1	-5.04	1.20	1.25
1	А	1149	CYS	CB-SG	-5.04	1.73	1.81
1	С	1086	GLU	CD-OE1	-5.04	1.20	1.25
1	D	1634	GLU	CD-OE1	-5.04	1.20	1.25
1	А	2308	GLU	CD-OE1	-5.04	1.20	1.25
1	В	1310	TYR	CB-CG	-5.03	1.44	1.51
1	Е	1800	TRP	CE2-CZ2	-5.03	1.31	1.39
1	А	1006	GLU	CD-OE2	-5.03	1.20	1.25
1	С	1095	SER	CB-OG	-5.02	1.35	1.42
1	D	1827	TRP	CB-CG	-5.02	1.41	1.50
1	А	996	TYR	CB-CG	-5.02	1.44	1.51
1	А	747	GLU	CD-OE2	-5.02	1.20	1.25
1	В	2019	PHE	CB-CG	-5.02	1.42	1.51
2	F	2064	GLU	CD-OE1	-5.01	1.20	1.25
1	D	747	GLU	CD-OE2	-5.01	1.20	1.25
1	D	515	PHE	CB-CG	-5.00	1.42	1.51
1	D	1139	ASN	CB-CG	-5.00	1.39	1.51
1	В	1853	PHE	CB-CG	-5.00	1.42	1.51
1	A	1725	PHE	CB-CG	-5.00	1.42	1.51

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All (373) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	445	ARG	NE-CZ-NH2	-13.57	113.52	120.30
1	А	462	ARG	NE-CZ-NH2	-13.26	113.67	120.30
1	Е	445	ARG	NE-CZ-NH1	11.68	126.14	120.30
1	С	1319	ARG	NE-CZ-NH2	-10.73	114.93	120.30
1	А	1319	ARG	NE-CZ-NH2	-10.70	114.95	120.30
2	F	472	ARG	NE-CZ-NH2	-10.54	115.03	120.30
1	Е	462	ARG	NE-CZ-NH1	10.46	125.53	120.30
2	F	1351	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	Е	2018	ARG	NE-CZ-NH2	-10.33	115.14	120.30



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Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	D	1319	ARG	NE-CZ-NH2	-10.26	115.17	120.30
1	Е	462	ARG	NE-CZ-NH2	-10.10	115.25	120.30
1	В	329	ARG	NE-CZ-NH2	-10.03	115.28	120.30
1	D	2333	ARG	NE-CZ-NH2	-9.69	115.45	120.30
1	А	462	ARG	NE-CZ-NH1	9.55	125.08	120.30
1	Е	445	ARG	NE-CZ-NH2	-9.50	115.55	120.30
2	F	588	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	Ε	1421	ARG	NE-CZ-NH2	-9.47	115.56	120.30
2	F	2051	ARG	NE-CZ-NH1	9.47	125.03	120.30
2	F	1585	ARG	NE-CZ-NH2	9.46	125.03	120.30
1	D	1421	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	В	2290	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	Е	1159	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	D	1819	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	А	1819	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	С	380	ARG	NE-CZ-NH2	-9.11	115.74	120.30
1	D	517	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	D	462	ARG	NE-CZ-NH1	9.03	124.81	120.30
2	F	1290	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	С	1909	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	D	1159	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	А	1421	ARG	NE-CZ-NH2	-8.80	115.90	120.30
2	F	472	ARG	NE-CZ-NH1	8.75	124.67	120.30
2	F	332	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	Е	1124	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	Ε	380	ARG	NE-CZ-NH2	-8.65	115.97	120.30
1	А	1426	ARG	NE-CZ-NH2	-8.63	115.98	120.30
2	F	131	ARG	NE-CZ-NH2	-8.61	115.99	120.30
1	В	1421	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	Ε	2243	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	D	462	ARG	NE-CZ-NH2	-8.56	116.02	120.30
2	F	1609	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	C	1300	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	Ε	1358	ARG	NE-CZ-NH2	-8.51	116.04	120.30
1	A	1782	ARG	NE-CZ-NH2	-8.47	116.06	120.30
1	С	$2\overline{272}$	ARG	$NE-\overline{CZ-NH2}$	-8.45	116.07	120.30
1	А	2411	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	Е	354	ARG	NE-CZ-NH2	-8.41	116.09	120.30
2	F	1979	ARG	NE-CZ-NH2	-8.35	116.12	120.30
2	F	81	ARG	NE-CZ-NH2	-8.31	116.15	120.30
1	D	1159	ARG	$NE-\overline{CZ-NH2}$	-8.26	116.17	120.30
1	Е	1342	TYR	CB-CG-CD1	-8.25	116.05	121.00



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	999	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	С	1159	ARG	NE-CZ-NH1	8.17	124.39	120.30
2	F	1389	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	D	1124	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	А	1369	ARG	NE-CZ-NH2	-8.10	116.25	120.30
2	F	1972	TYR	CB-CG-CD1	-8.09	116.15	121.00
1	D	2327	ARG	NE-CZ-NH2	-8.08	116.26	120.30
2	F	259	TYR	CB-CG-CD1	-8.05	116.17	121.00
2	F	2051	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	В	1159	ARG	NE-CZ-NH2	-7.95	116.32	120.30
1	Е	1159	ARG	NE-CZ-NH1	7.91	124.26	120.30
1	С	1421	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	В	354	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	С	1015	ARG	NE-CZ-NH2	-7.77	116.41	120.30
2	F	1511	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	Е	1782	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	Е	1863	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	В	1358	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	D	999	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	А	204	TYR	CB-CG-CD2	-7.71	116.38	121.00
1	А	517	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	В	1971	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	В	999	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	С	193	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	D	2189	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	А	1426	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	D	2216	ARG	NE-CZ-NH2	-7.53	116.54	120.30
2	F	289	ARG	NE-CZ-NH2	-7.52	116.54	120.30
2	F	1974	TYR	CB-CG-CD2	-7.50	116.50	121.00
1	С	547	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	В	193	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	С	208	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	В	2281	ARG	NE-CZ-NH2	-7.44	116.58	120.30
2	F	1139	ARG	NE-CZ-NH2	-7.42	116.59	120.30
2	F	332	ARG	NE-CZ-NH1	7.40	124.00	120.30
2	F	1725	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	D	284	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	В	2333	ARG	NE-CZ-NH2	-7.36	116.62	120.30
2	F	2114	TYR	CB-CG-CD2	-7.33	116.60	121.00
1	C	2327	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	С	204	TYR	$CB-\overline{CG}-\overline{CD2}$	-7.30	116.62	121.00
1	С	1124	ARG	NE-CZ-NH2	-7.27	116.67	120.30



