



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:05 PM UTC

PDB ID : 9HMZ / pdb\_00009hmz  
Title : Structure of Corynebacterium glutamicum SteA, a cell division regulator  
Authors : Gaday, Q.; Carloni, G.; Wehenkel, A.M.; Alzari, P.M.  
Deposited on : 2024-12-09  
Resolution : 2.05 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

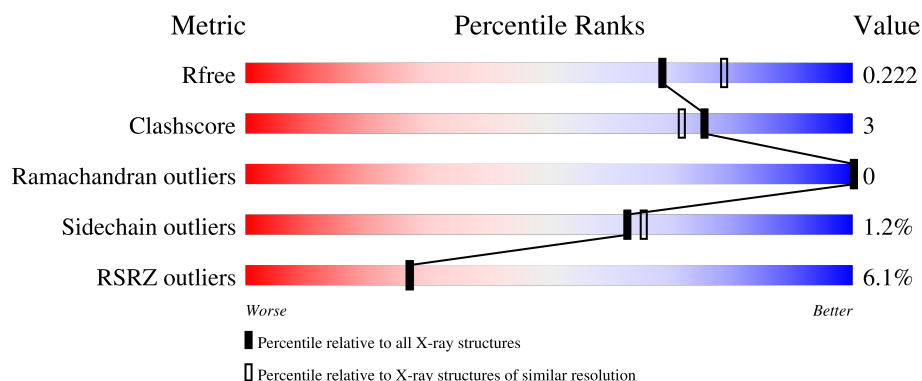
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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.



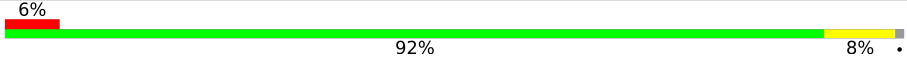


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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 of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	333	<div> <div>5%</div> <div> <div></div> <div>92%</div> <div>8%</div> </div> <div>.</div> </div>
1	B	333	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>10%</div> </div> <div>..</div> </div>
1	C	333	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> <div>.</div> </div>
1	D	333	<div> <div>13%</div> <div> <div></div> <div>88%</div> <div>9%</div> </div> <div>..</div> </div>
1	E	333	<div> <div>7%</div> <div> <div></div> <div>90%</div> <div>8%</div> </div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	333	 92% 8% •
1	G	333	 90% 9% •
1	H	333	 89% 9% •

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20802 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 SteA-like C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2448	1537	426	480	5			
1	B	331	Total	C	N	O	S	0	0	0
			2448	1537	426	480	5			
1	C	331	Total	C	N	O	S	0	0	0
			2448	1537	426	480	5			
1	D	327	Total	C	N	O	S	0	0	0
			2421	1520	422	474	5			
1	E	327	Total	C	N	O	S	0	0	0
			2421	1520	422	474	5			
1	F	331	Total	C	N	O	S	0	0	0
			2448	1537	426	480	5			
1	G	330	Total	C	N	O	S	0	0	0
			2440	1533	425	477	5			
1	H	327	Total	C	N	O	S	0	0	0
			2421	1520	422	474	5			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	208	Total	O	0	0
			208	208		
2	B	197	Total	O	0	0
			197	197		
2	C	165	Total	O	0	0
			165	165		
2	D	127	Total	O	0	0
			127	127		
2	E	132	Total	O	0	0
			132	132		
2	F	154	Total	O	0	0
			154	154		

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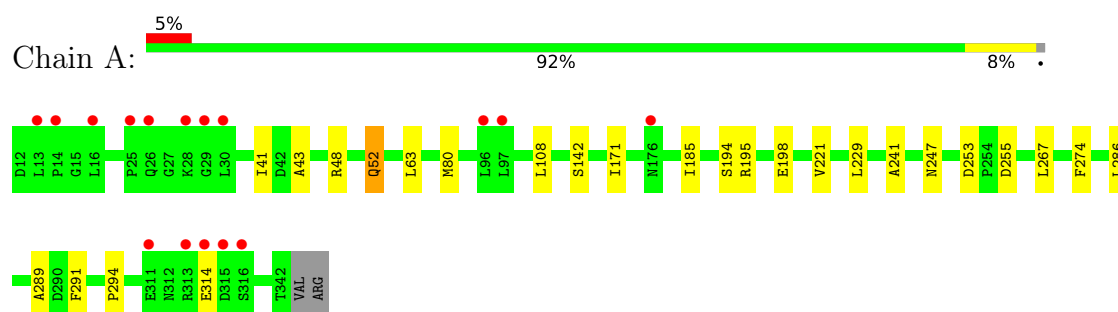
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	181	Total 181	O 181	0	0
2	H	143	Total 143	O 143	0	0

