



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2017 – 04:24 pm GMT

PDB ID : 1SJJ
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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29102

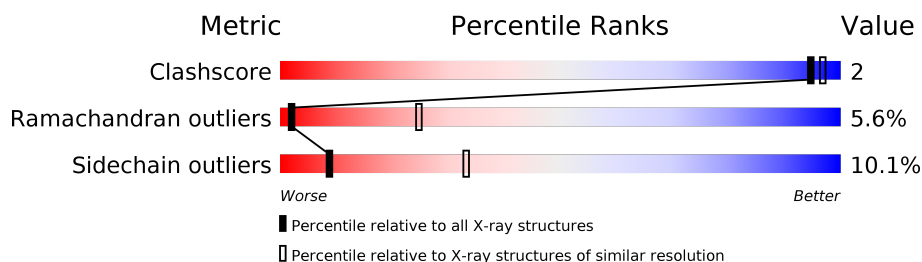
1 Overall quality at a glance

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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	1037 (15.00-3.80)
Ramachandran outliers	110173	1004 (11.50-3.76)
Sidechain outliers	110143	1099 (11.50-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	863	 75% 20% . .
1	B	863	 73% 22% . .

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 ZeroOcc column contains the number of atoms modelled with zero occupancy, 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.

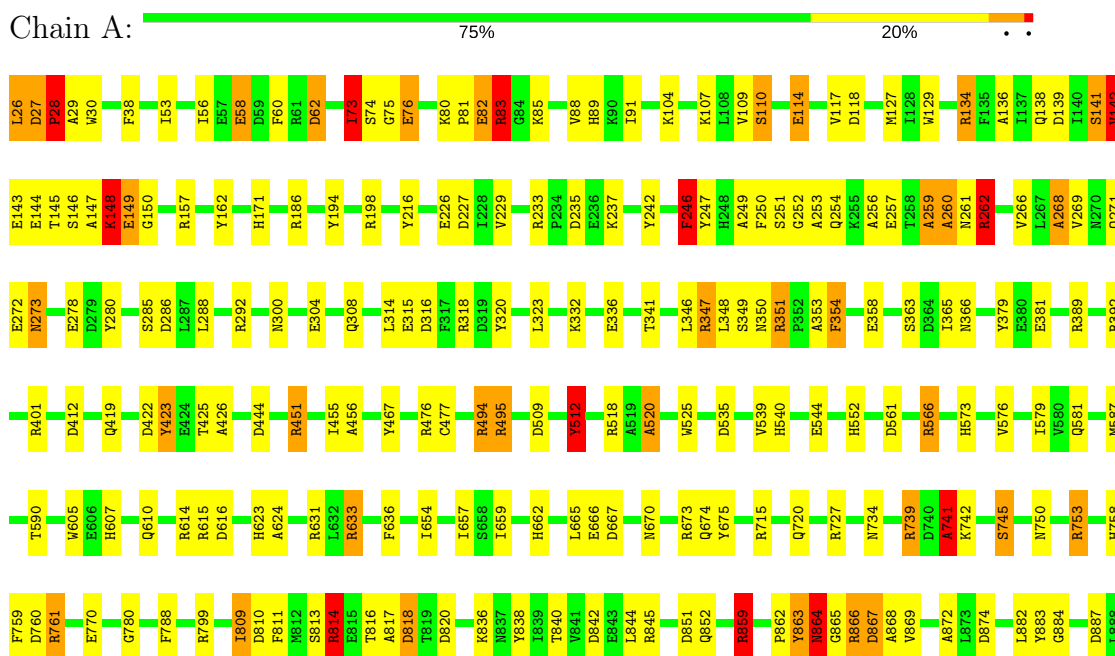
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	863	Total	C	N	O	S	0	0	0
			7007	4395	1236	1337	39			
1	B	863	Total	C	N	O	S	0	0	0
			7007	4395	1236	1337	39			

