



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 03:47 AM UTC

PDB ID : 3IBB / pdb\_00003ibb  
Title : Propionyl-CoA Carboxylase Beta Subunit, D422A  
Authors : Diacovich, L.; Arabolaza, A.; Shillito, E.M.; Lin, T.-W.; Mitchell, D.L.; Pham, H.; Melgar, M.M.  
Deposited on : 2009-07-15  
Resolution : 3.50 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](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  
Xtrriage (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

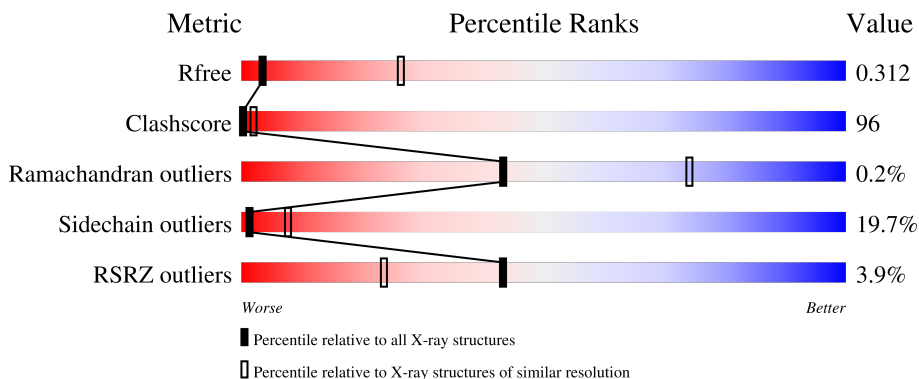
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

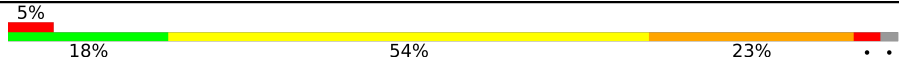
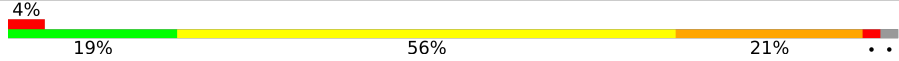
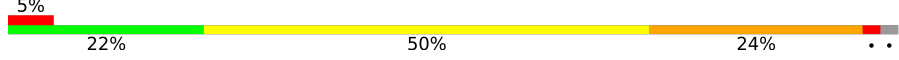
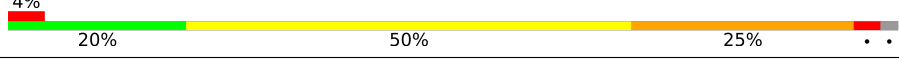
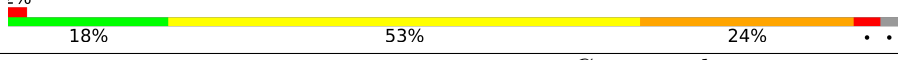
The reported resolution of this entry is 3.50 Å.

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.



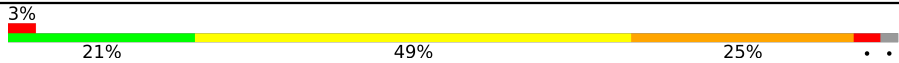
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	530	
1	B	530	
1	C	530	
1	D	530	
1	E	530	

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Mol	Chain	Length	Quality of chain
1	F	530	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment (3%), a green segment (21%), a large yellow segment (49%), and an orange segment (25%). The segments are separated by thin black lines. The percentages are labeled below each segment. The red segment is at the far left, followed by green, then yellow, and finally orange at the far right. There are two small black dots at the end of the orange segment.</p>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23700 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.