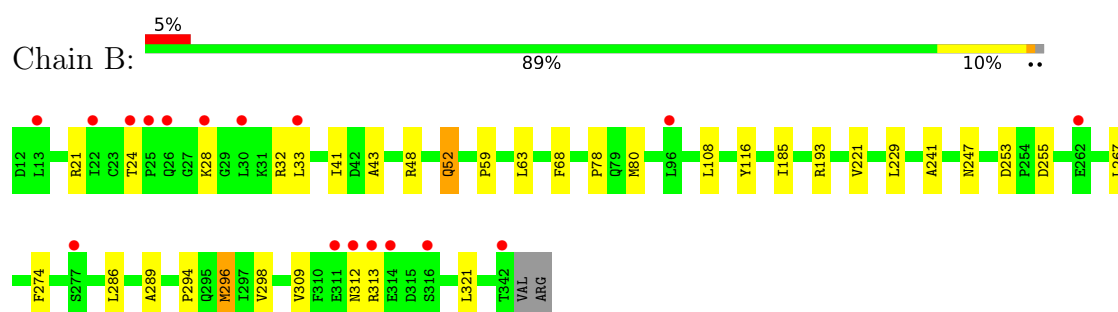
### 3 Residue-property plots [i](#)

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 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.

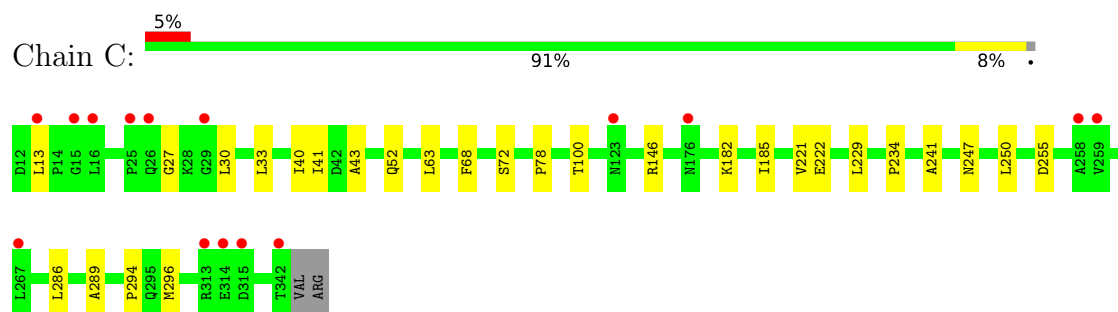
- Molecule 1: SteA-like C-terminal domain-containing protein



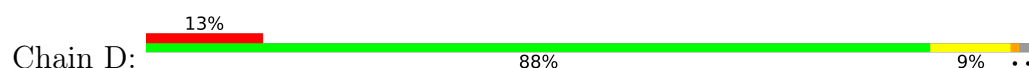
- Molecule 1: SteA-like C-terminal domain-containing protein