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Mol	Chain	\mathbf{Res}	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Е	2333	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	А	1863	ARG	NE-CZ-NH1	7.21	123.90	120.30
2	F	2117	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	С	1863	ARG	NE-CZ-NH1	7.19	123.90	120.30
1	Е	1287	ARG	NE-CZ-NH2	-7.17	116.72	120.30
2	F	919	TYR	CB-CG-CD2	-7.15	116.71	121.00
1	А	2243	ARG	NE-CZ-NH2	-7.15	116.72	120.30
2	F	1290	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	В	204	TYR	CB-CG-CD1	-7.12	116.73	121.00
1	А	1124	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	Е	2216	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	А	1855	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	Е	506	ARG	NE-CZ-NH2	-7.06	116.77	120.30
2	F	1575	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	С	1159	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	А	334	TYR	CB-CG-CD2	-7.03	116.78	121.00
2	F	80	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	С	1895	TYR	CB-CG-CD1	-7.00	116.80	121.00
2	F	2145	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	D	1782	ARG	NE-CZ-NH1	6.96	123.78	120.30
2	F	292	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	В	487	ARG	NE-CZ-NH2	-6.92	116.84	120.30
2	F	174	ARG	NE-CZ-NH2	-6.91	116.85	120.30
2	F	1521	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	А	1259	TYR	CB-CG-CD2	-6.89	116.87	121.00
1	D	2324	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	С	1664	TYR	CB-CG-CD2	-6.84	116.89	121.00
1	Ε	564	ARG	NE-CZ-NH1	6.84	123.72	120.30
2	F	2033	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	В	1782	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	D	564	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	А	2513	TYR	CB-CG-CD1	-6.82	116.91	121.00
1	D	1863	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	С	1230	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	А	2216	ARG	NE-CZ-NH2	-6.79	116.90	120.30
2	F	1969	ARG	NE-CZ-NH2	-6.76	$1\overline{16.92}$	120.30
1	Ε	2399	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	A	1154	TYR	$CB-CG-\overline{CD2}$	-6.74	116.96	121.00
1	В	$13\overline{69}$	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	В	1909	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	D	$12\overline{86}$	TYR	CB-CG-CD1	-6.68	116.99	121.00
1	В	2216	ARG	NE-CZ-NH2	-6.67	116.96	120.30



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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
1	D	1405	TYR	CB-CG-CD1	-6.65	117.01	121.00
2	F	130	TYR	CB-CG-CD2	-6.65	117.01	121.00
1	С	1782	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	А	193	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	С	1855	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	D	2456	ASP	CB-CG-OD1	6.63	124.27	118.30
1	Е	215	ASP	CB-CG-OD1	6.61	124.25	118.30
2	F	2077	TYR	CB-CG-CD1	-6.61	117.04	121.00
2	F	286	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	D	1154	TYR	CB-CG-CD2	-6.59	117.04	121.00
1	С	1050	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	С	2281	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	Ε	966	ASP	CB-CG-OD1	6.55	124.20	118.30
1	Е	2341	TYR	CB-CG-CD1	-6.55	117.07	121.00
1	D	204	TYR	CB-CG-CD1	-6.54	117.08	121.00
2	F	174	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	В	284	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	С	1868	TYR	CB-CG-CD1	-6.51	117.09	121.00
1	С	2189	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	F	1840	TYR	CB-CG-CD2	-6.50	117.10	121.00
1	А	2333	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	В	2018	ARG	NE-CZ-NH2	-6.49	117.06	120.30
2	F	1044	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	Е	1124	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	Е	332	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	В	2411	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	D	506	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	С	1552	ASP	CB-CG-OD1	6.44	124.09	118.30
1	С	141	ARG	NE-CZ-NH2	6.43	123.52	120.30
2	F	1419	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	А	1011	GLY	N-CA-C	-6.37	97.18	113.10
1	Е	2333	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	D	1148	ASP	CB-CG-OD2	6.31	123.98	118.30
1	D	1552	ASP	CB-CG-OD1	6.28	123.95	118.30
1	Е	2513	TYR	CB-CG-CD1	-6.26	117.24	121.00
1	А	332	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	E	966	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	С	859	LEU	C-N-CD	-6.22	106.92	120.60
2	F	1658	ARG	NE-CZ-NH1	6.21	123.41	120.30
2	F	859	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	В	2341	TYR	CB-CG-CD2	-6.17	117.30	121.00
1	D	328	TYR	CB-CG-CD2	-6.16	117.30	121.00



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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^{o})$	$Ideal(^{o})$
1	D	859	LEU	C-N-CD	-6.15	107.07	120.60
1	Е	1011	GLY	N-CA-C	-6.14	97.74	113.10
1	Е	328	TYR	CB-CG-CD2	-6.14	117.31	121.00
1	А	859	LEU	C-N-CD	-6.14	107.10	120.60
1	А	1552	ASP	CB-CG-OD1	6.13	123.82	118.30
1	В	1855	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	А	506	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	С	1287	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	D	1369	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	D	1971	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	В	2243	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	С	2147	PHE	CB-CG-CD2	-6.08	116.55	120.80
1	С	1259	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	С	2216	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	В	1148	ASP	CB-CG-OD1	-6.06	112.85	118.30
1	D	964	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	D	2196	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	А	332	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	В	329	ARG	NE-CZ-NH1	6.02	123.31	120.30
2	F	140	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	С	1148	ASP	CB-CG-OD2	6.00	123.70	118.30
1	С	328	TYR	CB-CG-CD2	-6.00	117.40	121.00
1	Е	999	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	Е	564	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	В	859	LEU	C-N-CD	-5.97	107.47	120.60
1	А	912	TYR	CB-CG-CD1	-5.96	117.42	121.00
1	С	332	ARG	NE-CZ-NH2	-5.96	117.32	120.30
2	F	838	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	С	1148	ASP	CB-CG-OD1	-5.92	112.97	118.30
1	D	1855	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	В	2512	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	Ε	859	LEU	C-N-CD	-5.91	107.60	120.60
1	Ε	2281	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	D	1148	ASP	CB-CG-OD1	-5.90	112.99	118.30
1	E	2186	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	В	1250	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	В	1148	ASP	CB-CG-OD2	5.88	123.59	118.30
1	D	1611	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	D	103	TYR	CB-CG-CD2	-5.87	117.48	121.00
2	F	1358	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	В	555	PHE	$CB-\overline{CG}-\overline{CD1}$	5.86	$1\overline{24.90}$	120.80
2	F	1449	ARG	NE-CZ-NH1	5.86	123.23	120.30