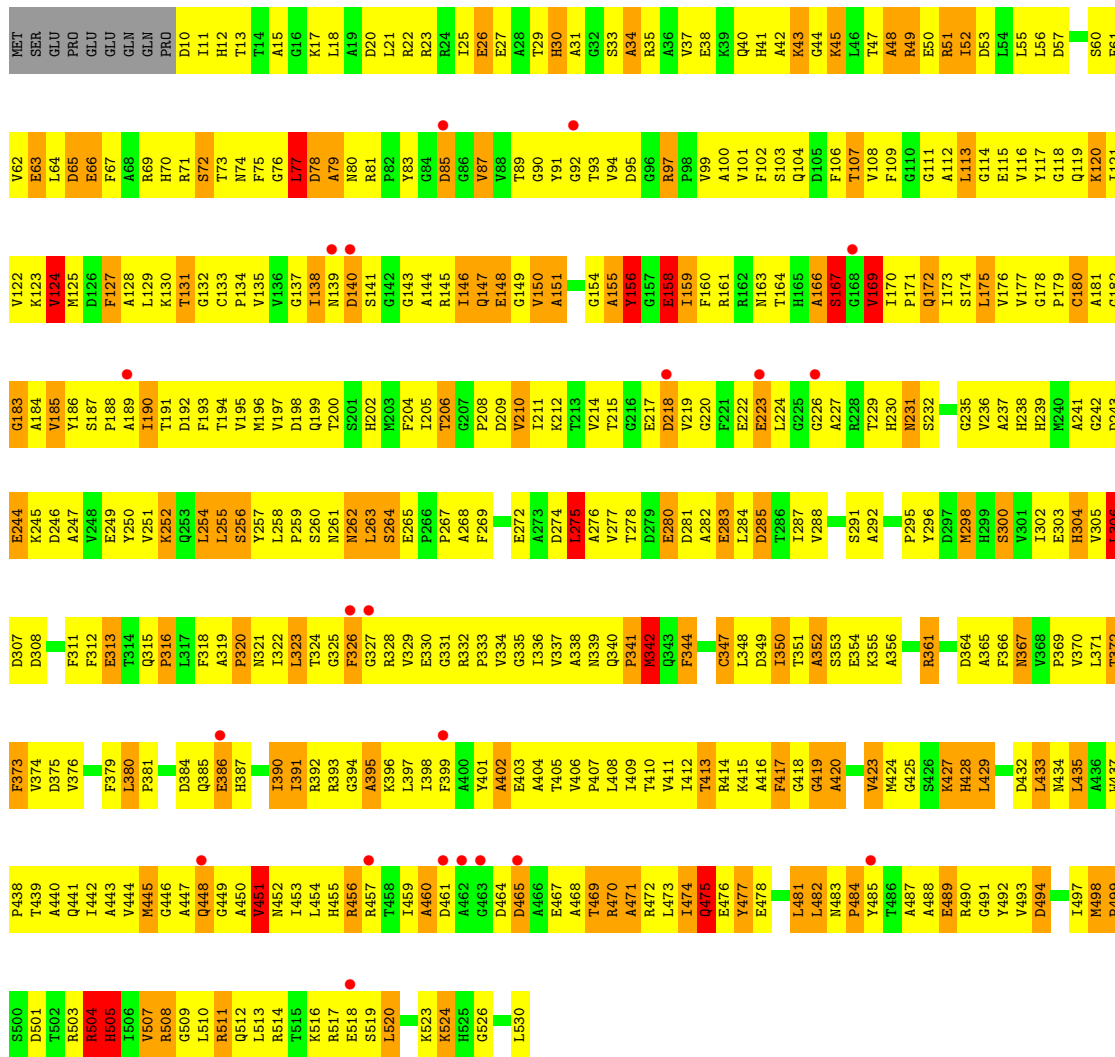
- Molecule 1 is a protein called Propionyl-CoA carboxylase complex B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	521	3950	2480	698	759	13	0	0	0
1	B	521	3950	2480	698	759	13	0	0	0
1	C	521	3950	2480	698	759	13	0	0	0
1	D	521	3950	2480	698	759	13	0	0	0
1	E	521	3950	2480	698	759	13	0	0	0
1	F	521	3950	2480	698	759	13	0	0	0

