



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:43 PM UTC

PDB ID : 1SJJ / pdb_00001sjj
Title : Cryo-EM Structure of Chicken Gizzard Smooth Muscle alpha-Actinin
Authors : Liu, J.; Taylor, D.W.; Taylor, K.A.
Deposited on : 2004-03-03
Resolution : 20.00 Å (reported)
Based on initial models : 1CFD, 1DXX, 1HCI

This is a Full wwPDB EM Validation Report for a publicly released PDB/EMDB 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

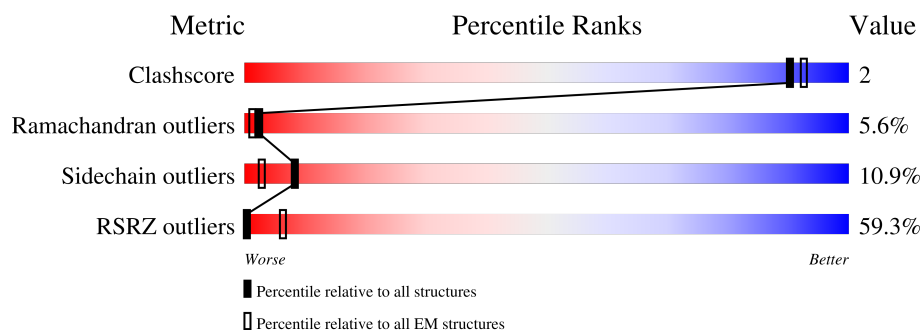
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 20.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RSRZ outliers	180361	209

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 ≥ 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	863	60% 67% 25% 6%
1	B	863	58% 66% 27% 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14014 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

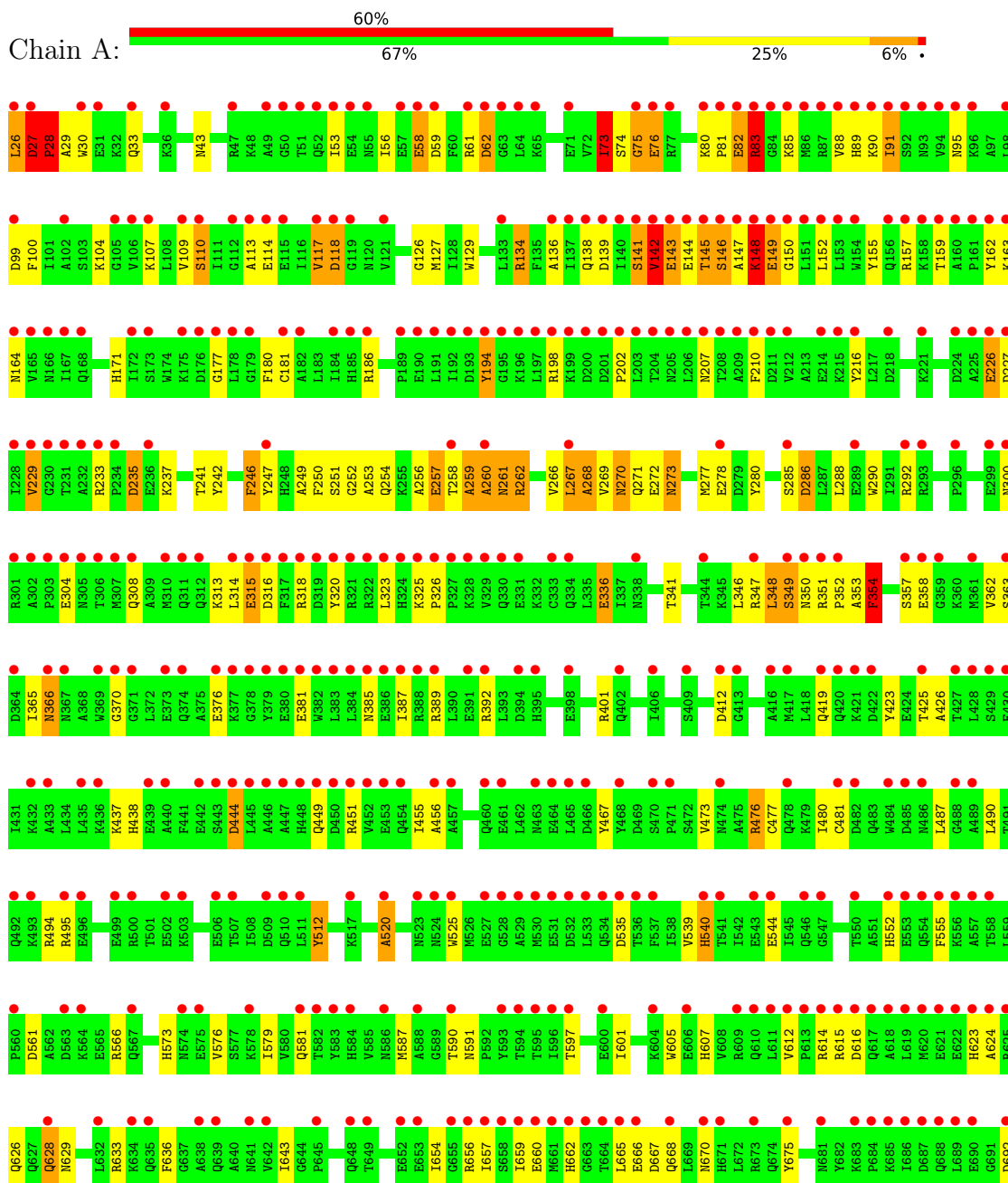
- Molecule 1 is a protein called actinin.

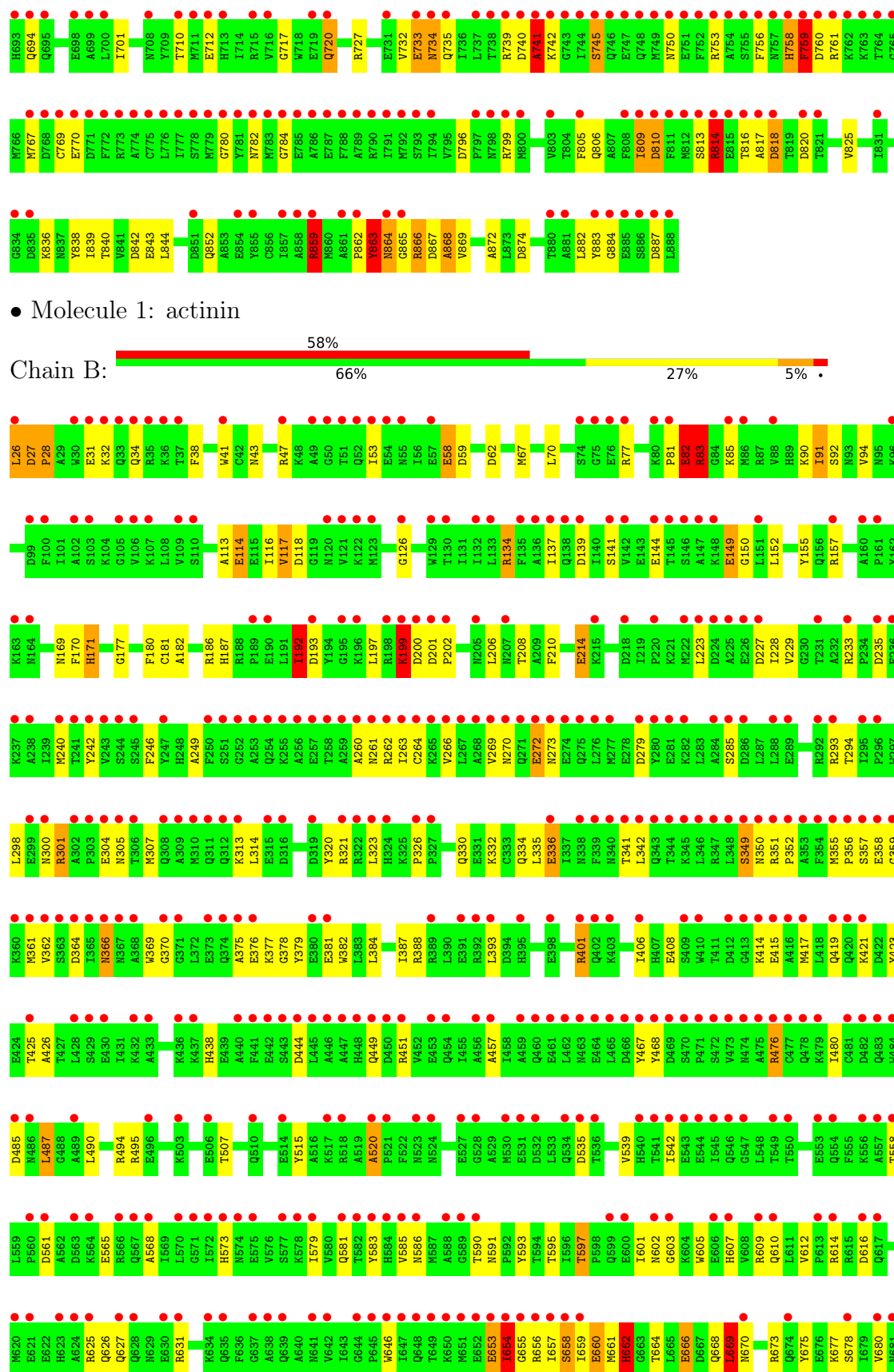
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	863	Total	C	N	O	S	0	0
			7007	4395	1236	1337	39		
1	B	863	Total	C	N	O	S	0	0
			7007	4395	1236	1337	39		

