



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 23, 2025 – 12:17 AM JST

PDB ID : 9KQ6 / pdb_00009kq6
Title : The structure of the apo-YcfA from *Erwinia amylovora*
Authors : Zhang, L.; Dou, C.; Zheng, Y.H.; Zhu, X.F.; Cheng, W.
Deposited on : 2024-11-25
Resolution : 2.34 Å(reported)

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

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

A user guide is available at

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

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 : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

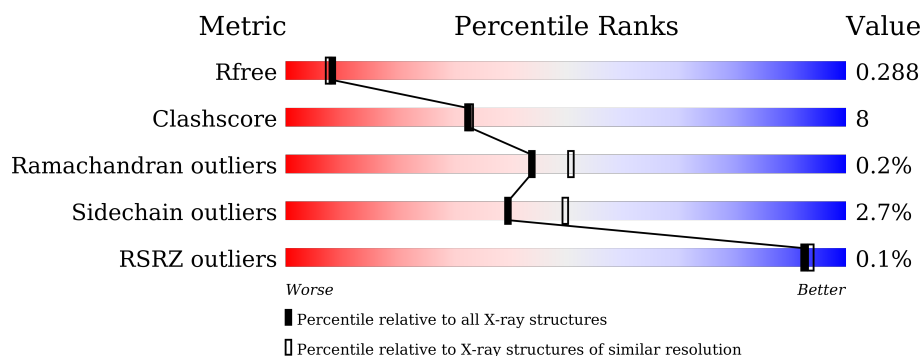
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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}	164625	2747 (2.36-2.32)
Clashscore	180529	2936 (2.36-2.32)
Ramachandran outliers	177936	2912 (2.36-2.32)
Sidechain outliers	177891	2912 (2.36-2.32)
RSRZ outliers	164620	2747 (2.36-2.32)

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 ≥ 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	234	<div> <div>79%</div> <div>14%</div> <div>• 5%</div> </div>
1	B	234	<div> <div>77%</div> <div>15%</div> <div>• 6%</div> </div>
1	C	234	<div> <div>77%</div> <div>16%</div> <div>• 5%</div> </div>
1	D	234	<div> <div>76%</div> <div>15%</div> <div>• 5%</div> </div>
1	E	234	<div> <div>59%</div> <div>28%</div> <div>• • 8%</div> </div>
1	F	234	<div> <div>78%</div> <div>15%</div> <div>• 6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	234	 78%12% • 7%
1	H	234	 79%14% • •
1	I	234	 76%17% • 6%
1	J	234	 79%12% • 6%
1	K	234	 74%18% • • 6%
1	L	234	 80%14% • 5%
1	M	234	 81%12% • 6%
1	N	234	 80%13% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24736 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 Asparagine synthetase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	N	222	Total	C	N	O	S	0	0	0
			1750	1115	300	325	10			
1	H	224	Total	C	N	O	S	0	0	0
			1761	1121	303	327	10			
1	D	222	Total	C	N	O	S	0	0	0
			1747	1114	300	323	10			
1	C	222	Total	C	N	O	S	0	0	0
			1750	1115	300	325	10			
1	L	222	Total	C	N	O	S	0	0	0
			1750	1115	300	325	10			
1	A	222	Total	C	N	O	S	0	0	0
			1745	1111	300	324	10			
1	M	221	Total	C	N	O	S	0	0	0
			1738	1106	299	323	10			
1	J	221	Total	C	N	O	S	0	0	0
			1739	1108	299	322	10			
1	F	221	Total	C	N	O	S	0	0	0
			1737	1106	299	322	10			
1	K	221	Total	C	N	O	S	0	0	0
			1738	1106	299	323	10			
1	E	216	Total	C	N	O	S	0	0	0
			1702	1083	293	316	10			
1	I	220	Total	C	N	O	S	0	0	0
			1732	1103	298	321	10			
1	B	220	Total	C	N	O	S	0	0	0
			1732	1103	298	321	10			
1	G	218	Total	C	N	O	S	0	0	0
			1720	1095	295	320	10			