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Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
2	F	2007	ARG	NE-CZ-NH2	-5.83	117.38	120.30
2	F	1436	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	D	2428	ASP	CB-CG-OD1	5.79	123.51	118.30
2	F	81	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	С	2513	TYR	CB-CG-CD1	-5.76	117.55	121.00
1	D	1604	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	В	1328	TYR	CB-CG-CD2	-5.75	117.55	121.00
2	F	1913	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	В	1204	ARG	NE-CZ-NH2	5.73	123.16	120.30
1	Е	1971	ARG	NE-CZ-NH2	-5.71	117.44	120.30
2	F	143	TYR	CB-CG-CD2	-5.71	117.57	121.00
2	F	1559	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	D	141	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	Е	268	PHE	CB-CG-CD1	-5.70	116.81	120.80
1	С	1611	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	D	1358	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	Е	484	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	D	268	PHE	CB-CG-CD1	-5.66	116.84	120.80
1	D	334	TYR	CB-CG-CD2	-5.65	117.61	121.00
1	Е	968	TYR	CB-CG-CD2	-5.64	117.61	121.00
2	F	1367	ARG	NE-CZ-NH2	5.64	123.12	120.30
2	F	871	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	С	1430	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	С	445	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	Е	1855	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	В	1868	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	С	2272	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	А	329	ARG	NE-CZ-NH1	5.57	123.09	120.30
2	F	2112	TYR	CB-CG-CD1	-5.56	117.66	121.00
2	F	1609	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	С	1168	TYR	CB-CG-CD1	-5.55	117.67	121.00
1	D	483	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	А	1971	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	Е	2266	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	D	2411	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	D	999	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	В	1552	ASP	CB-CG-OD1	5.50	123.25	118.30
1	Е	136	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	D	2327	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	C	547	ARG	NE-CZ-NH1	5.49	123.05	120.30
2	F	1001	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	В	215	ASP	CB-CG-OD1	5.48	123.23	118.30



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	В	356	ASP	CB-CG-OD1	5.48	123.23	118.30
1	Е	1295	ASP	CB-CG-OD1	5.48	123.23	118.30
1	С	1319	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	D	2243	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	D	2411	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	В	332	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	Е	334	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	В	1863	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	В	1124	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	D	1525	PHE	CB-CA-C	-5.44	99.52	110.40
1	В	1294	PHE	CB-CG-CD2	-5.44	116.99	120.80
1	В	506	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	Е	1405	TYR	CB-CG-CD1	-5.44	117.74	121.00
2	F	523	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	В	1287	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	А	204	TYR	CB-CG-CD1	5.42	124.25	121.00
2	F	478	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	Е	2018	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	D	942	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	D	2186	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	В	521	THR	N-CA-C	-5.39	96.44	111.00
1	А	1319	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	F	2080	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	В	1294	PHE	CB-CG-CD1	5.36	124.55	120.80
1	Е	376	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	С	488	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	D	1868	TYR	CB-CG-CD2	-5.34	117.80	121.00
1	С	141	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	Е	182	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	D	1319	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	В	1904	ASP	CB-CG-OD1	5.32	123.09	118.30
1	С	2399	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	D	182	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	С	1300	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	Е	1883	TYR	CB-CG-CD1	-5.29	117.83	121.00
1	В	2513	TYR	CB-CG-CD1	-5.29	117.83	121.00
1	Е	1358	ARG	NE-CZ-NH1	5.28	122.94	120.30
2	F	1763	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	С	462	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	F	766	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	A	672	ASP	CB-CG-OD1	5.28	123.05	118.30
1	В	1352	TYR	CB-CG-CD1	-5.27	117.83	121.00



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Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	1294	PHE	CB-CG-CD2	-5.27	117.11	120.80
2	F	1901	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	D	1358	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	Е	1328	TYR	CB-CG-CD2	-5.26	117.84	121.00
2	F	201	TYR	CB-CG-CD2	-5.26	117.84	121.00
2	F	825	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	Е	412	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	D	2255	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	Е	964	ARG	NE-CZ-NH2	-5.25	117.67	120.30
2	F	505	ASP	CB-CG-OD2	5.23	123.01	118.30
1	D	284	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	D	445	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	D	553	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	D	1011	GLY	N-CA-C	-5.21	100.07	113.10
1	А	1287	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	D	517	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	В	2333	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	547	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	А	1322	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	С	1405	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	С	182	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	D	1287	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	А	1286	TYR	CB-CG-CD1	-5.19	117.89	121.00
2	F	2117	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	D	1250	TYR	CB-CG-CD1	-5.17	117.90	121.00
1	В	1335	GLY	N-CA-C	-5.17	100.17	113.10
1	С	1868	TYR	CB-CG-CD2	5.17	124.10	121.00
1	D	2513	TYR	CB-CG-CD1	-5.17	117.90	121.00
2	F	1205	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	А	1868	TYR	CB-CG-CD2	-5.16	117.91	121.00
1	D	2189	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	В	2266	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	С	1470	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	D	694	PRO	N-CA-C	-5.13	98.76	112.10
1	А	1443	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	Е	1868	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	A	2266	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	В	2095	ARG	NE-CZ-NH2	-5.11	$117.7\overline{5}$	120.30
1	C	2186	ARG	NE-CZ-NH2	$-5.1\overline{1}$	$117.7\overline{5}$	120.30
1	В	1159	ARG	NE-CZ-NH1	5.10	122.85	120.30
2	F	302	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	В	2410	ARG	NE-CZ-NH2	-5.10	117.75	120.30