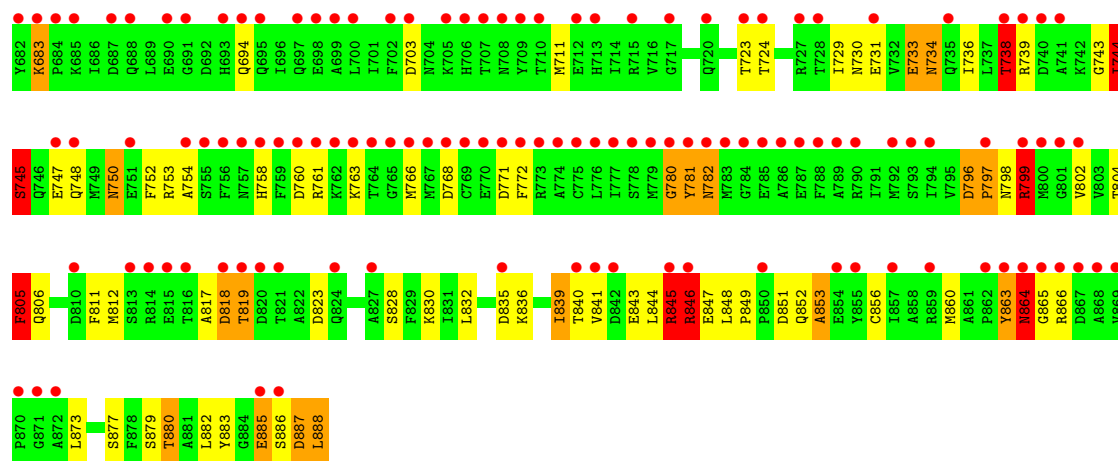
3 Residue-property plots

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. 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: actinin







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 1 2	Depositor
Cell constants a, b, c, α , β , γ	263.10Å 203.70Å 100.00Å 90.00° 90.00° 107.10°	Depositor
Resolution (Å)	(Not available) – 20.00 200.00 – 14.81	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-20.00) 29.2 (200.00-14.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available) 0.385 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	3.94 , 999.0	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	14014	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.97	1/7139 (0.0%)	1.90	183/9633 (1.9%)
1	B	0.99	1/7139 (0.0%)	1.90	155/9633 (1.6%)
All	All	0.98	2/14278 (0.0%)	1.90	338/19266 (1.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	55
1	B	0	56
All	All	0	111

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	149	GLU	CD-OE2	5.97	1.36	1.25
1	A	149	GLU	CD-OE2	5.95	1.36	1.25