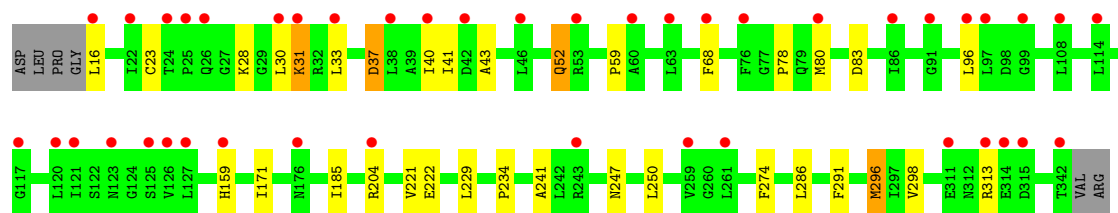


- Molecule 1: SteA-like C-terminal domain-containing protein

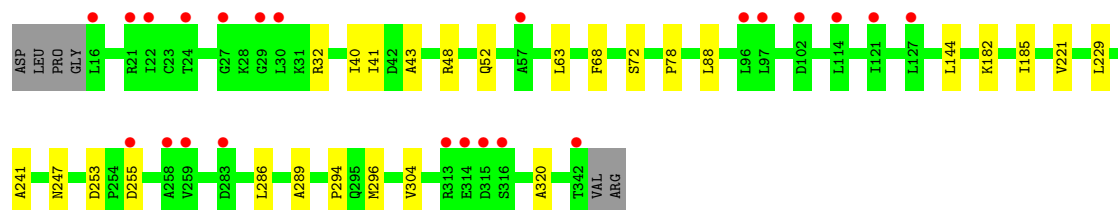
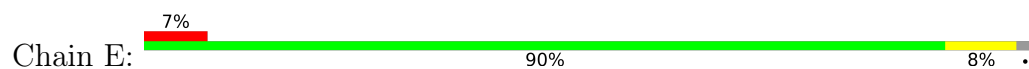


- Molecule 1: SteA-like C-terminal domain-containing protein

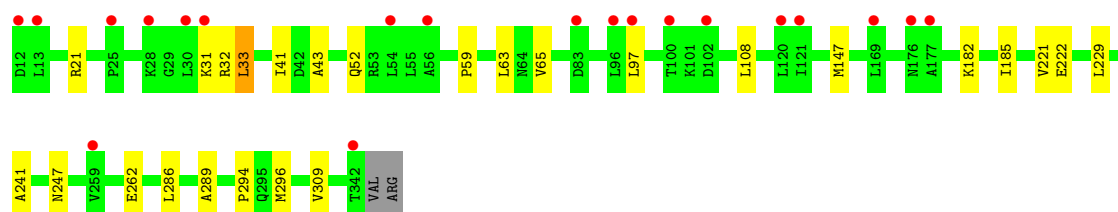
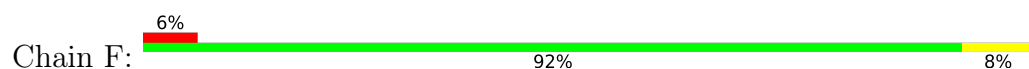




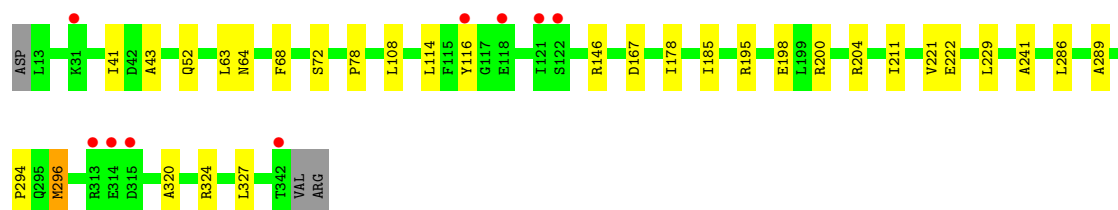
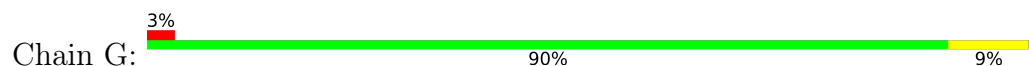
- Molecule 1: SteA-like C-terminal domain-containing protein



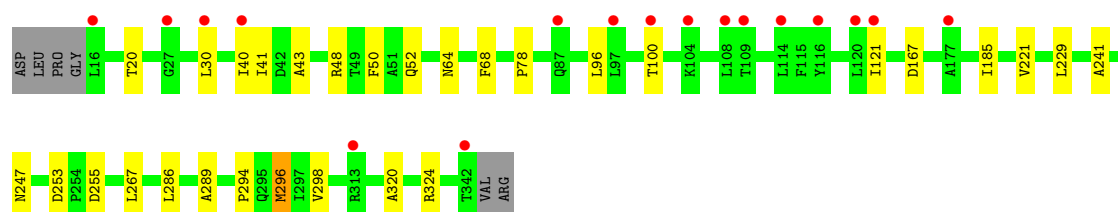
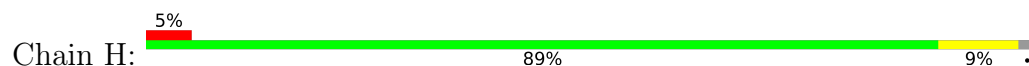
- Molecule 1: SteA-like C-terminal domain-containing protein