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Е	547	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	Е	487	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	А	1195	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	А	124	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	В	942	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	А	2186	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	D	1616	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	D	2216	ARG	NE-CZ-NH1	5.07	122.84	120.30
2	F	1210	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	D	2095	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	В	328	TYR	CB-CG-CD2	-5.06	117.97	121.00
1	С	1194	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	С	2095	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	Е	445	ARG	CD-NE-CZ	5.05	130.67	123.60
1	Е	1250	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	А	2411	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	Е	2095	ARG	NE-CZ-NH2	-5.04	117.78	120.30
2	F	233	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	С	1040	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	С	1782	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	А	328	TYR	CB-CG-CD2	-5.03	117.98	121.00
2	F	204	TYR	CB-CG-CD1	-5.03	117.98	121.00
2	F	1106	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	Е	1230	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	D	412	ARG	NE-CZ-NH1	-5.01	117.79	120.30
1	В	103	TYR	CB-CG-CD2	-5.01	117.99	121.00
1	А	215	ASP	CB-CG-OD1	5.00	122.80	118.30
1	Е	555	PHE	CB-CG-CD1	5.00	124.30	120.80

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There are no chirality outliers.

There are no planarity outliers.

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	А	19161	0	18735	50	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	19161	0	18735	52	0
1	С	19161	0	18735	44	0
1	D	19161	0	18735	64	0
1	Е	19161	0	18735	63	0
2	F	17117	0	16479	53	0
All	All	112922	0	110154	294	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 1.

All (294) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:2147:PHE:CD1	1:E:2147:PHE:CE1	1.83	1.63
1:D:2147:PHE:CD1	1:E:2147:PHE:HE1	0.95	1.59
1:D:2147:PHE:HD1	1:E:2147:PHE:CE1	1.29	1.24
1:D:2144:ILE:HG22	1:D:2148:ALA:O	1.65	0.95
1:D:2147:PHE:HB3	1:E:2147:PHE:HD1	1.33	0.93
1:D:2147:PHE:HB3	1:E:2147:PHE:CD1	2.10	0.86
1:D:2147:PHE:CE1	1:E:2147:PHE:CE1	2.66	0.81
1:D:2147:PHE:CG	1:E:2147:PHE:CE1	2.69	0.80
1:A:2147:PHE:HD1	1:E:2147:PHE:HB3	1.55	0.71
2:F:1442:THR:OG1	2:F:1443:ALA:N	2.26	0.68
1:B:2147:PHE:HB3	1:C:2147:PHE:CD1	2.32	0.65
1:D:2147:PHE:CD1	1:E:2147:PHE:CZ	2.76	0.65
1:A:1116:THR:HG1	1:E:1211:THR:HG1	1.46	0.61
1:B:859:LEU:O	1:B:860:PRO:C	2.40	0.59
1:E:1148:ASP:OD1	1:E:1148:ASP:N	2.32	0.58
1:E:521:THR:O	1:E:522:PRO:C	2.41	0.58
1:A:834:GLN:NE2	1:E:662:THR:OG1	2.37	0.58
1:B:1716:SER:OG	1:B:1717:ASP:N	2.37	0.58
1:A:521:THR:O	1:A:522:PRO:C	2.41	0.57
1:C:521:THR:O	1:C:522:PRO:C	2.41	0.57
1:B:1706:LYS:NZ	1:B:1717:ASP:OD1	2.36	0.56
1:D:2144:ILE:CG2	1:D:2148:ALA:O	2.48	0.56
1:C:1087:GLN:NE2	1:C:1114:SER:OG	2.38	0.56
1:C:1774:TYR:HH	1:C:1848:TYR:HH	1.52	0.56
1:E:859:LEU:O	1:E:860:PRO:C	2.44	0.56
1:A:1683:ASP:OD2	1:E:1377:LYS:NZ	2.39	0.56
1:B:2147:PHE:HA	1:D:1190:THR:HG21	1.88	0.55
1:B:817:LYS:NZ	1:B:837:ASP:OD2	2.35	0.55



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Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:859:LEU:O	1:A:860:PRO:C	2.45	0.55
1:D:859:LEU:O	1:D:860:PRO:C	2.45	0.55
1:B:1298:ASN:OD1	1:B:1298:ASN:N	2.37	0.55
1:E:1514:ASP:OD2	1:E:1515:LYS:NZ	2.40	0.55
1:D:733:TRP:NE1	1:D:748:THR:OG1	2.40	0.54
1:C:1377:LYS:NZ	1:D:1683:ASP:OD2	2.40	0.54
1:C:859:LEU:O	1:C:860:PRO:C	2.44	0.54
1:C:1148:ASP:OD1	1:C:1148:ASP:N	2.36	0.54
1:E:1350:LYS:NZ	1:E:1538:ASP:OD1	2.38	0.53
2:F:777:GLU:OE2	2:F:866:LYS:NZ	2.41	0.53
1:B:1148:ASP:OD1	1:B:1148:ASP:N	2.33	0.53
1:E:1622:ASP:OD1	1:E:1623:THR:N	2.41	0.53
2:F:1975:SER:OG	2:F:1977:ASP:OD1	2.26	0.53
1:B:1190:THR:HG21	1:E:2147:PHE:HA	1.90	0.53
2:F:78:THR:OG1	2:F:80:ARG:NH2	2.42	0.53
1:E:2144:ILE:HG22	1:E:2148:ALA:O	2.09	0.52
1:D:2147:PHE:CD1	1:E:2147:PHE:CD1	2.80	0.52
1:C:1311:GLU:HB3	1:C:1575:THR:HB	1.90	0.52
1:D:2287:ASP:OD1	1:D:2287:ASP:N	2.40	0.52
1:A:439:LYS:NZ	1:A:469:ASP:OD1	2.43	0.52
1:B:1120:GLU:OE2	1:B:1146:LYS:NZ	2.43	0.52
1:D:1087:GLN:NE2	1:D:1114:SER:OG	2.43	0.52
1:E:2207:ASP:OD2	1:E:2211:LYS:NZ	2.43	0.52
1:A:2147:PHE:O	1:B:2147:PHE:HD2	1.94	0.51
1:E:1398:SER:OG	1:E:1400:ASN:O	2.28	0.51
1:B:1447:ASN:ND2	1:B:1456:TYR:O	2.42	0.51
2:F:1914:ALA:O	2:F:2125:ARG:NH2	2.43	0.51
1:C:2280:TYR:OH	1:C:2324:ARG:NH1	2.44	0.51
2:F:991:SER:OG	2:F:1008:SER:OG	2.28	0.51
2:F:268:SER:OG	2:F:270:ASN:OD1	2.29	0.50
1:A:92:TYR:OH	1:A:99:ARG:NH1	2.45	0.50
1:D:198:THR:N	1:D:199:PRO:CD	2.75	0.50
1:A:1729:ASP:OD1	1:A:1729:ASP:N	2.43	0.50
1:D:2285:ASN:O	1:D:2286:ASP:C	2.49	0.50
1:C:2468:LYS:NZ	1:D:2325:ASP:OD2	2.39	0.49
1:D:1164:LYS:NZ	1:D:1243:ASP:OD2	2.45	0.49
1:E:1428:THR:OG1	1:E:1429:THR:N	2.45	0.49
1:A:198:THR:N	1:A:199:PRO:CD	2.76	0.49
1:B:141:ARG:HD3	1:B:970:TYR:O	2.11	0.49
1:C:1168:TYR:CD2	1:C:1202:HIS:HB3	2.47	0.49
1:A:418:SER:OG	1:A:419:TRP:N	2.45	0.49