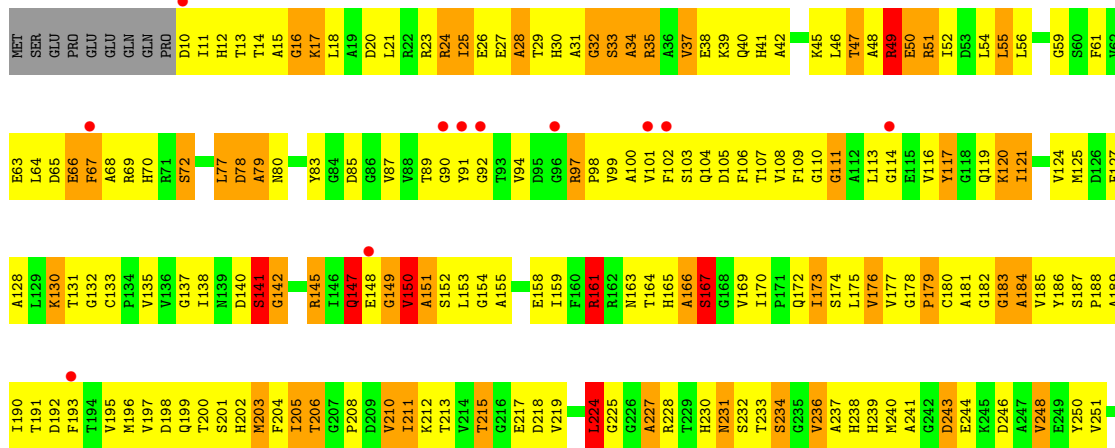
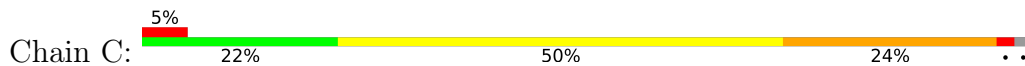
There are 6 discrepancies between the modelled and reference sequences:

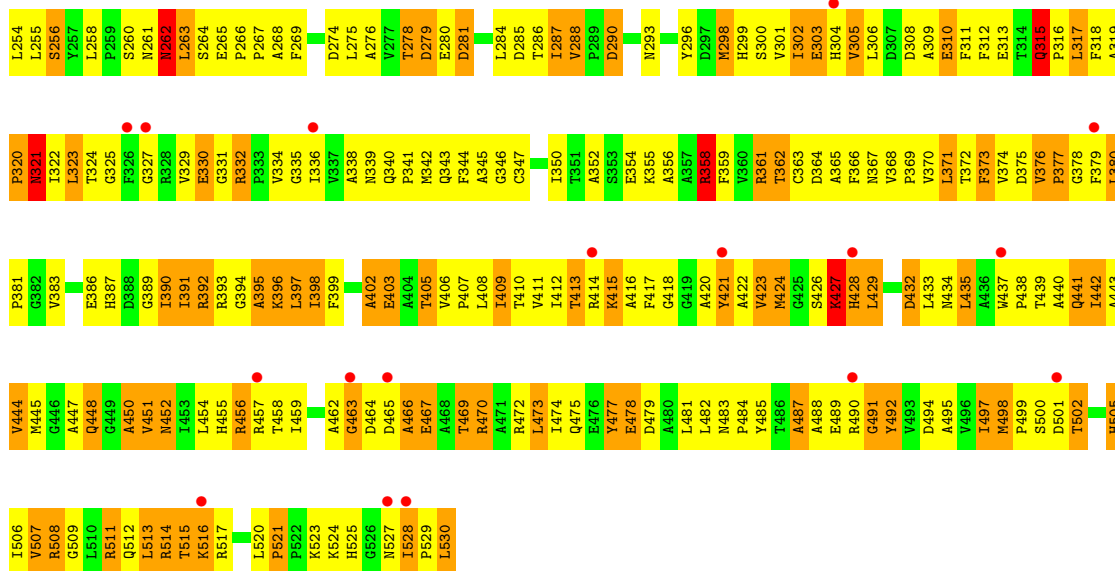
Chain	Residue	Modelled	Actual	Comment	Reference
A	422	ALA	ASP	engineered mutation	UNP Q9X4K7
B	422	ALA	ASP	engineered mutation	UNP Q9X4K7
C	422	ALA	ASP	engineered mutation	UNP Q9X4K7
D	422	ALA	ASP	engineered mutation	UNP Q9X4K7
E	422	ALA	ASP	engineered mutation	UNP Q9X4K7
F	422	ALA	ASP	engineered mutation	UNP Q9X4K7