3 Residue-property plots

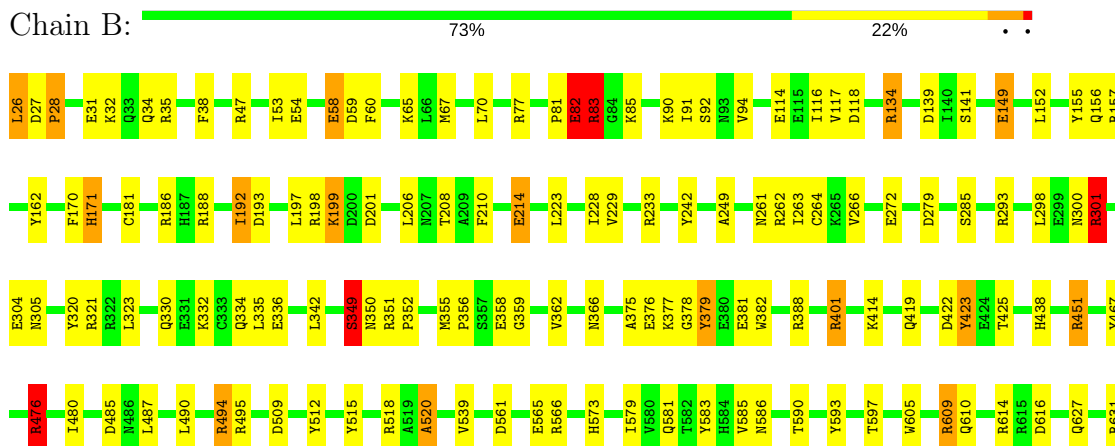
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

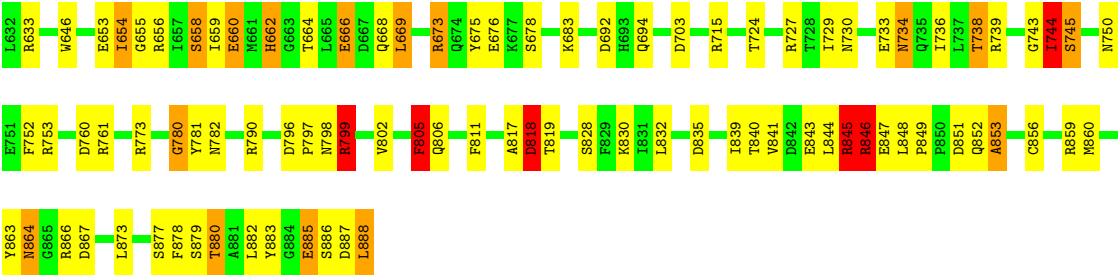
Note EDS was not executed.

• Molecule 1: actinin



• Molecule 1: actinin





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

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	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-20.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14014	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

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	0.77	1/7139 (0.0%)	1.37	53/9633 (0.6%)
1	B	0.78	1/7139 (0.0%)	1.36	53/9633 (0.6%)
All	All	0.78	2/14278 (0.0%)	1.36	106/19266 (0.6%)

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	10.05	1.36	1.25
1	A	149	GLU	CD-OE2	10.00	1.36	1.25

