



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:51 PM GMT

PDB ID : 3V9G  
Title : Crystal structure of human 1-pyrroline-5-carboxylate dehydrogenase  
Authors : Tanner, J.J.; Srivastava, D.  
Deposited on : 2011-12-27  
Resolution : 2.50 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

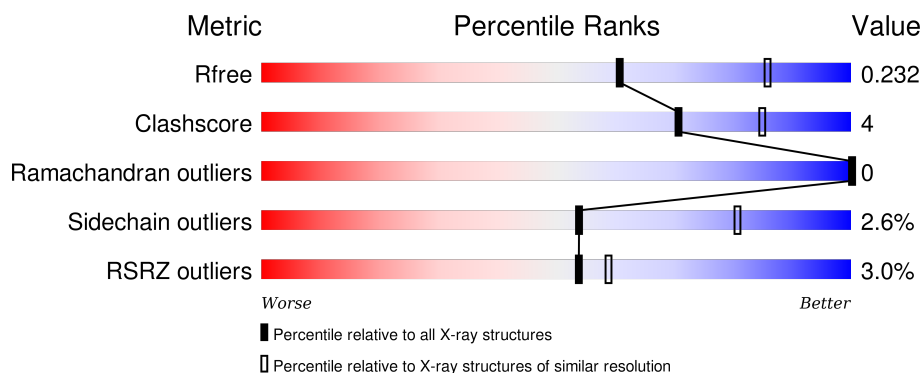
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	566	<div> <div></div> <div>84% 9% . .</div> </div>
1	B	566	<div> <div></div> <div>85% 9% . .</div> </div>
1	C	566	<div> <div>4%</div> <div>85% 9% . 5%</div> </div>
1	D	566	<div> <div>5%</div> <div>86% 8% . 5%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16032 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 Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	S	0	0	0
			4045	2590	683	757	15			
1	B	541	Total	C	N	O	S	0	0	0
			4033	2583	685	750	15			
1	C	540	Total	C	N	O	S	0	0	0
			3995	2566	671	743	15			
1	D	540	Total	C	N	O	S	0	0	0
			3959	2538	669	737	15			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	EXPRESSION TAG	UNP P30038
A	-1	GLY	-	EXPRESSION TAG	UNP P30038
A	0	SER	-	EXPRESSION TAG	UNP P30038
A	1	SER	-	EXPRESSION TAG	UNP P30038
A	2	HIS	-	EXPRESSION TAG	UNP P30038
A	3	HIS	-	EXPRESSION TAG	UNP P30038
A	4	HIS	-	EXPRESSION TAG	UNP P30038
A	5	HIS	-	EXPRESSION TAG	UNP P30038
A	6	HIS	-	EXPRESSION TAG	UNP P30038
A	7	HIS	-	EXPRESSION TAG	UNP P30038
A	8	SER	-	EXPRESSION TAG	UNP P30038
A	9	SER	-	EXPRESSION TAG	UNP P30038
A	10	GLY	-	EXPRESSION TAG	UNP P30038
A	11	LEU	-	EXPRESSION TAG	UNP P30038
A	12	VAL	-	EXPRESSION TAG	UNP P30038
A	13	PRO	-	EXPRESSION TAG	UNP P30038
A	14	ARG	-	EXPRESSION TAG	UNP P30038
A	15	GLY	-	EXPRESSION TAG	UNP P30038
A	16	SER	-	EXPRESSION TAG	UNP P30038
A	17	HIS	-	EXPRESSION TAG	UNP P30038
B	-2	MET	-	EXPRESSION TAG	UNP P30038