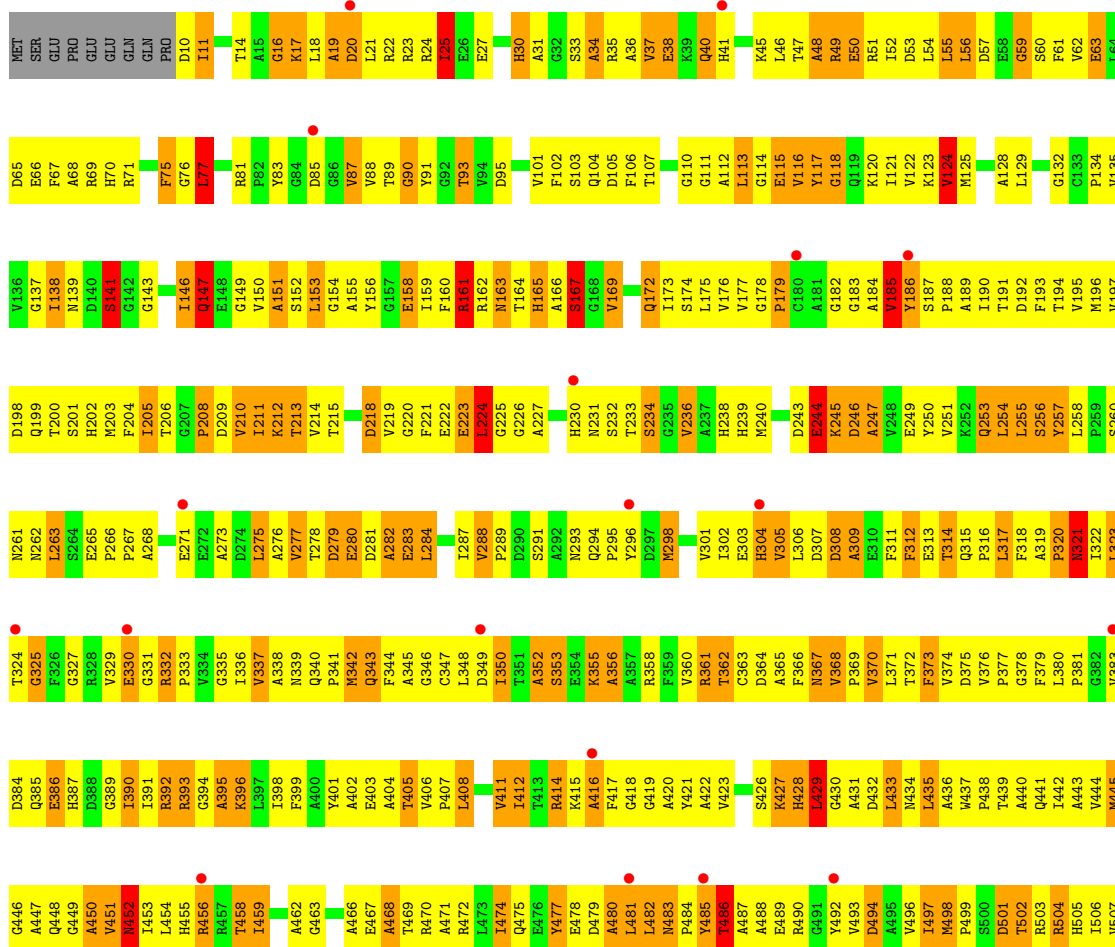
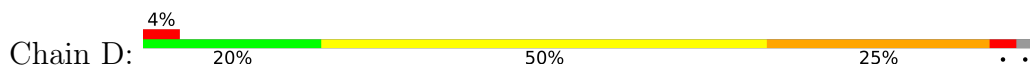