All (338) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	GLU	CB-CA-C	-13.51	84.44	110.10
1	B	62	ASP	CA-CB-CG	11.38	123.98	112.60
1	A	142	VAL	CB-CA-C	10.10	127.85	111.29
1	A	82	GLU	O-C-N	-9.73	114.65	123.41
1	A	660	GLU	N-CA-C	9.46	122.83	110.43
1	B	366	ASN	CA-CB-CG	9.25	121.85	112.60
1	B	263	ILE	CA-C-N	9.22	138.29	121.70
1	B	263	ILE	C-N-CA	9.22	138.29	121.70
1	A	148	LYS	CA-C-N	8.80	137.54	121.70
1	A	148	LYS	C-N-CA	8.80	137.54	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	262	ARG	CA-C-N	8.78	137.50	121.70
1	B	262	ARG	C-N-CA	8.78	137.50	121.70
1	A	62	ASP	CA-CB-CG	8.77	121.37	112.60
1	A	258	THR	N-CA-C	8.60	121.79	111.82
1	A	145	THR	CA-C-N	8.52	137.03	121.70
1	A	145	THR	C-N-CA	8.52	137.03	121.70
1	A	250	PHE	CA-C-N	8.49	136.98	121.70
1	A	250	PHE	C-N-CA	8.49	136.98	121.70
1	B	82	GLU	CA-C-N	8.30	136.63	121.70
1	B	82	GLU	C-N-CA	8.30	136.63	121.70
1	B	864	ASN	CA-CB-CG	8.23	120.83	112.60
1	A	259	ALA	CA-C-N	8.16	136.38	121.70
1	A	259	ALA	C-N-CA	8.16	136.38	121.70
1	B	744	ILE	CB-CA-C	8.12	124.60	111.29
1	A	82	GLU	CA-C-N	8.08	136.24	121.70
1	A	82	GLU	C-N-CA	8.08	136.24	121.70
1	A	227	ASP	CA-C-N	8.02	130.94	120.60
1	A	227	ASP	C-N-CA	8.02	130.94	120.60
1	B	307	MET	CA-C-N	7.86	131.15	120.38
1	B	307	MET	C-N-CA	7.86	131.15	120.38
1	B	476	ARG	CA-C-N	7.86	131.45	120.29
1	B	476	ARG	C-N-CA	7.86	131.45	120.29
1	B	364	ASP	CA-CB-CG	-7.76	104.84	112.60
1	B	262	ARG	O-C-N	-7.63	113.99	122.92
1	A	142	VAL	O-C-N	-7.62	113.05	122.57
1	A	259	ALA	O-C-N	-7.60	114.68	123.27
1	A	597	THR	O-C-N	-7.45	116.94	121.71
1	A	229	VAL	CA-C-N	7.44	128.20	119.94
1	A	229	VAL	C-N-CA	7.44	128.20	119.94
1	A	99	ASP	CA-CB-CG	-7.43	105.17	112.60
1	B	468	TYR	N-CA-C	7.43	119.02	111.07
1	A	139	ASP	CA-C-N	7.41	135.03	121.70
1	A	139	ASP	C-N-CA	7.41	135.03	121.70
1	A	591	ASN	CA-CB-CG	7.38	119.97	112.60
1	B	782	ASN	CA-CB-CG	7.34	119.94	112.60
1	B	677	LYS	CA-C-N	7.32	129.96	120.44
1	B	677	LYS	C-N-CA	7.32	129.96	120.44
1	B	417	MET	CA-C-N	7.26	130.02	120.28
1	B	417	MET	C-N-CA	7.26	130.02	120.28
1	A	805	PHE	CA-C-N	7.24	129.98	120.28
1	A	805	PHE	C-N-CA	7.24	129.98	120.28
1	A	141	SER	CB-CA-C	7.21	124.77	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	758	HIS	CA-CB-CG	-7.20	106.60	113.80
1	B	731	GLU	N-CA-C	-7.17	105.06	114.31
1	A	144	GLU	CA-C-N	7.16	134.58	121.70
1	A	144	GLU	C-N-CA	7.16	134.58	121.70
1	A	759	PHE	CA-CB-CG	-7.15	106.65	113.80
1	B	568	ALA	CA-C-N	7.06	130.02	120.77
1	B	568	ALA	C-N-CA	7.06	130.02	120.77
1	B	177	GLY	CA-C-N	7.03	130.01	120.38
1	B	177	GLY	C-N-CA	7.03	130.01	120.38
1	A	210	PHE	CA-CB-CG	-7.01	106.79	113.80
1	B	180	PHE	CA-CB-CG	-6.99	106.81	113.80
1	A	444	ASP	CA-CB-CG	6.98	119.58	112.60
1	B	370	GLY	CA-C-N	6.97	127.72	119.98
1	B	370	GLY	C-N-CA	6.97	127.72	119.98
1	A	370	GLY	CA-C-N	6.93	127.68	119.98
1	A	370	GLY	C-N-CA	6.93	127.68	119.98
1	A	735	GLN	N-CA-C	6.92	119.47	111.02
1	A	59	ASP	CA-CB-CG	-6.91	105.69	112.60
1	A	43	ASN	CA-CB-CG	-6.87	105.73	112.60
1	B	542	ILE	N-CA-C	6.83	117.62	110.72
1	B	865	GLY	N-CA-C	6.83	116.42	110.21
1	A	270	ASN	CA-CB-CG	-6.80	105.80	112.60
1	B	421	LYS	CA-C-N	6.80	130.07	120.28
1	B	421	LYS	C-N-CA	6.80	130.07	120.28
1	B	772	PHE	CA-C-N	6.79	129.68	120.38
1	B	772	PHE	C-N-CA	6.79	129.68	120.38
1	A	139	ASP	O-C-N	-6.70	113.67	122.59
1	B	444	ASP	CA-C-N	6.66	129.50	120.38
1	B	444	ASP	C-N-CA	6.66	129.50	120.38
1	A	194	TYR	CA-C-N	6.58	127.42	119.99
1	A	194	TYR	C-N-CA	6.58	127.42	119.99
1	A	100	PHE	CA-CB-CG	-6.55	107.25	113.80
1	A	110	SER	N-CA-CB	6.54	121.54	110.49
1	B	733	GLU	CB-CG-CD	6.54	123.71	112.60
1	A	286	ASP	CA-CB-CG	-6.48	106.12	112.60
1	A	142	VAL	CA-C-N	6.47	133.34	121.70
1	A	142	VAL	C-N-CA	6.47	133.34	121.70
1	A	366	ASN	CA-CB-CG	6.46	119.06	112.60
1	A	444	ASP	CA-C-N	6.44	129.23	120.54
1	A	444	ASP	C-N-CA	6.44	129.23	120.54
1	A	357	SER	CA-C-N	6.41	133.78	121.54
1	A	357	SER	C-N-CA	6.41	133.78	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	387	ILE	N-CA-CB	6.40	117.62	110.51
1	A	180	PHE	CA-CB-CG	-6.38	107.42	113.80
1	B	591	ASN	CA-CB-CG	6.38	118.97	112.60
1	B	781	TYR	N-CA-C	6.37	119.12	108.73
1	B	294	THR	N-CA-C	6.37	118.22	111.28
1	B	711	MET	N-CA-C	6.36	118.29	111.36
1	B	246	PHE	CA-C-N	6.32	129.04	120.38
1	B	246	PHE	C-N-CA	6.32	129.04	120.38
1	B	270	ASN	N-CA-C	6.32	118.30	110.91
1	B	744	ILE	N-CA-C	-6.31	96.22	109.34
1	A	261	ASN	CA-CB-CG	6.25	118.85	112.60
1	B	607	HIS	CA-C-N	6.21	128.62	120.60
1	B	607	HIS	C-N-CA	6.21	128.62	120.60
1	A	868	ALA	N-CA-C	6.21	119.22	109.96
1	A	316	ASP	N-CA-CB	-6.20	100.67	110.22
1	B	846	ARG	N-CA-C	-6.19	103.82	112.12
1	B	744	ILE	O-C-N	-6.19	114.83	122.57
1	B	202	PRO	CA-C-N	6.19	131.03	121.19
1	B	202	PRO	C-N-CA	6.19	131.03	121.19
1	A	487	LEU	CA-C-N	6.17	126.96	119.99
1	A	487	LEU	C-N-CA	6.17	126.96	119.99
1	A	806	GLN	N-CA-C	6.17	118.00	111.28
1	B	336	GLU	CA-C-N	6.16	129.22	120.53
1	B	336	GLU	C-N-CA	6.16	129.22	120.53
1	A	118	ASP	CA-CB-CG	-6.16	106.44	112.60
1	A	626	GLN	N-CA-C	6.13	121.49	111.37
1	B	182	ALA	CA-C-N	6.12	128.40	120.44
1	B	182	ALA	C-N-CA	6.12	128.40	120.44
1	B	625	ARG	CA-C-N	6.09	128.77	120.54
1	B	625	ARG	C-N-CA	6.09	128.77	120.54
1	A	387	ILE	N-CA-CB	6.09	118.37	110.57
1	B	748	GLN	CB-CG-CD	-6.08	102.27	112.60
1	B	507	THR	CA-C-N	6.07	128.43	120.60
1	B	507	THR	C-N-CA	6.07	128.43	120.60
1	B	82	GLU	O-C-N	-6.06	114.53	122.59
1	B	796	ASP	O-C-N	-6.06	114.36	121.32
1	A	62	ASP	CB-CA-C	6.05	121.13	110.85
1	A	692	ASP	CA-C-N	6.04	128.62	120.65
1	A	692	ASP	C-N-CA	6.04	128.62	120.65
1	B	863	TYR	N-CA-C	6.00	123.58	110.80
1	B	117	VAL	N-CA-C	6.00	116.06	110.42
1	B	661	MET	N-CA-C	5.98	118.70	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	393	LEU	CA-C-N	5.96	128.26	120.28
1	B	393	LEU	C-N-CA	5.96	128.26	120.28
1	A	809	ILE	CA-CB-CG1	5.95	120.52	110.40
1	B	200	ASP	CA-C-N	5.95	128.17	120.44
1	B	200	ASP	C-N-CA	5.95	128.17	120.44
1	B	487	LEU	CA-C-N	5.95	126.54	119.94
1	B	487	LEU	C-N-CA	5.95	126.54	119.94
1	A	143	GLU	CA-C-N	5.94	132.40	121.70
1	A	143	GLU	C-N-CA	5.94	132.40	121.70
1	A	473	VAL	CA-C-N	5.93	129.03	120.79
1	A	473	VAL	C-N-CA	5.93	129.03	120.79
1	B	768	ASP	O-C-N	-5.91	115.76	122.68
1	B	137	ILE	N-CA-C	-5.90	99.62	108.12
1	A	226	GLU	CA-C-N	5.89	129.90	121.71
1	A	226	GLU	C-N-CA	5.89	129.90	121.71
1	B	91	ILE	N-CA-CB	5.84	117.00	110.51
1	B	602	ASN	CA-C-N	5.84	126.31	119.94
1	B	602	ASN	C-N-CA	5.84	126.31	119.94
1	B	240	MET	N-CA-C	5.84	118.14	111.02
1	B	887	ASP	N-CA-C	-5.83	98.24	108.20
1	A	202	PRO	CA-C-N	5.82	128.40	120.54
1	A	202	PRO	C-N-CA	5.82	128.40	120.54
1	A	740	ASP	CB-CA-C	5.81	118.90	111.40
1	A	126	GLY	CA-C-N	5.79	128.03	120.28
1	A	126	GLY	C-N-CA	5.79	128.03	120.28
1	B	144	GLU	O-C-N	-5.75	116.66	123.22
1	A	290	TRP	N-CA-C	5.75	117.22	111.07
1	A	354	PHE	N-CA-C	5.73	123.01	110.80
1	B	662	HIS	CB-CG-CD2	-5.72	123.76	131.20
1	A	257	GLU	CA-C-N	5.72	129.00	120.31
1	A	257	GLU	C-N-CA	5.72	129.00	120.31
1	A	863	TYR	N-CA-C	5.70	119.77	113.21