- Molecule 1: SteA-like C-terminal domain-containing protein



- Molecule 1: SteA-like C-terminal domain-containing protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	126.51Å 128.72Å 211.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	105.92 – 2.05 105.92 – 2.05	Depositor EDS
% Data completeness (in resolution range)	58.7 (105.92-2.05) 58.7 (105.92-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.05Å)	Xtriage
Refinement program	BUSTER 2.10.4	Depositor
R, $R_{free}$	0.205 , 0.238 0.193 , 0.222	Depositor DCC
$R_{free}$ test set	6204 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 53.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	20802	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.64 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8430e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.72	0/2487	1.01	0/3375
1	B	0.72	1/2487 (0.0%)	1.01	2/3375 (0.1%)
1	C	0.72	0/2487	1.01	1/3375 (0.0%)
1	D	0.71	1/2459 (0.0%)	0.98	4/3336 (0.1%)
1	E	0.71	0/2459	0.98	0/3336
1	F	0.72	0/2487	1.00	0/3375
1	G	0.74	1/2479 (0.0%)	1.02	2/3364 (0.1%)
1	H	0.73	1/2459 (0.0%)	0.98	1/3336 (0.0%)
All	All	0.72	4/19804 (0.0%)	1.00	10/26872 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	296	MET	SD-CE	-10.77	1.52	1.79
1	H	296	MET	SD-CE	-8.32	1.58	1.79
1	B	296	MET	SD-CE	-7.40	1.61	1.79
1	G	296	MET	SD-CE	-5.93	1.64	1.79

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	178	ILE	N-CA-C	7.22	117.75	111.90
1	D	37	ASP	CA-CB-CG	6.33	118.94	112.60
1	C	255	ASP	CA-CB-CG	6.33	118.93	112.60
1	B	116	TYR	N-CA-C	-5.79	103.80	111.96
1	G	64	ASN	CA-CB-CG	5.49	118.09	112.60
1	H	64	ASN	CA-CB-CG	5.36	117.96	112.60
1	D	83	ASP	CA-CB-CG	5.21	117.81	112.60
1	D	30	LEU	CA-C-N	5.19	128.20	120.31
1	D	30	LEU	C-N-CA	5.19	128.20	120.31
1	B	274	PHE	CA-CB-CG	5.15	118.95	113.80

There are no chirality outliers.

There are no planarity outliers.

## 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	2448	0	2460	14	0
1	B	2448	0	2460	19	0
1	C	2448	0	2460	12	0
1	D	2421	0	2435	19	0
1	E	2421	0	2435	15	0
1	F	2448	0	2460	13	0
1	G	2440	0	2456	16	0
1	H	2421	0	2435	19	0
2	A	208	0	0	0	0
2	B	197	0	0	1	0
2	C	165	0	0	0	0
2	D	127	0	0	0	0
2	E	132	0	0	0	0
2	F	154	0	0	0	0
2	G	181	0	0	1	0
2	H	143	0	0	0	0
All	All	20802	0	19601	116	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 3.