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	GLU	CB-CA-C	-12.98	84.44	110.40
1	A	753	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	B	566	ARG	NE-CZ-NH1	10.16	125.38	120.30
1	B	162	TYR	CB-CG-CD1	8.98	126.39	121.00
1	B	162	TYR	CB-CG-CD2	-8.68	115.79	121.00
1	A	142	VAL	CB-CA-C	8.66	127.85	111.40
1	B	846	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	B	727	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	A	141	SER	CB-CA-C	7.72	124.77	110.10
1	B	188	ARG	NE-CZ-NH1	7.66	124.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	673	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	B	188	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	110	SER	N-CA-CB	7.36	121.54	110.50
1	B	633	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	A	741	ALA	CB-CA-C	7.24	120.95	110.10
1	A	38	PHE	CB-CG-CD1	7.18	125.83	120.80
1	A	495	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	715	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	451	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	B	520	ALA	CB-CA-C	6.91	120.46	110.10
1	B	673	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	520	ALA	CB-CA-C	6.80	120.30	110.10
1	B	263	ILE	C-N-CA	6.64	138.29	121.70
1	B	451	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	B	512	TYR	CB-CG-CD2	-6.50	117.10	121.00
1	B	744	ILE	CB-CA-C	6.50	124.60	111.60
1	B	845	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	859	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	B	67	MET	CG-SD-CE	-6.46	89.86	100.20
1	B	198	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	379	TYR	CB-CG-CD2	-6.44	117.14	121.00
1	A	83	ARG	NE-CZ-NH1	6.41	123.51	120.30
1	A	518	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	148	LYS	C-N-CA	6.33	137.54	121.70
1	B	262	ARG	C-N-CA	6.32	137.50	121.70
1	B	379	TYR	CB-CG-CD2	-6.22	117.27	121.00
1	A	512	TYR	CB-CG-CD2	-6.17	117.30	121.00
1	A	145	THR	C-N-CA	6.13	137.03	121.70
1	A	250	PHE	C-N-CA	6.11	136.98	121.70
1	B	38	PHE	CB-CG-CD1	6.11	125.08	120.80
1	B	715	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	B	494	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	B	423	TYR	CB-CG-CD1	-6.08	117.35	121.00
1	B	859	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	142	VAL	O-C-N	-6.03	113.05	122.70
1	A	38	PHE	CB-CG-CD2	-6.02	116.59	120.80
1	B	82	GLU	C-N-CA	5.97	136.63	121.70
1	A	347	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	B	818	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	A	512	TYR	CB-CG-CD1	5.93	124.56	121.00
1	B	509	ASP	CB-CG-OD1	-5.93	112.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	631	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	673	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	773	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	259	ALA	C-N-CA	5.87	136.38	121.70
1	A	739	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	82	GLU	C-N-CA	5.82	136.24	121.70
1	A	423	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	B	35	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	B	692	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	B	60	PHE	CB-CG-CD2	-5.77	116.76	120.80
1	A	139	ASP	O-C-N	-5.64	113.67	122.70
1	B	878	PHE	CB-CG-CD1	5.61	124.73	120.80
1	B	773	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	262	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	818	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	476	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	494	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	753	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	268	ALA	N-CA-CB	5.52	117.83	110.10
1	A	316	ASP	N-CA-CB	-5.51	100.67	110.60
1	B	349	SER	N-CA-CB	5.50	118.75	110.50
1	A	509	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	A	566	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	60	PHE	CB-CG-CD1	5.49	124.64	120.80
1	B	744	ILE	N-CA-C	-5.47	96.22	111.00
1	A	60	PHE	CB-CG-CD2	-5.47	116.97	120.80
1	B	262	ARG	O-C-N	-5.45	113.99	122.70
1	A	142	VAL	CA-CB-CG1	5.44	119.07	110.90
1	A	633	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	62	ASP	CB-CA-C	5.37	121.13	110.40
1	B	518	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	139	ASP	C-N-CA	5.33	135.03	121.70
1	A	139	ASP	CB-CA-C	5.33	121.06	110.40
1	B	263	ILE	O-C-N	-5.31	114.20	122.70
1	B	401	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	B	878	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	B	790	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	859	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	B	609	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	263	ILE	CA-C-N	5.22	128.69	117.20
1	A	246	PHE	CB-CG-CD2	-5.16	117.19	120.80
1	B	512	TYR	CB-CG-CD1	5.16	124.10	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	727	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	885	GLU	CB-CA-C	5.16	120.71	110.40
1	A	144	GLU	C-N-CA	5.15	134.58	121.70
1	B	301	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	60	PHE	CB-CG-CD1	5.12	124.38	120.80
1	B	82	GLU	O-C-N	-5.11	114.53	122.70
1	A	633	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	B	799	ARG	N-CA-CB	5.05	119.68	110.60
1	A	82	GLU	O-C-N	-5.03	114.65	122.70
1	A	259	ALA	O-C-N	-5.01	114.68	122.70
1	A	809	ILE	CA-CB-CG1	5.01	120.52	111.00
1	B	83	ARG	N-CA-CB	5.01	119.62	110.60

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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
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
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