1	A	278	GLU	CA-C-N	5.68	128.21	120.54
1	A	278	GLU	C-N-CA	5.68	128.21	120.54
1	A	449	GLN	CA-C-N	5.68	128.22	120.54
1	A	449	GLN	C-N-CA	5.68	128.22	120.54
1	B	754	ALA	CA-C-N	5.68	128.14	120.65
1	B	754	ALA	C-N-CA	5.68	128.14	120.65
1	A	117	VAL	N-CA-C	5.66	115.74	110.42
1	B	341	THR	N-CA-C	5.66	117.13	111.07
1	B	535	ASP	N-CA-C	5.66	122.86	110.80
1	A	352	PRO	N-CA-C	5.63	120.08	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	669	LEU	CA-C-N	5.63	129.26	120.82
1	B	669	LEU	C-N-CA	5.63	129.26	120.82
1	B	457	ALA	N-CA-C	5.62	118.14	111.33
1	B	670	ASN	CA-CB-CG	5.62	118.22	112.60
1	B	272	GLU	CA-C-N	5.62	127.81	120.28
1	B	272	GLU	C-N-CA	5.62	127.81	120.28
1	B	41	TRP	O-C-N	-5.62	116.17	122.12
1	B	595	THR	CA-C-N	5.61	129.21	120.34
1	B	595	THR	C-N-CA	5.61	129.21	120.34
1	A	782	ASN	CA-CB-CG	5.61	118.21	112.60
1	A	810	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	555	PHE	CA-CB-CG	-5.60	108.20	113.80
1	A	207	ASN	N-CA-C	5.60	119.62	112.34
1	B	738	THR	N-CA-C	5.58	122.69	110.80
1	A	152	LEU	N-CA-C	5.57	117.81	111.02
1	A	250	PHE	O-C-N	-5.56	115.19	122.59
1	B	235	ASP	CA-C-N	5.56	128.05	120.54
1	B	235	ASP	C-N-CA	5.56	128.05	120.54
1	A	315	GLU	CA-C-N	5.55	128.28	120.28
1	A	315	GLU	C-N-CA	5.55	128.28	120.28
1	B	839	ILE	O-C-N	-5.54	117.20	123.18
1	B	361	MET	CA-C-N	5.52	128.31	120.53
1	B	361	MET	C-N-CA	5.52	128.31	120.53
1	B	812	MET	CA-C-N	5.51	127.94	120.44
1	B	812	MET	C-N-CA	5.51	127.94	120.44
1	B	260	ALA	CA-C-N	5.51	132.06	121.54
1	B	260	ALA	C-N-CA	5.51	132.06	121.54
1	A	720	GLN	CA-C-N	5.51	127.66	120.28
1	A	720	GLN	C-N-CA	5.51	127.66	120.28
1	A	336	GLU	CA-C-N	5.50	127.99	120.46
1	A	336	GLU	C-N-CA	5.50	127.99	120.46
1	A	591	ASN	O-C-N	-5.50	116.02	121.19
1	B	263	ILE	O-C-N	-5.50	114.20	123.00
1	B	597	THR	O-C-N	-5.49	116.69	121.35
1	B	819	THR	N-CA-C	-5.47	104.86	112.30
1	A	859	ARG	N-CA-C	5.46	117.31	111.36
1	A	177	GLY	CA-C-N	5.45	129.00	120.82
1	A	177	GLY	C-N-CA	5.45	129.00	120.82
1	A	241	THR	N-CA-CB	5.44	118.60	110.22
1	A	155	TYR	CA-C-N	5.44	127.88	120.54
1	A	155	TYR	C-N-CA	5.44	127.88	120.54
1	B	799	ARG	N-CA-CB	5.44	119.68	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	27	ASP	CA-CB-CG	-5.44	107.16	112.60
1	A	476	ARG	CA-C-N	5.43	128.56	120.31
1	A	476	ARG	C-N-CA	5.43	128.56	120.31
1	A	142	VAL	N-CA-CB	-5.42	102.28	111.23
1	A	825	VAL	CA-C-N	5.41	127.80	120.38
1	A	825	VAL	C-N-CA	5.41	127.80	120.38
1	A	326	PRO	N-CA-C	5.41	117.30	110.70
1	A	362	VAL	CB-CA-C	-5.38	104.82	111.70
1	B	357	SER	N-CA-C	5.38	118.81	111.39
1	A	612	VAL	CA-C-N	5.37	126.56	119.84
1	A	612	VAL	C-N-CA	5.37	126.56	119.84
1	A	75	GLY	CA-C-N	5.37	131.79	121.54
1	A	75	GLY	C-N-CA	5.37	131.79	121.54
1	A	668	GLN	CA-C-N	5.37	128.47	120.31
1	A	668	GLN	C-N-CA	5.37	128.47	120.31
1	B	83	ARG	N-CA-CB	5.36	119.62	110.50
1	A	784	GLY	CA-C-N	5.35	131.75	121.54
1	A	784	GLY	C-N-CA	5.35	131.75	121.54
1	A	139	ASP	CB-CA-C	5.34	121.06	110.42
1	A	181	CYS	CA-C-N	5.34	127.70	120.44
1	A	181	CYS	C-N-CA	5.34	127.70	120.44
1	B	449	GLN	CA-C-N	5.33	127.69	120.38
1	B	449	GLN	C-N-CA	5.33	127.69	120.38
1	A	61	ARG	CA-C-N	5.32	127.85	120.29
1	A	61	ARG	C-N-CA	5.32	127.85	120.29
1	A	656	ARG	CA-C-N	5.32	131.55	121.97
1	A	656	ARG	C-N-CA	5.32	131.55	121.97
1	B	38	PHE	CA-C-N	5.32	127.67	120.44
1	B	38	PHE	C-N-CA	5.32	127.67	120.44
1	B	626	GLN	N-CA-C	5.32	117.49	111.11
1	A	148	LYS	O-C-N	-5.30	115.54	122.59
1	A	741	ALA	CB-CA-C	5.29	120.95	110.42
1	A	376	GLU	N-CA-C	5.28	117.04	111.28
1	A	257	GLU	O-C-N	-5.27	115.58	122.59
1	B	326	PRO	CA-C-O	-5.27	112.92	120.56
1	A	769	CYS	CA-C-N	5.27	127.34	120.28
1	A	769	CYS	C-N-CA	5.27	127.34	120.28
1	B	654	ILE	CA-C-N	5.26	131.73	121.41
1	B	654	ILE	C-N-CA	5.26	131.73	121.41
1	A	481	CYS	CA-C-N	5.26	127.85	120.28
1	A	481	CYS	C-N-CA	5.26	127.85	120.28
1	A	385	ASN	N-CA-C	5.25	117.01	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	ASP	CA-CB-CG	-5.25	107.35	112.60
1	B	43	ASN	CA-CB-CG	-5.24	107.36	112.60
1	A	113	ALA	CA-C-N	5.23	127.60	120.54
1	A	113	ALA	C-N-CA	5.23	127.60	120.54
1	A	277	MET	N-CA-C	5.23	118.45	111.75
1	B	169	ASN	N-CA-C	5.23	117.69	108.75
1	A	839	ILE	O-C-N	-5.22	117.02	123.03
1	B	520	ALA	CB-CA-C	5.22	120.46	110.17
1	A	163	LYS	CA-C-N	5.21	130.12	121.99
1	A	163	LYS	C-N-CA	5.21	130.12	121.99
1	A	733	GLU	CA-C-N	5.21	131.49	121.54
1	A	733	GLU	C-N-CA	5.21	131.49	121.54
1	B	187	HIS	CA-CB-CG	-5.20	108.60	113.80
1	B	558	THR	CA-CB-OG1	5.20	117.40	109.60
1	B	744	ILE	N-CA-CB	-5.20	102.65	111.23
1	A	629	ASN	N-CA-CB	5.20	118.22	110.22
1	A	712	GLU	N-CA-C	5.20	116.95	111.28
1	A	437	LYS	CA-C-N	5.20	127.24	120.28
1	A	437	LYS	C-N-CA	5.20	127.24	120.28
1	B	750	ASN	N-CA-CB	5.19	117.81	110.13
1	A	325	LYS	N-CA-C	5.18	119.22	112.17
1	B	369	TRP	CA-C-N	5.18	125.73	119.98
1	B	369	TRP	C-N-CA	5.18	125.73	119.98
1	B	384	LEU	N-CA-C	5.18	117.00	111.36
1	B	885	GLU	CB-CA-C	5.17	120.71	110.42
1	A	710	THR	N-CA-CB	5.17	119.22	110.49
1	A	628	GLN	CB-CG-CD	5.16	121.38	112.60
1	B	113	ALA	CA-C-N	5.16	127.20	120.28
1	B	113	ALA	C-N-CA	5.16	127.20	120.28
1	A	438	HIS	ND1-CG-CD2	5.16	111.26	106.10
1	A	229	VAL	CB-CA-C	-5.16	105.72	111.80
1	B	612	VAL	CA-C-N	5.15	126.27	119.84
1	B	612	VAL	C-N-CA	5.15	126.27	119.84
1	B	401	ARG	CD-NE-CZ	-5.15	117.20	124.40
1	A	520	ALA	CB-CA-C	5.14	120.30	110.17
1	B	745	SER	O-C-N	-5.14	115.75	122.59
1	B	823	ASP	N-CA-C	5.14	116.88	111.28
1	B	273	ASN	CA-CB-CG	-5.13	107.47	112.60
1	A	95	ASN	CA-CB-CG	-5.13	107.47	112.60
1	A	33	GLN	CA-C-N	5.13	127.40	120.38
1	A	33	GLN	C-N-CA	5.13	127.40	120.38
1	A	490	LEU	CA-C-N	5.13	128.10	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	490	LEU	C-N-CA	5.13	128.10	120.31
1	A	149	GLU	CA-C-N	5.12	130.92	121.70
1	A	149	GLU	C-N-CA	5.12	130.92	121.70
1	A	159	THR	CA-C-N	5.12	126.15	120.06
1	A	159	THR	C-N-CA	5.12	126.15	120.06
1	B	683	LYS	N-CA-C	5.12	121.12	109.81
1	A	717	GLY	CA-C-N	5.12	127.13	120.28
1	A	717	GLY	C-N-CA	5.12	127.13	120.28
1	A	796	ASP	O-C-N	-5.11	117.09	121.23
1	B	227	ASP	CA-C-N	5.11	128.54	120.47
1	B	227	ASP	C-N-CA	5.11	128.54	120.47
1	A	142	VAL	CA-CB-CG1	5.10	119.07	110.40
1	B	603	GLY	CA-C-N	5.08	127.35	120.38
1	B	603	GLY	C-N-CA	5.08	127.35	120.38
1	B	797	PRO	N-CA-C	-5.07	109.40	114.68
1	A	261	ASN	CA-C-N	5.07	131.23	121.54
1	A	261	ASN	C-N-CA	5.07	131.23	121.54
1	A	164	ASN	CA-CB-CG	-5.07	107.53	112.60
1	A	267	LEU	N-CA-C	-5.06	100.27	108.41
1	A	694	GLN	CA-C-N	5.06	127.82	120.79
1	A	694	GLN	C-N-CA	5.06	127.82	120.79
1	B	758	HIS	ND1-CG-CD2	5.06	111.16	106.10
1	A	540	HIS	CA-CB-CG	-5.05	108.75	113.80
1	B	150	GLY	CA-C-N	5.05	127.31	120.65
1	B	150	GLY	C-N-CA	5.05	127.31	120.65
1	A	250	PHE	CA-CB-CG	-5.03	108.77	113.80
1	B	67	MET	CG-SD-CE	-5.02	89.86	100.90
1	B	426	ALA	N-CA-C	5.02	114.26	108.49
1	B	126	GLY	CA-C-N	5.01	126.95	120.44
1	B	126	GLY	C-N-CA	5.01	126.95	120.44
1	A	235	ASP	CA-C-N	5.01	127.92	120.31
1	A	235	ASP	C-N-CA	5.01	127.92	120.31
1	B	657	ILE	CA-C-N	5.00	131.10	121.54
1	B	657	ILE	C-N-CA	5.00	131.10	121.54