• Molecule 1: Propionyl-CoA carboxylase complex B subunit

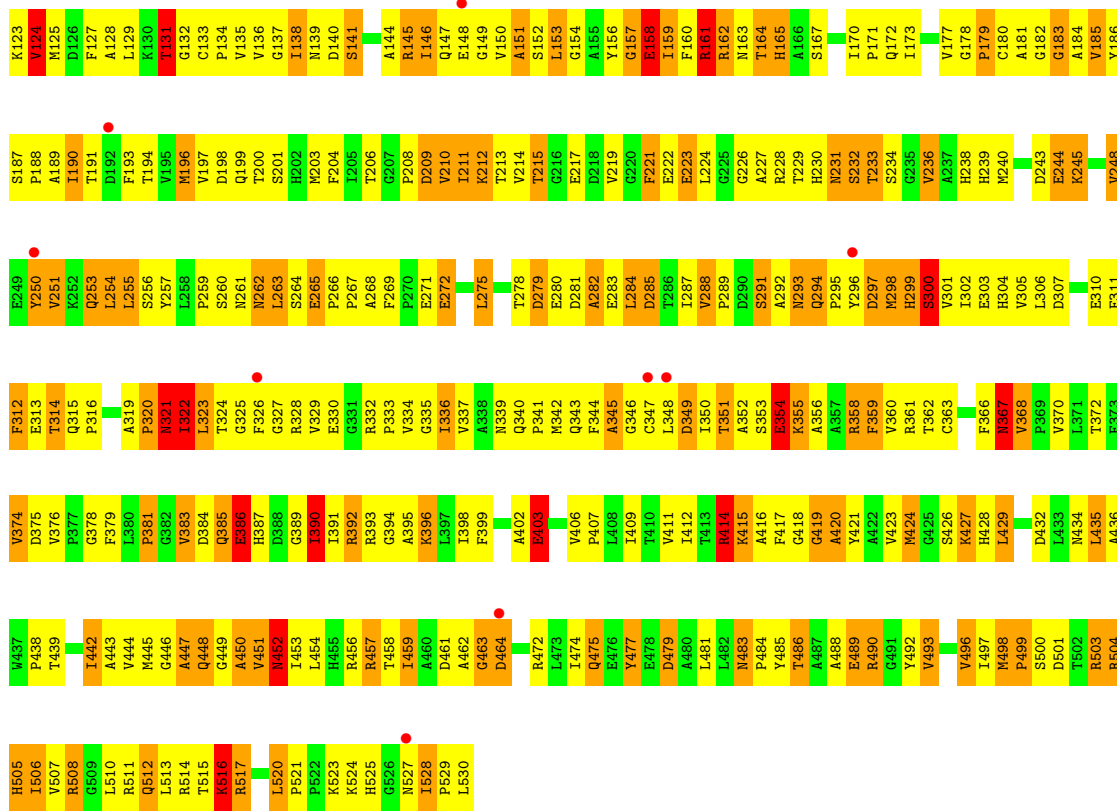




● Molecule 1: Propionyl-CoA carboxylase complex B subunit







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.06Å 183.33Å 228.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.50 50.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.4 (50.00-3.50) 95.2 (50.00-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.04 (at 3.48Å)	Xtrriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, $R_{free}$	0.190 , 0.269 0.299 , 0.312	Depositor DCC
$R_{free}$ test set	2294 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.3	Xtrriage
Anisotropy	0.084	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 0.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	23700	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	2.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.72	7/4030 (0.2%)	1.60	114/5474 (2.1%)
1	B	0.62	6/4030 (0.1%)	1.52	94/5474 (1.7%)
1	C	0.59	2/4030 (0.0%)	1.53	107/5474 (2.0%)
1	D	0.66	3/4030 (0.1%)	1.55	109/5474 (2.0%)
1	E	0.64	6/4030 (0.1%)	1.57	113/5474 (2.1%)
1	F	0.61	5/4030 (0.1%)	1.45	93/5474 (1.7%)
All	All	0.64	29/24180 (0.1%)	1.54	630/32844 (1.9%)