All (116) 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:48:ARG:HE	1:H:167:ASP:HB3	1.42	0.84
1:B:48:ARG:HE	1:G:167:ASP:HB3	1.51	0.76
1:C:27:GLY:HA2	1:C:30:LEU:HD12	1.69	0.74
1:D:296:MET:HE2	1:D:298:VAL:CG2	2.25	0.66
1:D:52:GLN:HG3	1:D:80:MET:HE1	1.77	0.65
1:D:296:MET:HE2	1:D:298:VAL:HG22	1.80	0.63
1:D:291:PHE:CZ	1:E:48:ARG:NH1	2.64	0.62
1:F:229:LEU:HD23	1:F:247:ASN:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:229:LEU:HD23	1:H:247:ASN:HB3	1.83	0.61
1:H:296:MET:HE2	1:H:298:VAL:CG2	2.32	0.59
1:B:229:LEU:HD23	1:B:247:ASN:HB3	1.85	0.59
1:F:33:LEU:HD11	1:F:59:PRO:HB3	1.84	0.59
1:D:229:LEU:HD23	1:D:247:ASN:HB3	1.84	0.58
1:H:30:LEU:HD21	1:H:50:PHE:HE1	1.68	0.58
1:G:195:ARG:NH1	1:G:198:GLU:OE1	2.37	0.58
1:A:229:LEU:HD23	1:A:247:ASN:HB3	1.87	0.57
1:D:291:PHE:HZ	1:E:48:ARG:HH12	1.49	0.57
1:E:229:LEU:HD23	1:E:247:ASN:HB3	1.86	0.56
1:D:291:PHE:HZ	1:E:48:ARG:NH1	2.02	0.56
1:H:20:THR:HG23	1:H:40:ILE:HD13	1.86	0.56
1:B:33:LEU:HD21	1:B:59:PRO:HB3	1.87	0.56
1:C:229:LEU:HD23	1:C:247:ASN:HB3	1.86	0.56
1:D:33:LEU:HD21	1:D:59:PRO:HB3	1.88	0.55
1:A:194:SER:O	1:A:198:GLU:HG3	2.07	0.55
1:C:234:PRO:HG3	1:C:250:LEU:HD11	1.90	0.54
1:B:296:MET:HE2	1:B:298:VAL:CG2	2.38	0.53
1:H:20:THR:HG22	1:H:100:THR:HG23	1.90	0.53
1:B:52:GLN:HG3	1:B:80:MET:HE1	1.90	0.53
1:C:41:ILE:HD12	1:C:43:ALA:HB3	1.91	0.52
1:B:267:LEU:HD21	1:D:222:GLU:HG2	1.91	0.52
1:H:296:MET:HE2	1:H:298:VAL:HG22	1.92	0.52
1:A:52:GLN:HG3	1:A:80:MET:HE1	1.91	0.51
1:G:185:ILE:HD12	1:G:286:LEU:HD23	1.92	0.51
1:C:40:ILE:HD13	1:C:100:THR:HG21	1.92	0.51
1:G:200:ARG:NH1	1:G:204:ARG:HH12	2.09	0.51
1:B:309:VAL:HG21	1:B:321:LEU:HD22	1.93	0.50
1:C:185:ILE:HD12	1:C:286:LEU:HD23	1.92	0.50
1:H:185:ILE:HD12	1:H:286:LEU:HD23	1.94	0.49
1:F:182:LYS:HE3	1:F:296:MET:HE3	1.94	0.49
1:D:159:HIS:CD2	1:E:144:LEU:HD22	2.48	0.48
1:C:68:PHE:HB3	1:C:78:PRO:HG3	1.95	0.48
1:F:63:LEU:HD21	1:F:108:LEU:HD22	1.94	0.48
1:G:200:ARG:NH1	1:G:204:ARG:NH1	2.61	0.48
1:A:267:LEU:HD21	1:C:222:GLU:HG2	1.95	0.48
1:D:185:ILE:HD12	1:D:286:LEU:HD23	1.96	0.48
1:F:185:ILE:HD12	1:F:286:LEU:HD23	1.95	0.48
1:F:147:MET:HE1	1:F:309:VAL:HG12	1.96	0.47
1:D:68:PHE:HB3	1:D:78:PRO:HG3	1.97	0.47
1:B:21:ARG:HH22	1:B:32:ARG:HH21	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:289:ALA:O	1:G:294:PRO:HD3	2.14	0.47
1:H:96:LEU:O	1:H:100:THR:OG1	2.28	0.47
1:B:185:ILE:HD12	1:B:286:LEU:HD23	1.97	0.47
1:A:291:PHE:CZ	1:H:48:ARG:NH1	2.83	0.47
1:E:185:ILE:HD12	1:E:286:LEU:HD23	1.96	0.46
1:H:41:ILE:HD12	1:H:43:ALA:HB3	1.97	0.46
1:E:304:VAL:HG21	1:E:320:ALA:HB1	1.98	0.46
1:E:41:ILE:HD12	1:E:43:ALA:HB3	1.98	0.46
1:G:41:ILE:HD12	1:G:43:ALA:HB3	1.97	0.46
1:G:72:SER:O	1:G:146:ARG:NH2	2.48	0.46
1:G:221:VAL:HG21	1:G:241:ALA:HA	1.98	0.46
1:H:20:THR:CG2	1:H:100:THR:HG23	2.45	0.46
1:D:41:ILE:HD12	1:D:43:ALA:HB3	1.97	0.46
1:E:32:ARG:HA	1:F:31:LYS:NZ	2.31	0.46
1:B:41:ILE:HD12	1:B:43:ALA:HB3	1.98	0.45
1:C:182:LYS:HE3	1:C:296:MET:HE3	1.97	0.45
1:G:63:LEU:HD21	1:G:108:LEU:HD22	1.98	0.44
1:G:68:PHE:HB3	1:G:78:PRO:HG3	1.99	0.44