	juo puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:F:692:THR:OG1	2:F:693:ASN:N	2.45	0.49
1:E:1311:GLU:HB3	1:E:1575:THR:HB	1.93	0.49
1:E:1524:SER:OG	1:E:1525:PHE:N	2.45	0.49
2:F:1329:ASP:N	2:F:1329:ASP:OD1	2.35	0.49
1:E:1229:ASN:OD1	1:E:1229:ASN:N	2.42	0.49
1:D:2468:LYS:NZ	1:E:2325:ASP:OD2	2.42	0.48
1:B:1657:ASP:OD1	1:B:1657:ASP:N	2.42	0.48
2:F:224:THR:O	2:F:227:ARG:NH1	2.46	0.48
1:D:1168:TYR:CD2	1:D:1202:HIS:HB3	2.49	0.48
2:F:530:ASP:OD1	2:F:530:ASP:N	2.40	0.48
1:A:193:ARG:N	1:A:194:PRO:CD	2.77	0.48
1:B:533:ASP:OD1	1:B:533:ASP:N	2.40	0.48
1:D:842:ASP:OD1	1:D:844:ASN:N	2.45	0.48
1:E:2382:ASP:OD1	1:E:2382:ASP:N	2.46	0.48
1:D:694:PRO:O	1:D:695:TYR:HB2	2.14	0.48
1:D:1148:ASP:N	1:D:1148:ASP:OD1	2.35	0.48
2:F:693:ASN:N	2:F:693:ASN:OD1	2.47	0.48
1:A:1311:GLU:HB3	1:A:1575:THR:HB	1.95	0.48
1:B:1426:ARG:NH2	1:B:1450:ALA:O	2.47	0.48
1:B:1507:LYS:NZ	1:B:1538:ASP:OD2	2.45	0.48
1:E:2319:ASP:OD2	1:E:2323:LYS:NZ	2.46	0.48
1:E:2082:LYS:NZ	1:E:2086:GLU:OE2	2.43	0.48
1:C:198:THR:N	1:C:199:PRO:CD	2.77	0.47
1:D:2380:GLY:N	1:D:2383:THR:OG1	2.47	0.47
1:D:521:THR:O	1:D:522:PRO:C	2.51	0.47
1:E:2287:ASP:N	1:E:2287:ASP:OD1	2.45	0.47
1:B:1168:TYR:CD2	1:B:1202:HIS:HB3	2.49	0.47
1:E:342:ASP:OD2	1:E:360:LYS:NZ	2.38	0.47
1:B:2147:PHE:HA	1:D:1190:THR:CG2	2.44	0.47
1:B:2147:PHE:HB3	1:C:2147:PHE:CG	2.49	0.47
1:C:1272:ASP:N	1:C:1272:ASP:OD1	2.46	0.47
1:E:1272:ASP:N	1:E:1272:ASP:OD1	2.43	0.47
1:A:1272:ASP:N	1:A:1272:ASP:OD1	2.44	0.47
1:B:447:SER:O	1:B:451:GLU:N	2.48	0.47
1:B:1890:LEU:HB3	1:B:1960:TRP:CH2	2.50	0.47
1:D:2147:PHE:CE1	1:E:2147:PHE:CZ	3.02	0.47
1:B:1272:ASP:OD1	1:B:1272:ASP:N	2.45	0.46
1:C:439:LYS:NZ	1:C:469:ASP:OD1	2.48	0.46
1:D:1657:ASP:OD1	1:D:1657:ASP:N	2.43	0.46
1:A:1890:LEU:HB3	1:A:1960:TRP:CH2	2.51	0.46
1:C:1836:ASP:OD1	1:C:1836:ASP:C	2.53	0.46