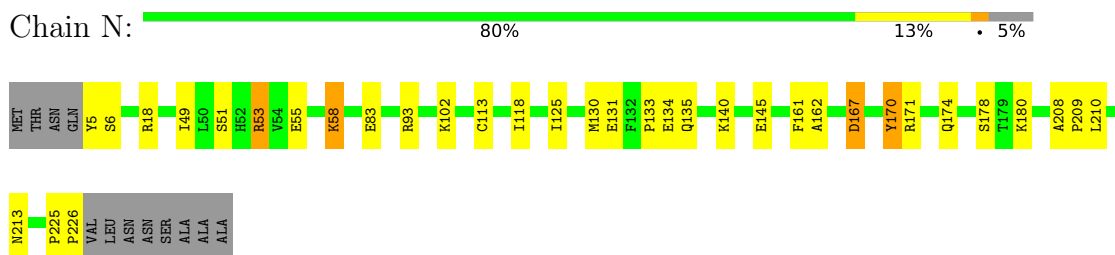
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	N	32	Total 32	O 32	0	0
2	H	22	Total 22	O 22	0	0
2	D	31	Total 31	O 31	0	0
2	C	32	Total 32	O 32	0	0
2	L	17	Total 17	O 17	0	0
2	A	37	Total 37	O 37	0	0
2	M	32	Total 32	O 32	0	0
2	J	24	Total 24	O 24	0	0
2	F	23	Total 23	O 23	0	0
2	K	10	Total 10	O 10	0	0
2	E	52	Total 52	O 52	0	0
2	I	18	Total 18	O 18	0	0
2	B	30	Total 30	O 30	0	0
2	G	35	Total 35	O 35	0	0

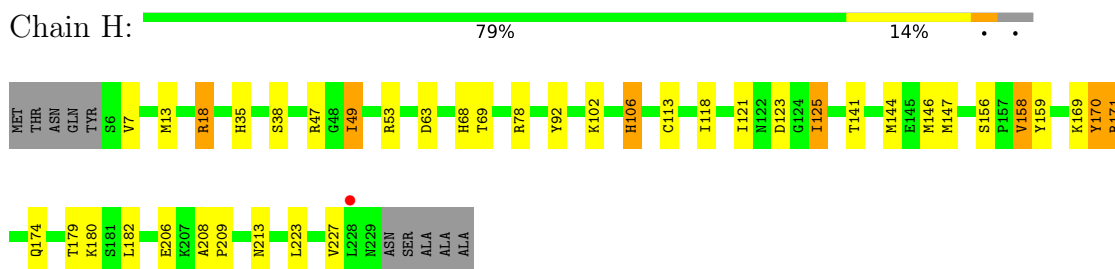
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

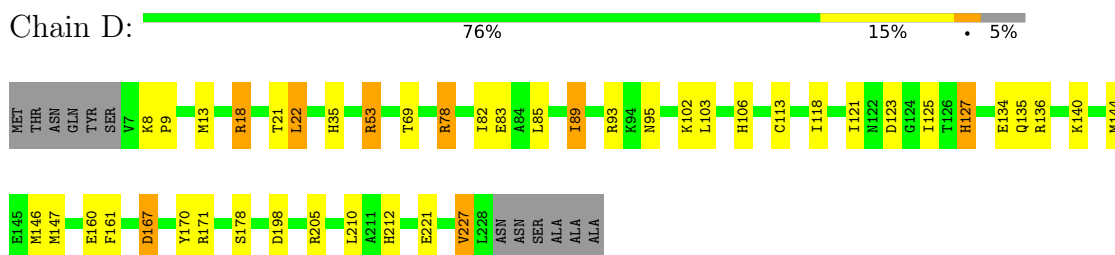
- Molecule 1: Asparagine synthetase domain-containing protein



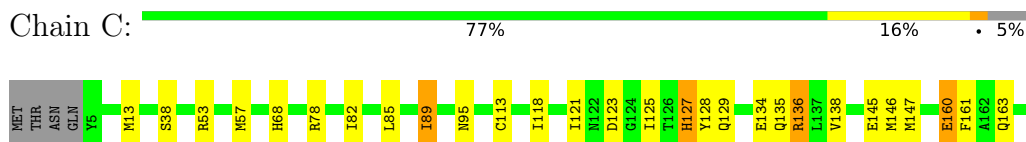
- Molecule 1: Asparagine synthetase domain-containing protein