1:B:296:MET:HE2	1:B:298:VAL:HG22	1.98	0.44
1:F:221:VAL:HG21	1:F:241:ALA:HA	2.00	0.44
1:B:63:LEU:HD11	1:B:108:LEU:HD22	1.99	0.44
1:H:221:VAL:HG21	1:H:241:ALA:HA	1.99	0.44
1:E:289:ALA:O	1:E:294:PRO:HD3	2.18	0.44
1:H:68:PHE:HB3	1:H:78:PRO:HG3	1.99	0.44
1:B:312:ASN:O	1:B:313:ARG:HB2	2.18	0.44
1:F:41:ILE:HD12	1:F:43:ALA:HB3	1.99	0.44
1:E:221:VAL:HG21	1:E:241:ALA:HA	1.99	0.43
1:G:320:ALA:O	1:G:324:ARG:HG2	2.18	0.43
1:F:222:GLU:HG2	1:H:267:LEU:CD2	2.48	0.43
1:B:68:PHE:HB3	1:B:78:PRO:HG3	1.99	0.43
1:C:72:SER:O	1:C:146:ARG:NH2	2.51	0.43
1:E:68:PHE:HB3	1:E:78:PRO:HG3	2.00	0.43
1:F:65:VAL:HG21	1:F:97:LEU:HG	1.99	0.43
1:A:185:ILE:HD12	1:A:286:LEU:HD23	1.99	0.43
1:G:286:LEU:HB3	1:G:327:LEU:HD21	2.00	0.43
1:E:182:LYS:HE3	1:E:296:MET:HE3	2.01	0.43
1:A:221:VAL:HG21	1:A:241:ALA:HA	2.00	0.43
1:D:31:LYS:H	1:D:31:LYS:HG2	1.62	0.43
1:H:20:THR:HG23	1:H:40:ILE:CD1	2.48	0.43
1:A:41:ILE:HD12	1:A:43:ALA:HB3	2.00	0.42
1:E:253:ASP:HB2	1:E:255:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:222:GLU:HG3	2:G:448:HOH:O	2.20	0.42
1:C:221:VAL:HG21	1:C:241:ALA:HA	2.01	0.42
1:H:320:ALA:O	1:H:324:ARG:HG2	2.19	0.42
1:B:253:ASP:HB2	1:B:255:ASP:OD1	2.19	0.42
1:H:289:ALA:O	1:H:294:PRO:HD3	2.19	0.42
1:B:289:ALA:O	1:B:294:PRO:HD3	2.20	0.42
1:E:40:ILE:HD11	1:E:63:LEU:HD22	2.01	0.42
1:B:221:VAL:HG21	1:B:241:ALA:HA	2.01	0.42
1:D:23:CYS:HA	1:D:28:LYS:O	2.19	0.42
1:H:253:ASP:HB2	1:H:255:ASP:OD1	2.20	0.42
1:F:21:ARG:HH22	1:F:32:ARG:HH21	1.68	0.41
1:D:221:VAL:HG21	1:D:241:ALA:HA	2.02	0.41
1:A:63:LEU:HD21	1:A:108:LEU:HD22	2.02	0.41
1:G:211:ILE:HG12	1:G:229:LEU:HB2	2.02	0.41
1:B:193:ARG:HD3	2:B:518:HOH:O	2.20	0.41
1:G:116:TYR:HD1	1:G:116:TYR:HA	1.82	0.41
1:D:234:PRO:HD3	1:D:250:LEU:HD22	2.02	0.41
1:A:289:ALA:O	1:A:294:PRO:HD3	2.20	0.41
1:C:289:ALA:O	1:C:294:PRO:HD3	2.21	0.41
1:D:171:ILE:HG12	1:D:274:PHE:CZ	2.56	0.41
1:A:253:ASP:HB2	1:A:255:ASP:OD1	2.21	0.40
1:F:289:ALA:O	1:F:294:PRO:HD3	2.20	0.40
1:B:24:THR:OG1	1:B:28:LYS:HB3	2.21	0.40
1:D:40:ILE:HD12	1:D:96:LEU:HD11	2.03	0.40
1:A:171:ILE:HG12	1:A:274:PHE:CZ	2.56	0.40
1:A:195:ARG:NH1	1:A:198:GLU:OE1	2.50	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 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	329/333 (99%)	319 (97%)	10 (3%)	0	100	100
1	B	329/333 (99%)	321 (98%)	8 (2%)	0	100	100
1	C	329/333 (99%)	321 (98%)	8 (2%)	0	100	100
1	D	325/333 (98%)	317 (98%)	8 (2%)	0	100	100
1	E	325/333 (98%)	314 (97%)	11 (3%)	0	100	100
1	F	329/333 (99%)	318 (97%)	11 (3%)	0	100	100
1	G	328/333 (98%)	320 (98%)	8 (2%)	0	100	100
1	H	325/333 (98%)	315 (97%)	10 (3%)	0	100	100
All	All	2619/2664 (98%)	2545 (97%)	74 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	259/261 (99%)	256 (99%)	3 (1%)	63	65
1	B	259/261 (99%)	258 (100%)	1 (0%)	84	88
1	C	259/261 (99%)	255 (98%)	4 (2%)	57	58
1	D	256/261 (98%)	250 (98%)	6 (2%)	44	42
1	E	256/261 (98%)	253 (99%)	3 (1%)	63	65
1	F	259/261 (99%)	256 (99%)	3 (1%)	63	65
1	G	258/261 (99%)	255 (99%)	3 (1%)	63	65
1	H	256/261 (98%)	254 (99%)	2 (1%)	73	77
All	All	2062/2088 (99%)	2037 (99%)	25 (1%)	63	65