There are no chirality outliers.

All (111) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ASP	Peptide
1	A	134	ARG	Sidechain
1	A	136	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	A	141	SER	Peptide
1	A	148	LYS	Peptide
1	A	157	ARG	Sidechain
1	A	162	TYR	Sidechain
1	A	186	ARG	Sidechain
1	A	194	TYR	Sidechain
1	A	198	ARG	Sidechain
1	A	216	TYR	Sidechain
1	A	242	TYR	Sidechain
1	A	247	TYR	Sidechain
1	A	256	ALA	Peptide
1	A	257	GLU	Peptide
1	A	26	LEU	Peptide
1	A	262	ARG	Sidechain
1	A	27	ASP	Peptide
1	A	280	TYR	Sidechain
1	A	292	ARG	Sidechain
1	A	318	ARG	Sidechain
1	A	320	TYR	Sidechain
1	A	389	ARG	Sidechain
1	A	401	ARG	Sidechain
1	A	423	TYR	Sidechain
1	A	451	ARG	Sidechain
1	A	467	TYR	Sidechain
1	A	476	ARG	Sidechain
1	A	494	ARG	Sidechain
1	A	495	ARG	Sidechain
1	A	512	TYR	Sidechain
1	A	540	HIS	Sidechain
1	A	552	HIS	Sidechain
1	A	56	ILE	Peptide
1	A	566	ARG	Sidechain
1	A	573	HIS	Sidechain
1	A	58	GLU	Peptide
1	A	607	HIS	Sidechain
1	A	614	ARG	Sidechain
1	A	623	HIS	Sidechain
1	A	624	ALA	Peptide
1	A	633	ARG	Sidechain
1	A	636	PHE	Sidechain
1	A	675	TYR	Sidechain
1	A	727	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	745	SER	Peptide
1	A	753	ARG	Sidechain
1	A	758	HIS	Sidechain
1	A	759	PHE	Peptide
1	A	799	ARG	Sidechain
1	A	814	ARG	Sidechain
1	A	83	ARG	Sidechain
1	A	859	ARG	Sidechain
1	A	863	TYR	Peptide
1	A	883	TYR	Sidechain
1	B	118	ASP	Peptide
1	B	134	ARG	Sidechain
1	B	155	TYR	Sidechain
1	B	157	ARG	Sidechain
1	B	186	ARG	Sidechain
1	B	199	LYS	Peptide
1	B	229	VAL	Peptide
1	B	233	ARG	Sidechain
1	B	26	LEU	Peptide
1	B	27	ASP	Peptide
1	B	293	ARG	Sidechain
1	B	301	ARG	Sidechain
1	B	320	TYR	Sidechain
1	B	321	ARG	Sidechain
1	B	355	MET	Peptide
1	B	376	GLU	Peptide
1	B	379	TYR	Sidechain
1	B	388	ARG	Sidechain
1	B	401	ARG	Sidechain
1	B	423	TYR	Sidechain
1	B	438	HIS	Sidechain
1	B	451	ARG	Sidechain
1	B	467	TYR	Sidechain
1	B	47	ARG	Sidechain
1	B	476	ARG	Sidechain
1	B	494	ARG	Sidechain
1	B	495	ARG	Sidechain
1	B	515	TYR	Sidechain
1	B	573	HIS	Sidechain
1	B	58	GLU	Peptide
1	B	583	TYR	Sidechain
1	B	593	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	614	ARG	Sidechain
1	B	631	ARG	Sidechain
1	B	656	ARG	Sidechain
1	B	660	GLU	Peptide
1	B	673	ARG	Sidechain
1	B	675	TYR	Sidechain
1	B	730	ASN	Peptide
1	B	738	THR	Peptide
1	B	739	ARG	Sidechain
1	B	745	SER	Peptide
1	B	761	ARG	Sidechain
1	B	77	ARG	Sidechain
1	B	780	GLY	Peptide
1	B	781	TYR	Peptide
1	B	799	ARG	Sidechain
1	B	805	PHE	Sidechain
1	B	818	ASP	Peptide
1	B	819	THR	Peptide
1	B	83	ARG	Sidechain
1	B	845	ARG	Sidechain
1	B	846	ARG	Sidechain
1	B	866	ARG	Sidechain
1	B	886	SER	Peptide
1	B	887	ASP	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	A	7007	0	6898	28	172
1	B	7007	0	6898	23	160
All	All	14014	0	13796	48	209

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 2.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLU:HB2	1:A:150:GLY:CA	2.09	0.81
1:B:585:VAL:HG12	1:B:586:ASN:H	1.64	0.61
1:A:741:ALA:HB1	1:A:742:LYS:HA	1.83	0.60
1:A:149:GLU:HB2	1:A:150:GLY:HA3	1.88	0.56
1:A:852:GLN:NE2	1:B:149:GLU:OE2	2.32	0.55
1:B:91:ILE:HA	1:B:117:VAL:HG21	1.89	0.54
1:B:605:TRP:HE1	1:B:609:ARG:CZ	2.21	0.53
1:A:114:GLU:CD	1:A:114:GLU:H	2.17	0.52
1:A:259:ALA:HA	1:A:260:ALA:HB3	1.90	0.52
1:A:761:ARG:HA	1:A:761:ARG:HE	1.74	0.52
1:B:662:HIS:CD2	1:B:830:LYS:HE2	2.45	0.51
1:B:736:ILE:HG21	1:B:888:LEU:HD22	1.93	0.50
1:B:298:LEU:HB2	1:B:375:ALA:HB1	1.94	0.50
1:A:348:LEU:HD13	1:B:743:GLY:C	2.38	0.49
1:B:654:ILE:HG21	1:B:724:THR:HG22	1.95	0.48
1:B:666:GLU:H	1:B:666:GLU:CD	2.22	0.48
1:A:91:ILE:HG22	1:A:117:VAL:HG21	1.97	0.46
1:A:512:TYR:CZ	1:A:576:VAL:HG11	2.51	0.45
1:A:142:VAL:CG1	1:A:143:GLU:HA	2.46	0.45
1:B:653:GLU:C	1:B:655:GLY:H	2.24	0.45
1:B:223:LEU:HD12	1:B:242:TYR:CD2	2.52	0.45
1:A:665:LEU:HD11	1:A:739:ARG:HH21	1.82	0.45
1:A:73:ILE:HD12	1:A:134:ARG:HH21	1.82	0.44
1:A:665:LEU:CD1	1:A:739:ARG:HH21	2.30	0.44
1:B:669:LEU:HD12	1:B:818:ASP:HB3	2.01	0.43
1:A:741:ALA:HB1	1:A:742:LYS:CA	2.49	0.43
1:A:269:VAL:O	1:A:273:ASN:HB2	2.19	0.42
1:A:288:LEU:HD21	1:A:365:ILE:HG23	2.00	0.42
1:B:192:ILE:HG13	1:B:193:ASP:H	1.84	0.42
1:A:272:GLU:HA	1:B:805:PHE:CG	2.54	0.42
1:A:346:LEU:HD13	1:A:353:ALA:HB2	2.02	0.42
1:B:181:CYS:HB3	1:B:197:LEU:HD13	2.02	0.41
1:B:85:LYS:HA	1:B:90:LYS:HE2	2.02	0.41
1:B:658:SER:HA	1:B:668:GLN:HG3	2.01	0.41
1:A:665:LEU:HG	1:A:739:ARG:HH21	1.86	0.41
1:B:114:GLU:H	1:B:114:GLU:CD	2.28	0.41
1:A:756:PHE:CE2	1:A:767:MET:HE3	2.55	0.41
1:B:669:LEU:HD22	1:B:669:LEU:HA	1.97	0.41
1:A:732:VAL:C	1:A:734:ASN:H	2.29	0.40
1:B:94:VAL:HG11	1:B:116:ILE:HB	2.02	0.40
1:A:455:ILE:HG22	1:A:477:CYS:SG	2.61	0.40
1:A:665:LEU:CG	1:A:739:ARG:HH21	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:THR:HA	1:A:146:SER:C	2.46	0.40
1:A:268:ALA:C	1:A:270:ASN:H	2.29	0.40
1:A:759:PHE:HB2	1:A:767:MET:HE2	2.02	0.40
1:B:199:LYS:C	1:B:199:LYS:HZ2	2.30	0.40
1:A:525:TRP:CZ3	1:A:605:TRP:CZ3	3.10	0.40
1:B:223:LEU:CD1	1:B:228:ILE:HD13	2.52	0.40