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Mol	Chain	Res	Type	Group
1	B	886	SER	Peptide
1	B	887	ASP	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7007	0	6898	23	172
1	B	7007	0	6898	22	160
All	All	14014	0	13796	42	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 (42) 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:259:ALA:HA	1:A:260:ALA:HB3	1.90	0.52
1:A:761:ARG:HE	1:A:761:ARG:HA	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:B:654:ILE:HG21	1:B:724:THR:HG22	1.95	0.48
1:A:114:GLU:H	1:A:114:GLU:CD	2.17	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:LEU:HD13	1:B:743:GLY:C	2.38	0.44
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:666:GLU:H	1:B:666:GLU:CD	2.22	0.43
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:54:GLU:CD	1:B:65:LYS:HZ2	2.23	0.42
1:B:181:CYS:HB3	1:B:197:LEU:HD13	2.02	0.41
1:B:658:SER:HA	1:B:668:GLN:HG3	2.01	0.41
1:B:85:LYS:HA	1:B:90:LYS:HE2	2.02	0.41
1:A:665:LEU:HG	1:A:739:ARG:HH21	1.86	0.41
1:B:669:LEU:HA	1:B:669:LEU:HD22	1.97	0.41
1:B:653:GLU:C	1:B:655:GLY:H	2.24	0.41
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:874:ASP:CG	1:B:849:PRO:CG[1_665]	1.07	1.13
1:A:81:PRO:CA	1:A:818:ASP:CB[1_445]	1.07	1.13
1:A:864:ASN:CB	1:B:845:ARG:NH2[1_665]	1.10	1.10
1:A:864:ASN:O	1:B:853:ALA:CB[1_665]	1.12	1.08
1:A:863:TYR:C	1:B:848:LEU:N[1_665]	1.12	1.08
1:B:352:PRO:CG	1:B:358:GLU:CB[2_555]	1.14	1.06
1:A:863:TYR:N	1:B:847:GLU:O[1_665]	1.16	1.04
1:A:836:LYS:NZ	1:B:828:SER:CB[1_665]	1.16	1.04
1:B:81:PRO:CG	1:B:301:ARG:NH2[2_555]	1.16	1.04
1:A:81:PRO:CB	1:A:818:ASP:CB[1_445]	1.16	1.04
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:868:ALA:O	1:B:832:LEU:O[1_665]	1.27	0.93
1:A:863:TYR:CB	1:B:847:GLU:CA[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:B:81:PRO:CG	1:B:301:ARG:NH1[2_555]	1.29	0.91
1:A:863:TYR:CG	1:B:847:GLU:N[1_665]	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:352:PRO:N	1:B:358:GLU:CB[2_555]	1.34	0.86
1:B:83:ARG:NH2	1:B:382:TRP:N[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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:836:LYS:CE	1:B:828:SER:OG[1_665]	1.42	0.78
1:A:81:PRO:O	1:A:817:ALA:CA[1_445]	1.42	0.78
1:A:869:VAL:CG1	1:B:832:LEU:N[1_665]	1.43	0.77
1:B:352:PRO:N	1:B:358:GLU:CG[2_555]	1.44	0.76
1:A:88:VAL:CG1	1:A:814:ARG:NE[1_445]	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:863:TYR:N	1:B:847:GLU:C[1_665]	1.48	0.72
1:A:89:HIS:CD2	1:A:813:SER:C[1_445]	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:872:ALA:N	1:B:847:GLU:OE1[1_665]	1.50	0.70
1:A:864:ASN:CG	1:B:845:ARG:NH2[1_665]	1.50	0.70
1:A:872:ALA:CB	1:B:847:GLU:OE1[1_665]	1.50	0.70
1:A:89:HIS:ND1	1:A:814:ARG:CG[1_445]	1.53	0.67
1:A:82:GLU:CG	1:A:817:ALA:CB[1_445]	1.53	0.67
1:A:865:GLY:N	1:B:845:ARG:CA[1_665]	1.54	0.66
1:A:81:PRO:CG	1:A:818:ASP:CB[1_445]	1.54	0.66
1:A:866:ARG:N	1:B:844:LEU:CG[1_665]	1.55	0.65
1:A:30:TRP:NE1	1:A:233:ARG:O[2_345]	1.55	0.65
1:A:864:ASN:CG	1:B:845:ARG:NE[1_665]	1.55	0.65
1:A:863:TYR:CB	1:B:848:LEU:N[1_665]	1.55	0.65
1:B:352:PRO:CG	1:B:358:GLU:C[2_555]	1.57	0.63
1:A:863:TYR:CB	1:B:847:GLU:CB[1_665]	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:874:ASP:OD1	1:B:849:PRO:CG[1_665]	1.63	0.57
1:A:868:ALA:C	1:B:832:LEU:O[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:864:ASN:OD1	1:B:845:ARG:NE[1_665]	1.66	0.54
1:A:836:LYS:CD	1:B:828:SER:CB[1_665]	1.66	0.54
1:B:81:PRO:CD	1:B:301:ARG:CZ[2_555]	1.67	0.53
1:B:81:PRO:CA	1:B:301:ARG:CZ[2_555]	1.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:81:PRO:C	1:A:818:ASP:N[1_445]	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:864:ASN:CA	1:B:845:ARG:CZ[1_665]	1.72	0.48