	had pagemi	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:796:HIS:ND1	1:D:796:HIS:N	2.64	0.46
1:E:512:PRO:O	1:E:517:ARG:NH1	2.48	0.46
1:A:306:GLN:NE2	1:A:314:ILE:O	2.48	0.46
1:A:2437:ASP:O	1:A:2438:LYS:C	2.54	0.46
1:D:133:ASP:N	1:D:133:ASP:OD1	2.46	0.46
1:D:2281:ARG:O	1:D:2282:TRP:C	2.53	0.46
1:E:831:THR:OG1	1:E:832:ALA:N	2.48	0.46
1:D:1426:ARG:NH2	1:D:1450:ALA:O	2.49	0.46
2:F:505:ASP:OD1	2:F:505:ASP:C	2.51	0.46
2:F:1087:ALA:HB1	2:F:1558:GLN:HB3	1.97	0.46
1:C:1220:LYS:NZ	1:C:1277:ASP:OD1	2.48	0.46
2:F:263:ASP:C	2:F:263:ASP:OD1	2.52	0.46
2:F:263:ASP:OD1	2:F:264:TYR:N	2.49	0.46
1:A:1432:SER:OG	1:A:1433:LYS:N	2.49	0.46
1:A:1514:ASP:N	1:A:1514:ASP:OD1	2.47	0.46
1:B:455:THR:OG1	1:B:456:ILE:N	2.49	0.46
2:F:902:THR:OG1	2:F:903:ASP:N	2.49	0.46
1:D:319:ASN:HB2	1:D:322:ASP:HB3	1.98	0.45
2:F:1109:THR:OG1	2:F:1110:ASN:N	2.49	0.45
2:F:1133:THR:OG1	2:F:1134:ALA:N	2.49	0.45
2:F:1698:ASP:OD1	2:F:1698:ASP:N	2.47	0.45
1:A:2143:ASN:N	1:A:2143:ASN:OD1	2.46	0.45
1:C:928:SER:OG	1:C:929:GLN:N	2.48	0.45
2:F:1208:THR:OG1	2:F:1209:LEU:N	2.49	0.45
1:B:1729:ASP:OD2	1:B:1730:LYS:NZ	2.43	0.45
1:E:1622:ASP:OD1	1:E:1622:ASP:N	2.49	0.45
2:F:390:PHE:CE1	2:F:396:TRP:HB3	2.51	0.45
2:F:584:LEU:O	2:F:588:ARG:NH2	2.50	0.45
1:A:831:THR:OG1	1:A:832:ALA:N	2.49	0.45
1:A:1348:ASP:OD1	1:A:1350:LYS:NZ	2.47	0.45
1:D:1272:ASP:OD1	1:D:1272:ASP:N	2.44	0.45
1:D:1769:TRP:CE3	1:D:1827:TRP:CZ2	3.04	0.45
1:A:398:ASN:O	1:A:399:THR:C	2.54	0.45
1:D:831:THR:OG1	1:D:832:ALA:N	2.50	0.45
1:E:92:TYR:OH	1:E:99:ARG:NE	2.49	0.45
2:F:446:SER:O	2:F:447:LEU:C	2.53	0.45
2:F:2120:GLN:HE21	2:F:2122:TRP:HE1	1.65	0.45
2:F:153:ASP:O	2:F:174:ARG:NH2	2.49	0.45
1:D:1907:LEU:O	1:D:1908:ASP:C	2.54	0.45
1:A:1168:TYR:CD2	1:A:1202:HIS:HB3	2.53	0.44
1:B:943:SER:O	1:B:944:ALA:C	2.55	0.44



	juo puge	Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
1:A:455:THR:OG1	1:A:456:ILE:N	2.50	0.44
1:E:1432:SER:OG	1:E:1433:LYS:N	2.50	0.44
1:C:193:ARG:N	1:C:194:PRO:CD	2.81	0.44
1:D:1447:ASN:ND2	1:D:1456:TYR:O	2.51	0.44
2:F:1444:LYS:HB3	2:F:1446:TRP:CE3	2.52	0.44
1:B:2487:PRO:O	1:B:2497:GLN:HG2	2.18	0.44
1:B:1729:ASP:OD1	1:B:1729:ASP:N	2.49	0.44
1:D:270:ASN:OD1	1:D:270:ASN:N	2.48	0.44
2:F:34:ASP:OD1	2:F:35:GLY:N	2.50	0.44
2:F:1687:ASP:OD1	2:F:1687:ASP:N	2.39	0.44
1:D:398:ASN:O	1:D:399:THR:C	2.56	0.44
1:E:137:TYR:CE2	1:E:139:ASP:HB2	2.53	0.44
1:A:575:ASP:OD2	1:A:577:LYS:NZ	2.36	0.44
1:A:1729:ASP:OD2	1:A:1730:LYS:NZ	2.50	0.44
1:B:193:ARG:HB2	1:B:194:PRO:HD3	2.00	0.44
1:B:1752:ASN:OD1	1:B:1752:ASN:N	2.43	0.44
1:D:2147:PHE:CB	1:E:2147:PHE:CD1	2.91	0.44
1:E:1168:TYR:CD2	1:E:1202:HIS:HB3	2.53	0.44
2:F:1882:ASP:OD1	2:F:1882:ASP:C	2.56	0.44
1:A:182:TYR:CD1	1:A:182:TYR:C	2.90	0.43
1:B:398:ASN:O	1:B:399:THR:C	2.56	0.43
1:B:2024:GLU:OE1	1:B:2027:ARG:NH1	2.51	0.43
1:C:1890:LEU:HB3	1:C:1960:TRP:CH2	2.53	0.43
2:F:1040:ASP:OD1	2:F:1042:LYS:HG3	2.18	0.43
2:F:1446:TRP:CZ3	2:F:1806:PRO:HA	2.53	0.43
2:F:2018:ASP:OD1	2:F:2018:ASP:C	2.56	0.43
1:B:137:TYR:CE2	1:B:139:ASP:HB2	2.53	0.43
1:B:521:THR:O	1:B:522:PRO:C	2.54	0.43
1:B:1907:LEU:O	1:B:1908:ASP:C	2.54	0.43
1:D:1432:SER:OG	1:D:1433:LYS:N	2.49	0.43
1:E:733:TRP:NE1	1:E:748:THR:OG1	2.51	0.43
2:F:326:GLY:N	2:F:327:PRO:HD2	2.32	0.43
1:A:2382:ASP:OD2	1:B:2404:ALA:N	2.51	0.43
1:C:1728:ASP:OD1	1:C:1728:ASP:C	2.57	0.43
1:D:366:SER:N	1:D:413:VAL:O	2.52	0.43
1:D:1729:ASP:OD1	1:D:1729:ASP:N	2.49	0.43
1:E:2380:GLY:N	1:E:2383:THR:OG1	2.52	0.43
1:A:2491:MET:N	1:A:2492:PRO:HD2	2.34	0.43
1:E:1264:MET:HB2	1:E:1283:SER:OG	2.19	0.43
2:F:369:ALA:HB3	2:F:701:GLU:HB2	2.01	0.43
1:C:1903:SER:O	1:C:1905:PRO:HD3	2.19	0.43