- Molecule 1: Asparagine synthetase domain-containing protein



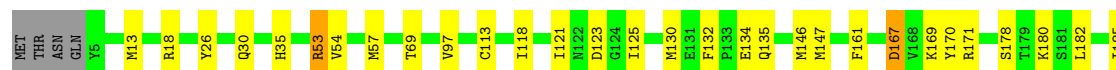
- Molecule 1: Asparagine synthetase domain-containing protein





- Molecule 1: Asparagine synthetase domain-containing protein

Chain L: 80% 14% 5%



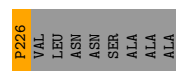
- Molecule 1: Asparagine synthetase domain-containing protein

Chain A: 79% 14% 5%



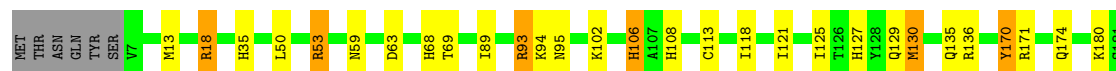
- Molecule 1: Asparagine synthetase domain-containing protein

Chain M: 81% 12% 6%



- Molecule 1: Asparagine synthetase domain-containing protein

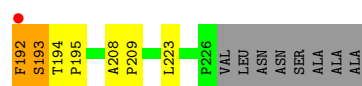
Chain J: 79% 12% 6%



- Molecule 1: Asparagine synthetase domain-containing protein

Chain F: 78% 15% 6%





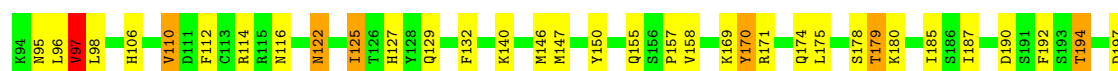
- Molecule 1: Asparagine synthetase domain-containing protein

Chain K: 74% 18% 6%



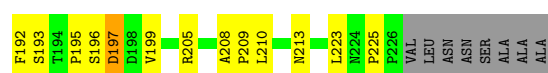
- Molecule 1: Asparagine synthetase domain-containing protein

Chain E: 59% 28% 8%



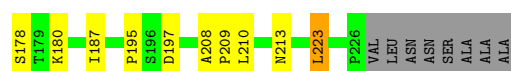
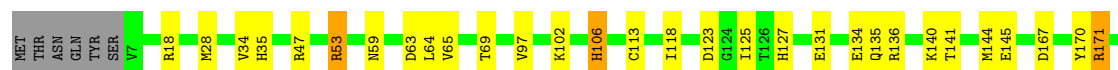
- Molecule 1: Asparagine synthetase domain-containing protein

Chain I: 76% 17% 6%



- Molecule 1: Asparagine synthetase domain-containing protein

Chain B: 77% 15% 6%



- Molecule 1: Asparagine synthetase domain-containing protein

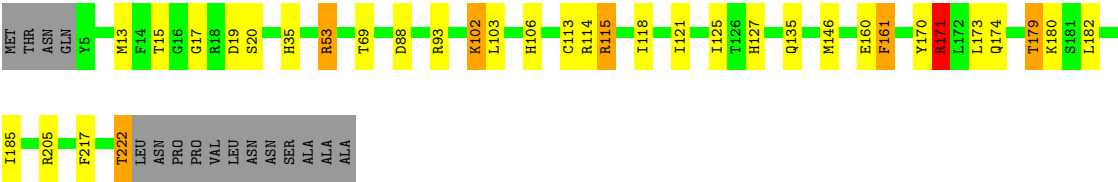
Chain G:

78%

12%

•

7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	69.76Å 134.92Å 234.27Å 90.00° 98.55° 90.00°	Depositor
Resolution (Å)	48.28 – 2.34 48.28 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.28-2.34) 99.2 (48.28-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.247 , 0.285 0.253 , 0.288	Depositor DCC
R_{free} test set	9081 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 24.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.287 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	24736	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.92	0/1780	1.27	11/2410 (0.5%)
1	B	0.86	0/1767	1.25	6/2392 (0.3%)
1	C	0.85	0/1786	1.22	6/2418 (0.2%)
1	D	0.83	0/1782	1.25	10/2413 (0.4%)
1	E	0.99	2/1735 (0.1%)	1.66	25/2346 (1.1%)
1	F	0.77	0/1772	1.15	2/2399 (0.1%)
1	G	0.86	0/1754	1.21	7/2372 (0.3%)
1	H	0.75	0/1796	1.16	4/2432 (0.2%)
1	I	0.75	0/1767	1.20	7/2392 (0.3%)
1	J	0.72	0/1774	1.20	9/2402 (0.4%)
1	K	0.72	0/1773	1.14	3/2400 (0.1%)
1	L	0.74	0/1786	1.14	6/2418 (0.2%)
1	M	0.85	0/1773	1.27	5/2400 (0.2%)
1	N	0.90	0/1786	1.26	6/2418 (0.2%)
All	All	0.82	2/24831 (0.0%)	1.25	107/33612 (0.3%)

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	2
1	B	0	2
1	C	0	1
1	D	0	4
1	E	0	1
1	F	0	1
1	G	0	4
1	H	0	1
1	I	0	4
1	J	0	3
1	K	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
1	M	0	2
1	N	0	3
All	All	0	33

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	44	SER	CA-CB	-5.77	1.44	1.53
1	E	208	ALA	C-O	-5.02	1.20	1.24

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ASP	CA-CB-CG	9.58	122.18	112.60
1	E	197	ASP	CA-CB-CG	9.14	121.74	112.60
1	J	59	ASN	CA-CB-CG	8.67	121.27	112.60
1	B	59	ASN	CA-CB-CG	8.33	120.93	112.60
1	E	194	THR	CA-CB-OG1	-7.61	98.19	109.60

There are no chirality outliers.

5 of 33 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	18	ARG	Sidechain
1	H	18	ARG	Sidechain
1	N	171	ARG	Sidechain
1	N	18	ARG	Sidechain
1	N	93	ARG	Sidechain

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	1745	0	1742	21	0
1	B	1732	0	1728	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1750	0	1742	30	1
1	D	1747	0	1748	25	0
1	E	1702	0	1697	41	1
1	F	1737	0	1730	36	0
1	G	1720	0	1711	23	0
1	H	1761	0	1759	32	0
1	I	1732	0	1728	23	0
1	J	1739	0	1737	26	0
1	K	1738	0	1733	58	0
1	L	1750	0	1742	19	0
1	M	1738	0	1733	22	0
1	N	1750	0	1742	19	0
2	A	37	0	0	1	0
2	B	30	0	0	3	0
2	C	32	0	0	0	0
2	D	31	0	0	1	0
2	E	52	0	0	4	0
2	F	23	0	0	1	0
2	G	35	0	0	0	0
2	H	22	0	0	2	0
2	I	18	0	0	1	0
2	J	24	0	0	2	0
2	K	10	0	0	0	0
2	L	17	0	0	0	0
2	M	32	0	0	0	0
2	N	32	0	0	1	0
All	All	24736	0	24272	379	1

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 8.

The worst 5 of 379 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:B:141:THR:HA	1:B:144:MET:HE3	1.31	1.12
1:K:28:MET:HE3	1:K:34:VAL:CG2	1.80	1.10
1:K:28:MET:CE	1:K:34:VAL:HG22	1.82	1.08
1:M:28:MET:CE	1:M:34:VAL:HG22	1.85	1.06
1:B:28:MET:CE	1:B:34:VAL:HG22	1.87	1.04

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:TYR:OH	1:E:190:ASP:OD2[2_555]	1.81	0.39