All (209) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:ASN:CB	1:B:845:ARG:CZ[1_665]	0.31	1.89
1:A:836:LYS:CE	1:B:828:SER:CB[1_665]	0.32	1.88
1:A:89:HIS:CD2	1:A:813:SER:O[1_445]	0.48	1.72
1:B:81:PRO:CD	1:B:301:ARG:NH1[2_555]	0.68	1.52
1:B:81:PRO:CB	1:B:301:ARG:NH2[2_555]	0.68	1.52
1:A:866:ARG:O	1:B:840:THR:O[1_665]	0.70	1.50
1:A:863:TYR:CA	1:B:847:GLU:C[1_665]	0.71	1.49
1:B:352:PRO:CB	1:B:358:GLU:CA[2_555]	0.75	1.45
1:B:352:PRO:CD	1:B:358:GLU:CB[2_555]	0.77	1.43
1:A:81:PRO:O	1:A:817:ALA:C[1_445]	0.79	1.41
1:A:863:TYR:CD1	1:B:847:GLU:N[1_665]	0.83	1.37
1:A:863:TYR:CE2	1:B:843:GLU:O[1_665]	0.83	1.37
1:A:89:HIS:NE2	1:A:813:SER:C[1_445]	0.90	1.30
1:A:869:VAL:CG1	1:B:832:LEU:CA[1_665]	0.92	1.28
1:B:81:PRO:CG	1:B:301:ARG:CZ[2_555]	0.94	1.26
1:B:352:PRO:CG	1:B:358:GLU:CA[2_555]	0.99	1.21
1:A:863:TYR:CB	1:B:847:GLU:C[1_665]	1.02	1.18
1:A:863:TYR:CA	1:B:848:LEU:N[1_665]	1.04	1.16
1:A:863:TYR:CG	1:B:847:GLU:CA[1_665]	1.04	1.16
1:A:81:PRO:CA	1:A:818:ASP:CB[1_445]	1.07	1.13
1:A:874:ASP:CG	1:B:849:PRO:CG[1_665]	1.07	1.13
1:A:864:ASN:CB	1:B:845:ARG:NH2[1_665]	1.10	1.10
1:A:863:TYR:C	1:B:848:LEU:N[1_665]	1.12	1.08
1:A:864:ASN:O	1:B:853:ALA:CB[1_665]	1.12	1.08
1:B:352:PRO:CG	1:B:358:GLU:CB[2_555]	1.14	1.06
1:A:81:PRO:CB	1:A:818:ASP:CB[1_445]	1.16	1.04
1:A:836:LYS:NZ	1:B:828:SER:CB[1_665]	1.16	1.04
1:A:863:TYR:N	1:B:847:GLU:O[1_665]	1.16	1.04
1:B:81:PRO:CG	1:B:301:ARG:NH2[2_555]	1.16	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:ALA:CB	1:B:843:GLU:CB[1_665]	1.18	1.02
1:A:89:HIS:NE2	1:A:813:SER:O[1_445]	1.19	1.01
1:A:836:LYS:NZ	1:B:828:SER:CA[1_665]	1.20	1.00
1:A:867:ASP:OD2	1:B:844:LEU:CD2[1_665]	1.23	0.97
1:B:81:PRO:CB	1:B:301:ARG:CZ[2_555]	1.24	0.96
1:A:866:ARG:NE	1:B:873:LEU:CD2[1_665]	1.25	0.95
1:A:89:HIS:CG	1:A:813:SER:O[1_445]	1.26	0.94
1:A:863:TYR:CA	1:B:847:GLU:O[1_665]	1.26	0.94
1:A:863:TYR:CB	1:B:847:GLU:CA[1_665]	1.27	0.93
1:A:868:ALA:O	1:B:832:LEU:O[1_665]	1.27	0.93
1:B:352:PRO:CB	1:B:358:GLU:N[2_555]	1.28	0.92
1:A:863:TYR:CG	1:B:847:GLU:CB[1_665]	1.29	0.91
1:A:863:TYR:CG	1:B:847:GLU:N[1_665]	1.29	0.91
1:B:81:PRO:CG	1:B:301:ARG:NH1[2_555]	1.29	0.91
1:A:866:ARG:C	1:B:840:THR:O[1_665]	1.32	0.88
1:A:864:ASN:CB	1:B:845:ARG:NH1[1_665]	1.33	0.87
1:B:83:ARG:NH2	1:B:382:TRP:N[2_555]	1.34	0.86
1:B:352:PRO:N	1:B:358:GLU:CB[2_555]	1.34	0.86
1:B:352:PRO:CD	1:B:358:GLU:CG[2_555]	1.35	0.85
1:A:863:TYR:CD1	1:B:847:GLU:CA[1_665]	1.36	0.84
1:A:838:TYR:CZ	1:B:832:LEU:CD1[1_665]	1.37	0.83
1:A:865:GLY:O	1:B:841:VAL:O[1_665]	1.37	0.83
1:A:866:ARG:CD	1:B:873:LEU:CD2[1_665]	1.38	0.82
1:A:864:ASN:CA	1:B:845:ARG:NH2[1_665]	1.39	0.81
1:A:81:PRO:O	1:A:817:ALA:CA[1_445]	1.42	0.78
1:A:836:LYS:CE	1:B:828:SER:OG[1_665]	1.42	0.78
1:A:865:GLY:O	1:B:845:ARG:N[1_665]	1.42	0.78
1:A:872:ALA:CA	1:B:847:GLU:OE1[1_665]	1.42	0.78
1:A:869:VAL:CG1	1:B:832:LEU:N[1_665]	1.43	0.77
1:A:88:VAL:CG1	1:A:814:ARG:NE[1_445]	1.44	0.76
1:B:352:PRO:N	1:B:358:GLU:CG[2_555]	1.44	0.76
1:A:864:ASN:CG	1:B:845:ARG:CZ[1_665]	1.45	0.75
1:A:81:PRO:CB	1:A:818:ASP:CA[1_445]	1.46	0.74
1:A:89:HIS:CD2	1:A:813:SER:C[1_445]	1.48	0.72
1:A:863:TYR:N	1:B:847:GLU:C[1_665]	1.48	0.72
1:A:863:TYR:O	1:B:848:LEU:N[1_665]	1.48	0.72
1:A:863:TYR:CZ	1:B:843:GLU:O[1_665]	1.49	0.71
1:A:81:PRO:O	1:A:818:ASP:N[1_445]	1.50	0.70
1:A:864:ASN:CG	1:B:845:ARG:NH2[1_665]	1.50	0.70
1:A:872:ALA:N	1:B:847:GLU:OE1[1_665]	1.50	0.70
1:A:872:ALA:CB	1:B:847:GLU:OE1[1_665]	1.50	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:GLU:CG	1:A:817:ALA:CB[1_445]	1.53	0.67
1:A:89:HIS:ND1	1:A:814:ARG:CG[1_445]	1.53	0.67
1:A:81:PRO:CG	1:A:818:ASP:CB[1_445]	1.54	0.66
1:A:865:GLY:N	1:B:845:ARG:CA[1_665]	1.54	0.66
1:A:30:TRP:NE1	1:A:233:ARG:O[2_345]	1.55	0.65
1:A:863:TYR:CB	1:B:848:LEU:N[1_665]	1.55	0.65
1:A:864:ASN:CG	1:B:845:ARG:NE[1_665]	1.55	0.65
1:A:866:ARG:N	1:B:844:LEU:CG[1_665]	1.55	0.65
1:A:863:TYR:CB	1:B:847:GLU:CB[1_665]	1.57	0.63
1:B:352:PRO:CG	1:B:358:GLU:C[2_555]	1.57	0.63
1:A:866:ARG:NH1	1:B:860:MET:CG[1_665]	1.58	0.62
1:B:81:PRO:N	1:B:301:ARG:NH1[2_555]	1.59	0.61
1:A:864:ASN:N	1:B:848:LEU:O[1_665]	1.61	0.59
1:A:864:ASN:CB	1:B:845:ARG:NE[1_665]	1.61	0.59
1:B:352:PRO:CB	1:B:358:GLU:CB[2_555]	1.62	0.58
1:A:868:ALA:C	1:B:832:LEU:O[1_665]	1.63	0.57
1:A:874:ASP:OD1	1:B:849:PRO:CG[1_665]	1.63	0.57
1:A:867:ASP:CG	1:B:844:LEU:CD2[1_665]	1.64	0.56
1:A:874:ASP:CB	1:B:849:PRO:CG[1_665]	1.65	0.55
1:A:89:HIS:CE1	1:A:814:ARG:CB[1_445]	1.66	0.54
1:A:836:LYS:CD	1:B:828:SER:CB[1_665]	1.66	0.54
1:A:864:ASN:OD1	1:B:845:ARG:NE[1_665]	1.66	0.54
1:B:81:PRO:CD	1:B:301:ARG:CZ[2_555]	1.67	0.53
1:A:81:PRO:N	1:A:818:ASP:CB[1_445]	1.68	0.52
1:A:863:TYR:CE1	1:B:847:GLU:N[1_665]	1.68	0.52
1:B:81:PRO:CA	1:B:301:ARG:CZ[2_555]	1.68	0.52
1:A:81:PRO:C	1:A:818:ASP:N[1_445]	1.69	0.51
1:A:88:VAL:CG1	1:A:814:ARG:CD[1_445]	1.69	0.51
1:A:866:ARG:NH1	1:B:860:MET:SD[1_665]	1.69	0.51
1:A:864:ASN:N	1:B:845:ARG:NH2[1_665]	1.70	0.50
1:A:81:PRO:CA	1:A:818:ASP:CA[1_445]	1.71	0.49
1:A:89:HIS:CE1	1:A:814:ARG:CG[1_445]	1.72	0.48
1:A:864:ASN:CA	1:B:845:ARG:CZ[1_665]	1.72	0.48
1:A:89:HIS:NE2	1:A:814:ARG:N[1_445]	1.73	0.47
1:A:865:GLY:C	1:B:845:ARG:N[1_665]	1.73	0.47
1:A:867:ASP:N	1:B:844:LEU:CB[1_665]	1.73	0.47