1:A:89:HIS:CE1	1:A:814:ARG:CG[1_445]	1.72	0.48
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:89:HIS:NE2	1:A:814:ARG:N[1_445]	1.73	0.47
1:A:83:ARG:NH2	1:A:820:ASP:CG[1_445]	1.74	0.46
1:A:81:PRO:O	1:A:817:ALA:O[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
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:865:GLY:N	1:B:845:ARG:N[1_665]	1.80	0.40
1:A:863:TYR:C	1:B:848:LEU:CA[1_665]	1.80	0.40
1:A:867:ASP:OD2	1:B:844:LEU:CG[1_665]	1.80	0.40
1:B:352:PRO:CA	1:B:358:GLU:CB[2_555]	1.81	0.39
1:B:81:PRO:N	1:B:301:ARG:CZ[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:868:ALA:CB	1:B:843:GLU:CA[1_665]	1.89	0.31
1:A:29:ALA:CA	1:A:235:ASP:OD2[2_345]	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:874:ASP:CB	1:B:849:PRO:CD[1_665]	1.91	0.29
1:A:867:ASP:CB	1:B:839:ILE:CD1[1_665]	1.91	0.29
1:A:874:ASP:OD2	1:B:849:PRO:CG[1_665]	1.92	0.28
1:A:863:TYR:CA	1:B:848:LEU:CA[1_665]	1.92	0.28
1:A:838:TYR:OH	1:B:828:SER:O[1_665]	1.92	0.28
1:A:866:ARG:N	1:B:844:LEU:CD1[1_665]	1.92	0.28
1:B:82:GLU:OE2	1:B:378:GLY:CA[2_555]	1.93	0.27
1:A:863:TYR:O	1:B:844:LEU:O[1_665]	1.93	0.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:NE2	1:A:813:SER:CA[1_445]	1.94	0.26
1:A:838:TYR:CE2	1:B:832:LEU:CD1[1_665]	1.94	0.26
1:A:89:HIS:ND1	1:A:813:SER:O[1_445]	1.94	0.26
1:A:89:HIS:CE1	1:A:814:ARG:N[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:89:HIS:CE1	1:A:813:SER:C[1_445]	1.95	0.25
1:A:869:VAL:N	1:B:832:LEU:O[1_665]	1.95	0.25
1:A:867:ASP:O	1:B:839:ILE:CD1[1_665]	1.95	0.25
1:A:863:TYR:CE2	1:B:843:GLU:C[1_665]	1.95	0.25
1:B:352:PRO:CG	1:B:359:GLY:N[2_555]	1.96	0.24
1:B:352:PRO:CG	1:B:358:GLU:CG[2_555]	1.98	0.22
1:A:836:LYS:NZ	1:B:828:SER:C[1_665]	1.98	0.22
1:B:83:ARG:NE	1:B:382:TRP:N[2_555]	1.99	0.21
1:A:836:LYS:NZ	1:B:828:SER:OG[1_665]	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:B:351:ARG:C	1:B:358:GLU:CG[2_555]	2.03	0.17
1:A:866:ARG:CB	1:B:841:VAL:CA[1_665]	2.03	0.17
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:81:PRO:CB	1:A:818:ASP:N[1_445]	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:865:GLY:O	1:B:845:ARG:CA[1_665]	2.06	0.14
1:A:863:TYR:C	1:B:848:LEU:O[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:867:ASP:CA	1:B:839:ILE:CD1[1_665]	2.09	0.11
1:A:254:GLN:OE1	1:A:254:GLN:NE2[2_345]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:PRO:CB	1:A:817:ALA:O[1_445]	2.09	0.11
1:A:866:ARG:CA	1:B:841:VAL:CA[1_665]	2.09	0.11
1:A:88:VAL:CB	1:A:814:ARG:CD[1_445]	2.10	0.10
1:B:83:ARG:NH2	1:B:381:GLU:C[2_555]	2.11	0.09
1:A:868:ALA:CB	1:B:843:GLU:CG[1_665]	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:866:ARG:CB	1:B:841:VAL:N[1_665]	2.14	0.06
1:A:863:TYR:CD2	1:B:844:LEU:O[1_665]	2.14	0.06
1:A:867:ASP:C	1:B:839:ILE:CD1[1_665]	2.14	0.06
1:A:81:PRO:N	1:A:818:ASP:CG[1_445]	2.14	0.06
1:B:352:PRO:CA	1:B:358:GLU:CA[2_555]	2.14	0.06
1:A:865:GLY:CA	1:B:845:ARG:N[1_665]	2.14	0.06
1:B:81:PRO:CA	1:B:301:ARG:NH2[2_555]	2.14	0.06
1:A:865:GLY:C	1:B:841:VAL:O[1_665]	2.15	0.05
1:A:81:PRO:CB	1:A:818:ASP:C[1_445]	2.15	0.05
1:B:83:ARG:NH2	1:B:381:GLU:N[2_555]	2.15	0.05
1:A:872:ALA:C	1:B:847:GLU:OE1[1_665]	2.15	0.05
1:A:863:TYR:CD2	1:B:843:GLU:O[1_665]	2.15	0.05
1:A:865:GLY:O	1:B:845:ARG:CB[1_665]	2.15	0.05
1:A:863:TYR:CD1	1:B:847:GLU:CB[1_665]	2.16	0.04
1:A:129:TRP:CH2	1:A:237:LYS:O[2_345]	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:867:ASP:OD2	1:B:844:LEU:CD1[1_665]	2.18	0.02
1:A:864:ASN:C	1:B:853:ALA:CB[1_665]	2.18	0.02
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
1:A:28:PRO:O	1:A:235:ASP:CA[2_345]	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 X-ray entries followed by that with respect to entries of similar resolution.