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	A	142	SER

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Mol	Chain	Res	Type
1	A	314	GLU
1	B	52	GLN
1	C	13	LEU
1	C	33	LEU
1	C	52	GLN
1	C	63	LEU
1	D	16	LEU
1	D	31	LYS
1	D	37	ASP
1	D	52	GLN
1	D	204	ARG
1	D	313	ARG
1	E	52	GLN
1	E	72	SER
1	E	88	LEU
1	F	33	LEU
1	F	52	GLN
1	F	262	GLU
1	G	52	GLN
1	G	114	LEU
1	G	296	MET
1	H	52	GLN
1	H	121	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	87	GLN
1	A	94	GLN
1	A	159	HIS
1	B	87	GLN
1	B	94	GLN
1	B	113	GLN
1	B	140	GLN
1	B	299	ASN
1	C	94	GLN
1	C	156	GLN
1	D	94	GLN
1	D	156	GLN
1	D	159	HIS
1	E	94	GLN

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Mol	Chain	Res	Type
1	E	156	GLN
1	E	159	HIS
1	F	52	GLN
1	F	94	GLN
1	F	113	GLN
1	F	156	GLN
1	G	156	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

### 5.7 Other polymers ⓘ

There are no such residues in this entry.

### 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	331/333 (99%)	0.18	16 (4%) 35 36	32, 48, 92, 115	0
1	B	331/333 (99%)	0.21	17 (5%) 33 33	31, 48, 104, 123	0
1	C	331/333 (99%)	0.31	15 (4%) 38 38	32, 56, 89, 123	0
1	D	327/333 (98%)	0.81	43 (13%) 7 6	31, 66, 171, 188	0
1	E	327/333 (98%)	0.55	23 (7%) 22 22	29, 64, 123, 142	0
1	F	331/333 (99%)	0.43	20 (6%) 27 28	35, 60, 110, 144	0
1	G	330/333 (99%)	0.19	9 (2%) 56 58	30, 50, 97, 125	0
1	H	327/333 (98%)	0.47	17 (5%) 33 33	35, 57, 124, 145	0
All	All	2635/2664 (98%)	0.39	160 (6%) 27 27	29, 55, 118, 188	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	16	LEU	5.4
1	D	114	LEU	4.9
1	D	25	PRO	4.3
1	D	108	LEU	4.3
1	D	63	LEU	4.1
1	H	342	THR	4.1
1	D	97	LEU	4.0
1	H	16	LEU	4.0
1	E	16	LEU	3.9
1	B	316	SER	3.8
1	C	342	THR	3.7
1	E	30	LEU	3.7
1	D	342	THR	3.7
1	C	25	PRO	3.6
1	F	100	THR	3.5
1	B	24	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	342	THR	3.5
1	G	313	ARG	3.5
1	A	316	SER	3.4
1	D	26	GLN	3.3
1	B	342	THR	3.3
1	H	121	ILE	3.3
1	D	259	VAL	3.2
1	C	13	LEU	3.2
1	H	30	LEU	3.2
1	H	120	LEU	3.2
1	E	29	GLY	3.2
1	C	259	VAL	3.2
1	C	315	ASP	3.1
1	F	12	ASP	3.1
1	G	315	ASP	3.1
1	F	97	LEU	3.1
1	A	96	LEU	3.0
1	D	22	ILE	3.0
1	B	30	LEU	3.0
1	D	96	LEU	3.0