	A h O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:2319:ASP:OD2	1:C:2323:LYS:NZ	2.47	0.43
1:D:1890:LEU:HB3	1:D:1960:TRP:CZ2	2.54	0.43
1:A:286:TYR:O	1:A:448:ARG:NH1	2.52	0.43
1:A:1907:LEU:O	1:A:1908:ASP:C	2.55	0.43
1:B:702:LEU:HG	1:B:704:SER:H	1.84	0.43
1:C:1729:ASP:OD1	1:C:1729:ASP:N	2.45	0.43
1:C:1752:ASN:OD1	1:C:1752:ASN:N	2.41	0.43
1:D:2148:ALA:HA	1:E:2145:PHE:O	2.19	0.43
1:C:270:ASN:N	1:C:270:ASN:OD1	2.44	0.42
1:D:1229:ASN:N	1:D:1229:ASN:OD1	2.42	0.42
1:E:1729:ASP:OD1	1:E:1729:ASP:N	2.49	0.42
1:E:1244:THR:OG1	1:E:1245:LEU:N	2.52	0.42
2:F:209:ASP:C	2:F:209:ASP:OD1	2.56	0.42
1:B:2027:ARG:NH2	1:B:2318:GLU:OE1	2.52	0.42
1:C:831:THR:OG1	1:C:832:ALA:N	2.52	0.42
1:C:1016:GLN:O	1:C:1017:PHE:C	2.58	0.42
1:D:1670:ASP:OD1	1:D:1670:ASP:C	2.57	0.42
1:D:2147:PHE:CG	1:E:2147:PHE:CD1	3.07	0.42
1:A:1271:ALA:O	1:B:1611:ARG:NH1	2.53	0.42
1:D:516:ASP:O	1:D:520:ASN:N	2.52	0.42
1:D:1311:GLU:HB3	1:D:1575:THR:HB	2.01	0.42
2:F:1153:THR:OG1	2:F:1154:LEU:N	2.51	0.42
1:A:432:ASN:O	1:A:435:SER:N	2.52	0.42
1:A:827:ALA:O	1:A:829:SER:N	2.52	0.42
1:B:1531:GLN:OE1	1:C:1752:ASN:ND2	2.53	0.42
1:C:581:ASN:O	1:C:582:LEU:C	2.56	0.42
1:C:1657:ASP:OD1	1:C:1657:ASP:N	2.44	0.42
1:C:1907:LEU:O	1:C:1908:ASP:C	2.57	0.42
2:F:1549:ASN:OD1	2:F:1549:ASN:N	2.51	0.42
2:F:2044:ASP:OD1	2:F:2044:ASP:N	2.46	0.42
1:A:319:ASN:HB3	1:A:322:ASP:HB3	2.01	0.42
1:D:1293:GLN:HE22	1:D:1304:ASN:HB2	1.83	0.42
1:D:1872:GLU:O	1:D:1873:ARG:C	2.56	0.42
1:D:1890:LEU:HB3	1:D:1960:TRP:CH2	2.55	0.42
1:E:1752:ASN:OD1	1:E:1752:ASN:N	2.43	0.42
2:F:315:GLN:HB2	2:F:325:ASN:ND2	2.35	0.42
2:F:1168:ASP:OD1	2:F:1169:ALA:N	2.52	0.42
1:A:1125:SER:H	1:A:1142:SER:HG	1.68	0.42
1:B:133:ASP:OD1	1:B:133:ASP:N	2.47	0.42
1:B:2468:LYS:NZ	1:C:2325:ASP:OD2	2.53	0.42
1:C:1229:ASN:OD1	1:C:1229:ASN:N	2.45	0.42



	h l	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:C:1484:SER:OG	1:C:1485:GLY:N	2.52	0.42
1:C:2371:GLY:O	1:C:2374:ASN:ND2	2.53	0.42
1:D:581:ASN:O	1:D:582:LEU:C	2.58	0.42
1:E:545:ASP:OD1	1:E:545:ASP:C	2.58	0.42
2:F:1432:ASP:HB2	2:F:1433:PRO:HD2	2.01	0.42
1:A:581:ASN:O	1:A:582:LEU:C	2.58	0.42
1:C:137:TYR:CE2	1:C:139:ASP:HB2	2.55	0.42
2:F:2114:TYR:O	2:F:2116:TYR:N	2.51	0.42
1:D:694:PRO:O	1:D:695:TYR:CB	2.65	0.42
1:B:85:PRO:HG2	1:B:89:LEU:HB2	2.02	0.42
1:C:1670:ASP:OD1	1:C:1670:ASP:C	2.58	0.42
1:C:1729:ASP:OD2	1:C:1730:LYS:NZ	2.53	0.42
1:B:510:ASN:OD1	1:B:510:ASN:N	2.51	0.41
1:E:1168:TYR:CE2	1:E:1202:HIS:HB3	2.55	0.41
2:F:196:ARG:HB2	2:F:198:GLU:OE1	2.19	0.41
1:D:1124:ARG:HD2	1:D:1144:TRP:CE2	2.55	0.41
2:F:1729:ASP:OD1	2:F:1729:ASP:C	2.59	0.41
1:B:1890:LEU:HB3	1:B:1960:TRP:CZ2	2.54	0.41
1:E:510:ASN:OD1	1:E:510:ASN:N	2.52	0.41
1:E:733:TRP:HE1	1:E:748:THR:HG1	1.67	0.41
1:A:133:ASP:N	1:A:133:ASP:OD1	2.46	0.41
1:B:1016:GLN:O	1:B:1017:PHE:C	2.58	0.41
1:C:398:ASN:O	1:C:399:THR:C	2.58	0.41
1:E:1890:LEU:HB3	1:E:1960:TRP:CH2	2.55	0.41
1:A:1426:ARG:NH2	1:A:1450:ALA:O	2.53	0.41
1:A:2496:LYS:NZ	1:B:2400:GLU:OE1	2.54	0.41
1:D:2382:ASP:OD2	1:E:2404:ALA:N	2.54	0.41
1:A:731:TRP:O	1:A:732:ASP:C	2.58	0.41
1:A:842:ASP:OD1	1:A:843:ALA:N	2.54	0.41
1:A:432:ASN:O	1:A:433:GLN:C	2.59	0.41
1:B:1716:SER:HG	1:B:1717:ASP:N	2.19	0.41
1:E:1164:LYS:NZ	1:E:1243:ASP:OD1	2.48	0.41
2:F:350:ARG:NH2	2:F:362:THR:OG1	2.54	0.41
2:F:1067:THR:OG1	2:F:1068:ARG:N	2.53	0.41
1:A:552:LYS:O	1:A:556:ASN:N	2.54	0.41
1:A:975:ASN:OD1	1:A:975:ASN:N	2.46	0.41
1:A:1010:SER:C	1:A:1011:GLY:O	2.56	0.41
1:A:1447:ASN:ND2	1:A:1456:TYR:O	2.54	0.41
1:C:204:TYR:OH	1:C:241:ALA:O	2.39	0.41
1:D:552:LYS:O	1:D:556:ASN:N	2.54	0.41
1:E:731:TRP:O	1:E:732:ASP:C	2.59	0.41