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	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
1	B	218/234 (93%)	213 (98%)	5 (2%)	0	100	100
1	C	220/234 (94%)	212 (96%)	8 (4%)	0	100	100
1	D	220/234 (94%)	215 (98%)	5 (2%)	0	100	100
1	E	214/234 (92%)	204 (95%)	8 (4%)	2 (1%)	14	14
1	F	219/234 (94%)	210 (96%)	7 (3%)	2 (1%)	14	14
1	G	216/234 (92%)	212 (98%)	4 (2%)	0	100	100
1	H	222/234 (95%)	218 (98%)	4 (2%)	0	100	100
1	I	218/234 (93%)	208 (95%)	9 (4%)	1 (0%)	25	27
1	J	219/234 (94%)	215 (98%)	4 (2%)	0	100	100
1	K	219/234 (94%)	211 (96%)	6 (3%)	2 (1%)	14	14
1	L	220/234 (94%)	214 (97%)	6 (3%)	0	100	100
1	M	219/234 (94%)	212 (97%)	7 (3%)	0	100	100
1	N	220/234 (94%)	212 (96%)	8 (4%)	0	100	100
All	All	3064/3276 (94%)	2973 (97%)	84 (3%)	7 (0%)	44	51

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	K	162	ALA
1	E	221	GLU

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Mol	Chain	Res	Type
1	F	191	SER
1	F	193	SER
1	K	163	GLN

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	191/200 (96%)	187 (98%)	4 (2%)	48	60
1	B	189/200 (94%)	184 (97%)	5 (3%)	41	51
1	C	191/200 (96%)	188 (98%)	3 (2%)	58	70
1	D	191/200 (96%)	184 (96%)	7 (4%)	29	37
1	E	185/200 (92%)	172 (93%)	13 (7%)	12	13
1	F	189/200 (94%)	188 (100%)	1 (0%)	86	92
1	G	187/200 (94%)	182 (97%)	5 (3%)	40	50
1	H	193/200 (96%)	187 (97%)	6 (3%)	35	44
1	I	189/200 (94%)	183 (97%)	6 (3%)	34	42
1	J	190/200 (95%)	185 (97%)	5 (3%)	41	51
1	K	190/200 (95%)	187 (98%)	3 (2%)	58	70
1	L	191/200 (96%)	187 (98%)	4 (2%)	48	60
1	M	190/200 (95%)	185 (97%)	5 (3%)	41	51
1	N	191/200 (96%)	186 (97%)	5 (3%)	41	51
All	All	2657/2800 (95%)	2585 (97%)	72 (3%)	40	50

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	49	ILE
1	G	222	THR
1	I	97	VAL
1	B	178	SER

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Mol	Chain	Res	Type
1	L	185	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	135	GLN
1	G	163	GLN
1	I	68	HIS
1	B	135	GLN
1	L	213	ASN

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.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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 ²)	Q<0.9
1	A	222/234 (94%)	-1.31	0 100 100	30, 42, 62, 96	0
1	B	220/234 (94%)	-1.24	0 100 100	35, 47, 73, 98	0
1	C	222/234 (94%)	-1.28	0 100 100	30, 45, 83, 98	0
1	D	222/234 (94%)	-1.15	0 100 100	35, 51, 99, 127	0
1	E	216/234 (92%)	-1.37	0 100 100	27, 39, 56, 70	0
1	F	221/234 (94%)	-1.25	1 (0%) 87 89	37, 55, 81, 141	0
1	G	218/234 (93%)	-1.28	0 100 100	31, 44, 61, 80	0
1	H	224/234 (95%)	-1.26	1 (0%) 89 90	35, 54, 72, 121	0
1	I	220/234 (94%)	-1.23	0 100 100	44, 58, 86, 113	0
1	J	221/234 (94%)	-1.23	0 100 100	43, 60, 77, 96	0
1	K	221/234 (94%)	-1.18	0 100 100	44, 64, 100, 133	0
1	L	222/234 (94%)	-1.25	0 100 100	30, 58, 88, 121	0
1	M	221/234 (94%)	-1.33	0 100 100	34, 50, 68, 94	0
1	N	222/234 (94%)	-1.36	0 100 100	33, 46, 64, 128	0
All	All	3092/3276 (94%)	-1.27	2 (0%) 92 94	27, 51, 80, 141	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	192	PHE	2.8
1	H	228	LEU	2.5

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.