1:A:81:PRO:O	1:A:817:ALA:O[1_445]	1.74	0.46
1:A:83:ARG:NH2	1:A:820:ASP:CG[1_445]	1.74	0.46
1:A:253:ALA:CB	1:A:253:ALA:CB[2_345]	1.75	0.45
1:A:838:TYR:OH	1:B:832:LEU:CD1[1_665]	1.76	0.44
1:A:867:ASP:N	1:B:844:LEU:CG[1_665]	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:LYS:CE	1:B:828:SER:CA[1_665]	1.78	0.42
1:A:864:ASN:ND2	1:B:845:ARG:NH2[1_665]	1.78	0.42
1:A:81:PRO:C	1:A:817:ALA:C[1_445]	1.79	0.41
1:A:863:TYR:C	1:B:848:LEU:CA[1_665]	1.80	0.40
1:A:865:GLY:N	1:B:845:ARG:N[1_665]	1.80	0.40
1:A:867:ASP:OD2	1:B:844:LEU:CG[1_665]	1.80	0.40
1:B:81:PRO:N	1:B:301:ARG:CZ[2_555]	1.81	0.39
1:B:352:PRO:CA	1:B:358:GLU:CB[2_555]	1.81	0.39
1:A:83:ARG:NH2	1:A:820:ASP:CB[1_445]	1.84	0.36
1:A:866:ARG:O	1:B:840:THR:C[1_665]	1.85	0.35
1:A:89:HIS:CE1	1:A:813:SER:O[1_445]	1.87	0.33
1:A:29:ALA:CA	1:A:235:ASP:OD2[2_345]	1.89	0.31
1:A:868:ALA:CB	1:B:843:GLU:CA[1_665]	1.89	0.31
1:B:83:ARG:CZ	1:B:382:TRP:N[2_555]	1.89	0.31
1:A:867:ASP:CA	1:B:839:ILE:CG1[1_665]	1.90	0.30
1:A:89:HIS:CE1	1:A:814:ARG:CA[1_445]	1.91	0.29
1:A:867:ASP:CB	1:B:839:ILE:CD1[1_665]	1.91	0.29
1:A:874:ASP:CB	1:B:849:PRO:CD[1_665]	1.91	0.29
1:A:838:TYR:OH	1:B:828:SER:O[1_665]	1.92	0.28
1:A:863:TYR:CA	1:B:848:LEU:CA[1_665]	1.92	0.28
1:A:866:ARG:N	1:B:844:LEU:CD1[1_665]	1.92	0.28
1:A:874:ASP:OD2	1:B:849:PRO:CG[1_665]	1.92	0.28
1:A:863:TYR:O	1:B:844:LEU:O[1_665]	1.93	0.27
1:A:867:ASP:N	1:B:844:LEU:CD2[1_665]	1.93	0.27
1:B:81:PRO:CA	1:B:301:ARG:NE[2_555]	1.93	0.27
1:B:82:GLU:OE2	1:B:378:GLY:CA[2_555]	1.93	0.27
1:A:89:HIS:NE2	1:A:813:SER:CA[1_445]	1.94	0.26
1:A:89:HIS:ND1	1:A:813:SER:O[1_445]	1.94	0.26
1:A:838:TYR:CE2	1:B:832:LEU:CD1[1_665]	1.94	0.26
1:A:863:TYR:O	1:B:848:LEU:CA[1_665]	1.94	0.26
1:B:82:GLU:OE2	1:B:377:LYS:O[2_555]	1.94	0.26
1:A:89:HIS:CE1	1:A:814:ARG:N[1_445]	1.95	0.25
1:A:89:HIS:CE1	1:A:813:SER:C[1_445]	1.95	0.25
1:A:863:TYR:CD1	1:B:846:ARG:C[1_665]	1.95	0.25
1:A:863:TYR:O	1:B:848:LEU:CB[1_665]	1.95	0.25
1:A:863:TYR:CE2	1:B:843:GLU:C[1_665]	1.95	0.25
1:A:867:ASP:O	1:B:839:ILE:CD1[1_665]	1.95	0.25
1:A:869:VAL:N	1:B:832:LEU:O[1_665]	1.95	0.25
1:B:352:PRO:CG	1:B:359:GLY:N[2_555]	1.96	0.24
1:A:836:LYS:NZ	1:B:828:SER:C[1_665]	1.98	0.22
1:B:352:PRO:CG	1:B:358:GLU:CG[2_555]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:836:LYS:NZ	1:B:828:SER:OG[1_665]	1.99	0.21
1:B:83:ARG:NE	1:B:382:TRP:N[2_555]	1.99	0.21
1:A:81:PRO:CA	1:A:818:ASP:N[1_445]	2.00	0.20
1:A:81:PRO:CD	1:A:818:ASP:CB[1_445]	2.00	0.20
1:A:83:ARG:NH1	1:A:816:THR:O[1_445]	2.01	0.19
1:A:862:PRO:C	1:B:847:GLU:O[1_665]	2.01	0.19
1:B:81:PRO:CB	1:B:301:ARG:NE[2_555]	2.01	0.19
1:A:863:TYR:CE1	1:B:846:ARG:CB[1_665]	2.02	0.18
1:A:866:ARG:CB	1:B:841:VAL:CA[1_665]	2.03	0.17
1:B:351:ARG:C	1:B:358:GLU:CG[2_555]	2.03	0.17
1:A:81:PRO:CB	1:A:818:ASP:N[1_445]	2.04	0.16
1:A:863:TYR:CD2	1:B:847:GLU:CB[1_665]	2.04	0.16
1:A:863:TYR:C	1:B:847:GLU:C[1_665]	2.04	0.16
1:A:866:ARG:CZ	1:B:873:LEU:CD2[1_665]	2.05	0.15
1:A:869:VAL:CG1	1:B:832:LEU:CB[1_665]	2.05	0.15
1:A:863:TYR:C	1:B:848:LEU:O[1_665]	2.06	0.14
1:A:865:GLY:O	1:B:845:ARG:CA[1_665]	2.06	0.14
1:A:80:LYS:O	1:A:818:ASP:OD1[1_445]	2.07	0.13
1:A:863:TYR:CB	1:B:847:GLU:O[1_665]	2.07	0.13
1:A:866:ARG:CA	1:B:840:THR:O[1_665]	2.07	0.13
1:A:863:TYR:OH	1:B:843:GLU:O[1_665]	2.08	0.12
1:A:863:TYR:CG	1:B:847:GLU:C[1_665]	2.08	0.12
1:A:81:PRO:CB	1:A:817:ALA:O[1_445]	2.09	0.11
1:A:254:GLN:OE1	1:A:254:GLN:NE2[2_345]	2.09	0.11
1:A:866:ARG:CA	1:B:841:VAL:CA[1_665]	2.09	0.11
1:A:867:ASP:CA	1:B:839:ILE:CD1[1_665]	2.09	0.11
1:A:88:VAL:CB	1:A:814:ARG:CD[1_445]	2.10	0.10
1:A:868:ALA:CB	1:B:843:GLU:CG[1_665]	2.11	0.09
1:B:83:ARG:NH2	1:B:381:GLU:C[2_555]	2.11	0.09
1:A:81:PRO:CA	1:A:818:ASP:CG[1_445]	2.13	0.07
1:B:352:PRO:CD	1:B:358:GLU:CD[2_555]	2.13	0.07
1:A:81:PRO:N	1:A:818:ASP:CG[1_445]	2.14	0.06
1:A:863:TYR:CD2	1:B:844:LEU:O[1_665]	2.14	0.06
1:A:865:GLY:CA	1:B:845:ARG:N[1_665]	2.14	0.06
1:A:866:ARG:CB	1:B:841:VAL:N[1_665]	2.14	0.06
1:A:867:ASP:C	1:B:839:ILE:CD1[1_665]	2.14	0.06
1:B:81:PRO:CA	1:B:301:ARG:NH2[2_555]	2.14	0.06
1:B:352:PRO:CA	1:B:358:GLU:CA[2_555]	2.14	0.06
1:A:81:PRO:CB	1:A:818:ASP:C[1_445]	2.15	0.05
1:A:863:TYR:CD2	1:B:843:GLU:O[1_665]	2.15	0.05
1:A:865:GLY:C	1:B:841:VAL:O[1_665]	2.15	0.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:GLY:O	1:B:845:ARG:CB[1_665]	2.15	0.05
1:A:872:ALA:C	1:B:847:GLU:OE1[1_665]	2.15	0.05
1:B:83:ARG:NH2	1:B:381:GLU:N[2_555]	2.15	0.05
1:A:129:TRP:CH2	1:A:237:LYS:O[2_345]	2.16	0.04
1:A:863:TYR:CD1	1:B:847:GLU:CB[1_665]	2.16	0.04
1:A:863:TYR:CD2	1:B:847:GLU:N[1_665]	2.16	0.04
1:B:81:PRO:CG	1:B:301:ARG:NE[2_555]	2.16	0.04
1:A:863:TYR:CA	1:B:847:GLU:CA[1_665]	2.17	0.03
1:A:866:ARG:NH2	1:B:856:CYS:O[1_665]	2.17	0.03
1:A:838:TYR:CE1	1:B:832:LEU:CD1[1_665]	2.18	0.02
1:A:864:ASN:OD1	1:B:845:ARG:CZ[1_665]	2.18	0.02
1:A:864:ASN:C	1:B:853:ALA:CB[1_665]	2.18	0.02
1:A:867:ASP:OD2	1:B:844:LEU:CD1[1_665]	2.18	0.02
1:A:28:PRO:O	1:A:235:ASP:CA[2_345]	2.19	0.01
1:A:81:PRO:O	1:A:817:ALA:CB[1_445]	2.19	0.01
1:A:869:VAL:CB	1:B:832:LEU:CA[1_665]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	861/863 (100%)	688 (80%)	123 (14%)	50 (6%)	1	14
1	B	861/863 (100%)	698 (81%)	116 (14%)	47 (6%)	1	15
All	All	1722/1726 (100%)	1386 (80%)	239 (14%)	97 (6%)	2	14