Atom_1	Atom_2	Interatomic	Clash			
	Atom-2	distance (Å)	overlap (Å)			
1:A:137:TYR:CE2	1:A:139:ASP:HB2	2.57	0.40			
1:B:1040:TYR:CE2	1:B:1953:ASN:HB2	2.56	0.40			
1:D:1484:SER:OG	1:D:1485:GLY:N	2.54	0.40			
1:D:2266:TYR:CZ	1:D:2297:TRP:HB2	2.56	0.40			
1:B:198:THR:N	1:B:199:PRO:CD	2.85	0.40			
1:B:1834:SER:OG	1:B:1835:VAL:N	2.55	0.40			
1:C:2491:MET:N	1:C:2492:PRO:CD	2.85	0.40			
1:E:1834:SER:OG	1:E:1835:VAL:N	2.52	0.40			
2:F:963:TYR:N	2:F:964:PRO:CD	2.84	0.40			
2:F:112:ASP:OD2	2:F:147:LYS:NZ	2.49	0.40			
1:B:1432:SER:OG	1:B:1433:LYS:N	2.54	0.40			
1:C:1124:ARG:HD2	1:C:1144:TRP:CE2	2.56	0.40			
1:C:1298:ASN:OD1	1:C:1298:ASN:N	2.52	0.40			
1:E:149:ALA:O	1:E:154:ASN:ND2	2.48	0.40			
1:E:173:ILE:O	1:E:174:LYS:C	2.60	0.40			
1:E:198:THR:N	1:E:199:PRO:CD	2.84	0.40			
2:F:247:ASP:N	2:F:247:ASP:OD1	2.44	0.40			
2:F:1347:ASP:C	2:F:1347:ASP:OD1	2.60	0.40			
2:F:1560:ASP:C	2:F:1560:ASP:OD1	2.60	0.40			
2:F:2066:ASP:C	2:F:2066:ASP:OD1	2.60	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	Perce	ntiles
1	А	2411/2516~(96%)	2371~(98%)	34 (1%)	6~(0%)	47	79
1	В	2411/2516~(96%)	2365~(98%)	41 (2%)	5~(0%)	47	79
1	С	2411/2516~(96%)	2359~(98%)	44 (2%)	8 (0%)	41	74
1	D	2411/2516~(96%)	2361 (98%)	45 (2%)	5~(0%)	47	79



	$J \sim J \sim I \sim J$							
Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles		
1	Е	2411/2516~(96%)	2360~(98%)	47 (2%)	4 (0%)	47 79		
2	F	2142/2434~(88%)	2077 (97%)	56 (3%)	9 (0%)	34 70		
All	All	14197/15014~(95%)	13893 (98%)	267 (2%)	37~(0%)	44 74		

All (37) Ramachandran outliers are listed below:

\mathbf{Mol}	Chain	Res	Type
1	А	860	PRO
1	В	860	PRO
1	С	688	LEU
1	С	860	PRO
1	С	911	THR
1	D	860	PRO
1	Е	522	PRO
1	Е	860	PRO
2	F	1208	THR
1	А	522	PRO
1	А	908	GLU
1	С	522	PRO
2	F	1336	GLU
1	А	745	ALA
1	А	2106	ASN
1	С	2106	ASN
2	F	402	LYS
2	F	1920	THR
1	С	687	ASP
1	С	1985	ILE
1	D	107	GLY
1	D	1985	ILE
1	Е	1985	ILE
2	F	136	SER
1	В	521	THR
1	В	1985	ILE
1	В	2425	PRO
1	D	745	ALA
1	Е	1527	GLU
2	F	404	GLU
1	А	1985	ILE
1	D	827	ALA
2	F	683	SER
1	В	198	THR



Continued from previous page...

Mol	Chain	Res	Type
1	С	1478	GLY
2	F	1529	ILE
2	F	2115	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	ntiles
1	А	2067/2157~(96%)	2065 (100%)	2~(0%)	93	96
1	В	2067/2157~(96%)	2065 (100%)	2~(0%)	93	96
1	С	2067/2157~(96%)	2065 (100%)	2~(0%)	93	96
1	D	2067/2157~(96%)	2066 (100%)	1 (0%)	100	100
1	Ε	2067/2157~(96%)	2065 (100%)	2~(0%)	93	96
2	F	1853/2105~(88%)	1849 (100%)	4 (0%)	93	96
All	All	12188/12890~(95%)	12175 (100%)	13 (0%)	93	96

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	968	TYR
1	А	1868	TYR
1	В	341	MET
1	В	1868	TYR
1	С	341	MET
1	С	1868	TYR
1	D	1868	TYR
1	Е	968	TYR
1	Е	1868	TYR
2	F	267	ARG
2	F	1044	ARG
2	F	1848	ARG
2	F	1969	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such



sidechains are listed below:

Mol	Chain	Res	Type
1	А	935	HIS
1	В	1087	GLN
1	В	2021	HIS
1	D	1087	GLN
1	D	1748	ASN
1	D	2143	ASN
1	Е	1087	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0149. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map



The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 240

Y Index: 240



Z Index: 240

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 227

Y Index: 227

Z Index: 139

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



7.2 Volume estimate (i)



The volume at the recommended contour level is 825 nm^3 ; this corresponds to an approximate mass of 745 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.253 \AA^{-1}



8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0149 and PDB model 6H6E. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).



9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 73% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7309	0.3710
А	0.7307	0.3750
В	0.7321	0.3760
С	0.7335	0.3750
D	0.7324	0.3780
Е	0.7325	0.3770
F	0.7235	0.3400