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	525	HIS	C-N	13.51	1.40	1.33
1	D	363	CYS	C-N	9.24	1.46	1.34
1	E	414	ARG	C-N	9.11	1.46	1.33
1	A	238	HIS	C-N	-8.94	1.21	1.33
1	A	357	ALA	C-N	-8.76	1.22	1.33

The worst 5 of 630 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	VAL	N-CA-C	12.41	122.20	110.53
1	A	456	ARG	N-CA-C	-12.39	97.46	111.71
1	A	448	GLN	N-CA-C	-12.35	97.82	111.28
1	B	419	GLY	N-CA-C	-12.22	100.83	114.40
1	E	492	TYR	N-CA-C	-12.21	97.67	111.71

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3950	0	3881	869	0
1	B	3950	0	3881	814	0
1	C	3950	0	3881	809	0
1	D	3950	0	3881	833	0
1	E	3950	0	3881	803	0
1	F	3950	0	3881	812	0
All	All	23700	0	23286	4502	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 96.

The worst 5 of 4502 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:F:497:ILE:HD13	1:F:505:HIS:CD2	1.40	1.54
1:C:379:PHE:CE2	1:D:205:ILE:HD11	1.38	1.54
1:A:318:PHE:CZ	1:A:351:THR:HB	1.42	1.53
1:F:311:PHE:CE1	1:F:325:GLY:HA3	1.45	1.49
1:F:215:THR:CG2	1:F:217:GLU:HG2	1.43	1.47

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	519/530 (98%)	503 (97%)	14 (3%)	2 (0%)	30 62

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	519/530 (98%)	501 (96%)	18 (4%)	0	100	100
1	C	519/530 (98%)	501 (96%)	17 (3%)	1 (0%)	43	74
1	D	519/530 (98%)	501 (96%)	17 (3%)	1 (0%)	43	74
1	E	519/530 (98%)	505 (97%)	14 (3%)	0	100	100
1	F	519/530 (98%)	503 (97%)	13 (2%)	3 (1%)	21	54
All	All	3114/3180 (98%)	3014 (97%)	93 (3%)	7 (0%)	43	74

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	416	ALA
1	F	145	ARG
1	F	516	LYS
1	A	389	GLY
1	F	381	PRO

### 5.3.2 Protein sidechains [i](#)

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	411/420 (98%)	340 (83%)	71 (17%)	2	11
1	B	411/420 (98%)	337 (82%)	74 (18%)	2	10
1	C	411/420 (98%)	340 (83%)	71 (17%)	2	11
1	D	411/420 (98%)	324 (79%)	87 (21%)	1	6
1	E	411/420 (98%)	326 (79%)	85 (21%)	1	6
1	F	411/420 (98%)	312 (76%)	99 (24%)	1	4
All	All	2466/2520 (98%)	1979 (80%)	487 (20%)	1	8

5 of 487 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	124	VAL

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Mol	Chain	Res	Type
1	F	321	ASN
1	D	456	ARG
1	F	298	MET
1	F	483	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	40	GLN
1	E	315	GLN
1	F	505	HIS
1	E	80	ASN
1	E	231	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, 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	521/530 (98%)	0.45	26 (4%) 34 19	2, 2, 2, 2	0
1	B	521/530 (98%)	0.48	21 (4%) 42 23	2, 2, 2, 16	0
1	C	521/530 (98%)	0.51	28 (5%) 31 18	2, 2, 2, 14	0
1	D	521/530 (98%)	0.63	20 (3%) 44 24	2, 2, 2, 2	0
1	E	521/530 (98%)	0.42	12 (2%) 61 37	2, 2, 2, 2	0
1	F	521/530 (98%)	0.53	15 (2%) 53 31	2, 2, 2, 13	0
All	All	3126/3180 (98%)	0.50	122 (3%) 43 23	2, 2, 2, 16	0

The worst 5 of 122 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	85	ASP	6.4
1	A	85	ASP	5.3
1	C	67	PHE	5.2
1	F	91	TYR	5.0
1	F	527	ASN	5.0

### 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.