All (97) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	PRO
1	A	109	VAL
1	A	142	VAL
1	A	148	LYS

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Mol	Chain	Res	Type
1	A	251	SER
1	A	300	ASN
1	A	336	GLU
1	A	354	PHE
1	A	358	GLU
1	A	392	ARG
1	B	28	PRO
1	B	305	ASN
1	B	349	SER
1	B	350	ASN
1	B	658	SER
1	B	734	ASN
1	B	738	THR
1	B	745	SER
1	B	799	ARG
1	B	853	ALA
1	B	863	TYR
1	A	74	SER
1	A	83	ARG
1	A	104	LYS
1	A	110	SER
1	A	146	SER
1	A	260	ALA
1	A	268	ALA
1	A	347	ARG
1	A	349	SER
1	A	350	ASN
1	A	426	ALA
1	A	535	ASP
1	A	657	ILE
1	A	741	ALA
1	A	760	ASP
1	A	887	ASP
1	B	31	GLU
1	B	34	GLN
1	B	82	GLU
1	B	170	PHE
1	B	520	ALA
1	B	703	ASP
1	B	733	GLU
1	B	835	ASP
1	A	76	GLU

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Mol	Chain	Res	Type
1	A	85	LYS
1	A	246	PHE
1	A	341	THR
1	A	520	ALA
1	B	83	ARG
1	B	214	GLU
1	B	249	ALA
1	B	261	ASN
1	B	336	GLU
1	B	356	PRO
1	B	660	GLU
1	B	760	ASP
1	B	811	PHE
1	B	864	ASN
1	B	880	THR
1	A	147	ALA
1	A	249	ALA
1	A	262	ARG
1	A	456	ALA
1	A	544	GLU
1	A	587	MET
1	A	814	ARG
1	A	864	ASN
1	B	208	THR
1	B	335	LEU
1	B	414	LYS
1	B	664	THR
1	B	817	ALA
1	A	662	HIS
1	A	842	ASP
1	B	206	LEU
1	B	264	CYS
1	B	300	ASN
1	B	796	ASP
1	A	171	HIS
1	A	252	GLY
1	A	412	ASP
1	B	92	SER
1	B	171	HIS
1	B	654	ILE
1	B	192	ILE
1	A	27	ASP

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Mol	Chain	Res	Type
1	B	780	GLY
1	A	75	GLY
1	A	654	ILE
1	A	780	GLY
1	A	884	GLY
1	B	683	LYS
1	A	73	ILE
1	B	729	ILE
1	B	744	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	750/750 (100%)	680 (91%)	70 (9%)	8	26
1	B	750/750 (100%)	657 (88%)	93 (12%)	4	17
All	All	1500/1500 (100%)	1337 (89%)	163 (11%)	8	21

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	28	PRO
1	A	53	ILE
1	A	58	GLU
1	A	62	ASP
1	A	73	ILE
1	A	76	GLU
1	A	90	LYS
1	A	91	ILE
1	A	107	LYS
1	A	127	MET
1	A	138	GLN
1	A	148	LYS
1	A	226	GLU

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Mol	Chain	Res	Type
1	A	229	VAL
1	A	246	PHE
1	A	261	ASN
1	A	266	VAL
1	A	267	LEU
1	A	271	GLN
1	A	273	ASN
1	A	285	SER
1	A	286	ASP
1	A	304	GLU
1	A	308	GLN
1	A	313	LYS
1	A	314	LEU
1	A	315	GLU
1	A	323	LEU
1	A	348	LEU
1	A	349	SER
1	A	351	ARG
1	A	354	PHE
1	A	363	SER
1	A	366	ASN
1	A	381	GLU
1	A	419	GLN
1	A	425	THR
1	A	444	ASP
1	A	480	ILE
1	A	539	VAL
1	A	561	ASP
1	A	579	ILE
1	A	581	GLN
1	A	590	THR
1	A	601	ILE
1	A	615	ARG
1	A	616	ASP
1	A	628	GLN
1	A	643	ILE
1	A	659	ILE
1	A	666	GLU
1	A	667	ASP
1	A	670	ASN
1	A	701	ILE
1	A	720	GLN

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Mol	Chain	Res	Type
1	A	733	GLU
1	A	734	ASN
1	A	745	SER
1	A	750	ASN
1	A	770	GLU
1	A	809	ILE
1	A	810	ASP
1	A	818	ASP
1	A	840	THR
1	A	843	GLU
1	A	844	LEU
1	A	859	ARG
1	A	866	ARG
1	A	882	LEU
1	B	26	LEU
1	B	28	PRO
1	B	32	LYS
1	B	53	ILE
1	B	58	GLU
1	B	59	ASP
1	B	70	LEU
1	B	114	GLU
1	B	134	ARG
1	B	139	ASP
1	B	141	SER
1	B	152	LEU
1	B	171	HIS
1	B	192	ILE
1	B	199	LYS
1	B	201	ASP
1	B	210	PHE
1	B	214	GLU
1	B	266	VAL
1	B	269	VAL
1	B	272	GLU
1	B	279	ASP
1	B	285	SER
1	B	304	GLU
1	B	313	LYS
1	B	314	LEU
1	B	323	LEU
1	B	330	GLN

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Mol	Chain	Res	Type
1	B	332	LYS
1	B	334	GLN
1	B	342	LEU
1	B	349	SER
1	B	362	VAL
1	B	366	ASN
1	B	406	ILE
1	B	408	GLU
1	B	415	GLU
1	B	419	GLN
1	B	425	THR
1	B	480	ILE
1	B	485	ASP
1	B	487	LEU
1	B	490	LEU
1	B	539	VAL
1	B	561	ASP
1	B	565	GLU
1	B	579	ILE
1	B	581	GLN
1	B	590	THR
1	B	597	THR
1	B	601	ILE
1	B	610	GLN
1	B	616	ASP
1	B	627	GLN
1	B	646	TRP
1	B	653	GLU
1	B	659	ILE
1	B	662	HIS
1	B	666	GLU
1	B	669	LEU
1	B	678	SER
1	B	680	VAL
1	B	694	GLN
1	B	723	THR
1	B	734	ASN
1	B	744	ILE
1	B	747	GLU
1	B	750	ASN
1	B	752	PHE
1	B	753	ARG

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Mol	Chain	Res	Type
1	B	763	LYS
1	B	766	MET
1	B	771	ASP
1	B	782	ASN
1	B	797	PRO
1	B	798	ASN
1	B	799	ARG
1	B	802	VAL
1	B	804	THR
1	B	805	PHE
1	B	806	GLN
1	B	836	LYS
1	B	845	ARG
1	B	851	ASP
1	B	852	GLN
1	B	864	ASN
1	B	877	SER
1	B	879	SER
1	B	880	THR
1	B	882	LEU
1	B	883	TYR
1	B	885	GLU
1	B	888	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	93	ASN
1	A	95	ASN
1	A	187	HIS
1	A	510	GLN
1	A	573	HIS
1	A	574	ASN
1	A	629	ASN
1	A	697	GLN
1	A	782	ASN
1	A	824	GLN
1	B	43	ASN
1	B	156	GLN
1	B	248	HIS
1	B	270	ASN

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Mol	Chain	Res	Type
1	B	338	ASN
1	B	534	GLN
1	B	573	HIS
1	B	574	ASN
1	B	623	HIS
1	B	626	GLN
1	B	674	GLN
1	B	720	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 oligosaccharides 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.