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%)	2	24
1	B	861/863 (100%)	698 (81%)	116 (14%)	47 (6%)	2	25
All	All	1722/1726 (100%)	1386 (80%)	239 (14%)	97 (6%)	2	25

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 X-ray entries followed by that with respect to entries of similar resolution.

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%)	679 (90%)	71 (10%)	10	36
1	B	750/750 (100%)	669 (89%)	81 (11%)	7	31
All	All	1500/1500 (100%)	1348 (90%)	152 (10%)	9	33

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU

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Mol	Chain	Res	Type
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	107	LYS
1	A	114	GLU
1	A	127	MET
1	A	138	GLN
1	A	148	LYS
1	A	226	GLU
1	A	227	ASP
1	A	229	VAL
1	A	246	PHE
1	A	261	ASN
1	A	266	VAL
1	A	271	GLN
1	A	273	ASN
1	A	278	GLU
1	A	285	SER
1	A	286	ASP
1	A	304	GLU
1	A	308	GLN
1	A	314	LEU
1	A	315	GLU
1	A	323	LEU
1	A	332	LYS
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	422	ASP
1	A	425	THR
1	A	444	ASP
1	A	539	VAL
1	A	561	ASP
1	A	579	ILE
1	A	581	GLN
1	A	590	THR

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Mol	Chain	Res	Type
1	A	610	GLN
1	A	615	ARG
1	A	616	ASP
1	A	659	ILE
1	A	666	GLU
1	A	667	ASP
1	A	670	ASN
1	A	674	GLN
1	A	720	GLN
1	A	734	ASN
1	A	745	SER
1	A	750	ASN
1	A	761	ARG
1	A	770	GLU
1	A	788	PHE
1	A	809	ILE
1	A	810	ASP
1	A	811	PHE
1	A	818	ASP
1	A	840	THR
1	A	844	LEU
1	A	845	ARG
1	A	851	ASP
1	A	859	ARG
1	A	864	ASN
1	A	866	ARG
1	A	867	ASP
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	156	GLN
1	B	171	HIS

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Mol	Chain	Res	Type
1	B	199	LYS
1	B	201	ASP
1	B	210	PHE
1	B	214	GLU
1	B	266	VAL
1	B	272	GLU
1	B	279	ASP
1	B	285	SER
1	B	304	GLU
1	B	323	LEU
1	B	330	GLN
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	419	GLN
1	B	422	ASP
1	B	425	THR
1	B	476	ARG
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	610	GLN
1	B	616	ASP
1	B	627	GLN
1	B	646	TRP
1	B	659	ILE
1	B	662	HIS
1	B	666	GLU
1	B	669	LEU
1	B	676	GLU
1	B	678	SER

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Mol	Chain	Res	Type
1	B	694	GLN
1	B	734	ASN
1	B	744	ILE
1	B	750	ASN
1	B	752	PHE
1	B	753	ARG
1	B	782	ASN
1	B	797	PRO
1	B	798	ASN
1	B	799	ARG
1	B	802	VAL
1	B	805	PHE
1	B	806	GLN
1	B	845	ARG
1	B	851	ASP
1	B	852	GLN
1	B	864	ASN
1	B	867	ASP
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	574	ASN
1	A	586	ASN
1	B	156	GLN
1	B	248	HIS
1	B	534	GLN
1	B	546	GLN
1	B	573	HIS
1	B	623	HIS
1	B	694	GLN
1	B	720	GLN
1	B	852	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.