1	E	313	ARG	2.9
1	A	314	GLU	2.9
1	E	258	ALA	2.9
1	H	177	ALA	2.9
1	C	176	ASN	2.9
1	D	30	LEU	2.9
1	E	315	ASP	2.9
1	D	123	ASN	2.8
1	D	91	GLY	2.8
1	D	33	LEU	2.8
1	B	28	LYS	2.8
1	A	97	LEU	2.8
1	D	38	LEU	2.8
1	C	26	GLN	2.7
1	D	40	ILE	2.7
1	E	22	ILE	2.7
1	B	314	GLU	2.7
1	D	315	ASP	2.7
1	F	56	ALA	2.7
1	E	259	VAL	2.7
1	E	342	THR	2.7
1	H	108	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	114	LEU	2.7
1	B	25	PRO	2.7
1	E	255	ASP	2.7
1	H	27	GLY	2.7
1	B	26	GLN	2.6
1	B	312	ASN	2.6
1	D	127	LEU	2.6
1	F	96	LEU	2.6
1	F	169	LEU	2.6
1	E	24	THR	2.6
1	A	14	PRO	2.6
1	E	96	LEU	2.6
1	E	316	SER	2.6
1	E	121	ILE	2.6
1	E	114	LEU	2.6
1	H	97	LEU	2.6
1	C	313	ARG	2.6
1	E	314	GLU	2.6
1	E	57	ALA	2.6
1	A	29	GLY	2.5
1	A	13	LEU	2.5
1	D	46	LEU	2.5
1	E	97	LEU	2.5
1	B	33	LEU	2.5
1	F	176	ASN	2.5
1	D	86	ILE	2.5
1	D	120	LEU	2.4
1	A	311	GLU	2.4
1	E	102	ASP	2.4
1	A	313	ARG	2.4
1	F	28	LYS	2.4
1	D	68	PHE	2.4
1	D	53	ARG	2.4
1	D	313	ARG	2.4
1	A	30	LEU	2.4
1	B	13	LEU	2.4
1	E	127	LEU	2.4
1	D	314	GLU	2.4
1	D	121	ILE	2.4
1	B	277	SER	2.4
1	F	31	LYS	2.4
1	G	116	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	314	GLU	2.3
1	E	27	GLY	2.3
1	H	40	ILE	2.3
1	A	25	PRO	2.3
1	F	342	THR	2.3
1	C	123	ASN	2.3
1	A	16	LEU	2.3
1	F	30	LEU	2.3
1	F	83	ASP	2.3
1	D	243	ARG	2.3
1	G	121	ILE	2.3
1	F	13	LEU	2.3
1	F	102	ASP	2.3
1	D	80	MET	2.3
1	F	25	PRO	2.3
1	A	176	ASN	2.3
1	D	60	ALA	2.3
1	C	16	LEU	2.3
1	G	118	GLU	2.2
1	F	121	ILE	2.2
1	H	100	THR	2.2
1	D	42	ASP	2.2
1	D	117	GLY	2.2
1	D	159	HIS	2.2
1	F	259	VAL	2.2
1	C	15	GLY	2.2
1	C	29	GLY	2.2
1	C	258	ALA	2.2
1	B	96	LEU	2.2
1	A	28	LYS	2.2
1	B	311	GLU	2.2
1	G	314	GLU	2.2
1	D	204	ARG	2.2
1	D	76	PHE	2.1
1	A	26	GLN	2.1
1	H	313	ARG	2.1
1	G	122	SER	2.1
1	D	24	THR	2.1
1	F	177	ALA	2.1
1	D	31	LYS	2.1
1	F	54	LEU	2.1
1	D	311	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	109	THR	2.1
1	B	22	ILE	2.1
1	G	31	LYS	2.1
1	H	104	LYS	2.1
1	H	116	TYR	2.1
1	D	99	GLY	2.1
1	D	176	ASN	2.0
1	E	283	ASP	2.0
1	H	87	GLN	2.0
1	B	313	ARG	2.0
1	E	21	ARG	2.0
1	B	262	GLU	2.0
1	D	126	VAL	2.0
1	D	125	SER	2.0
1	C	267	LEU	2.0
1	D	261	LEU	2.0
1	F	120	LEU	2.0
1	A	315	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.