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	EXPRESSION TAG	UNP P30038
B	0	SER	-	EXPRESSION TAG	UNP P30038
B	1	SER	-	EXPRESSION TAG	UNP P30038
B	2	HIS	-	EXPRESSION TAG	UNP P30038
B	3	HIS	-	EXPRESSION TAG	UNP P30038
B	4	HIS	-	EXPRESSION TAG	UNP P30038
B	5	HIS	-	EXPRESSION TAG	UNP P30038
B	6	HIS	-	EXPRESSION TAG	UNP P30038
B	7	HIS	-	EXPRESSION TAG	UNP P30038
B	8	SER	-	EXPRESSION TAG	UNP P30038
B	9	SER	-	EXPRESSION TAG	UNP P30038
B	10	GLY	-	EXPRESSION TAG	UNP P30038
B	11	LEU	-	EXPRESSION TAG	UNP P30038
B	12	VAL	-	EXPRESSION TAG	UNP P30038
B	13	PRO	-	EXPRESSION TAG	UNP P30038
B	14	ARG	-	EXPRESSION TAG	UNP P30038
B	15	GLY	-	EXPRESSION TAG	UNP P30038
B	16	SER	-	EXPRESSION TAG	UNP P30038
B	17	HIS	-	EXPRESSION TAG	UNP P30038
C	-2	MET	-	EXPRESSION TAG	UNP P30038
C	-1	GLY	-	EXPRESSION TAG	UNP P30038
C	0	SER	-	EXPRESSION TAG	UNP P30038
C	1	SER	-	EXPRESSION TAG	UNP P30038
C	2	HIS	-	EXPRESSION TAG	UNP P30038
C	3	HIS	-	EXPRESSION TAG	UNP P30038
C	4	HIS	-	EXPRESSION TAG	UNP P30038
C	5	HIS	-	EXPRESSION TAG	UNP P30038
C	6	HIS	-	EXPRESSION TAG	UNP P30038
C	7	HIS	-	EXPRESSION TAG	UNP P30038
C	8	SER	-	EXPRESSION TAG	UNP P30038
C	9	SER	-	EXPRESSION TAG	UNP P30038
C	10	GLY	-	EXPRESSION TAG	UNP P30038
C	11	LEU	-	EXPRESSION TAG	UNP P30038
C	12	VAL	-	EXPRESSION TAG	UNP P30038
C	13	PRO	-	EXPRESSION TAG	UNP P30038
C	14	ARG	-	EXPRESSION TAG	UNP P30038
C	15	GLY	-	EXPRESSION TAG	UNP P30038
C	16	SER	-	EXPRESSION TAG	UNP P30038
C	17	HIS	-	EXPRESSION TAG	UNP P30038
D	-2	MET	-	EXPRESSION TAG	UNP P30038
D	-1	GLY	-	EXPRESSION TAG	UNP P30038
D	0	SER	-	EXPRESSION TAG	UNP P30038

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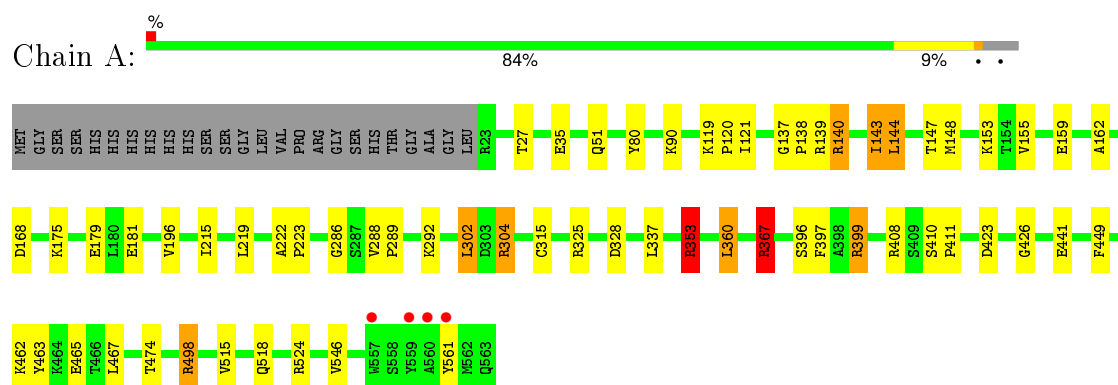
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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	SER	-	EXPRESSION TAG	UNP P30038
D	2	HIS	-	EXPRESSION TAG	UNP P30038
D	3	HIS	-	EXPRESSION TAG	UNP P30038
D	4	HIS	-	EXPRESSION TAG	UNP P30038
D	5	HIS	-	EXPRESSION TAG	UNP P30038
D	6	HIS	-	EXPRESSION TAG	UNP P30038
D	7	HIS	-	EXPRESSION TAG	UNP P30038
D	8	SER	-	EXPRESSION TAG	UNP P30038
D	9	SER	-	EXPRESSION TAG	UNP P30038
D	10	GLY	-	EXPRESSION TAG	UNP P30038
D	11	LEU	-	EXPRESSION TAG	UNP P30038
D	12	VAL	-	EXPRESSION TAG	UNP P30038
D	13	PRO	-	EXPRESSION TAG	UNP P30038
D	14	ARG	-	EXPRESSION TAG	UNP P30038
D	15	GLY	-	EXPRESSION TAG	UNP P30038
D	16	SER	-	EXPRESSION TAG	UNP P30038
D	17	HIS	-	EXPRESSION TAG	UNP P30038

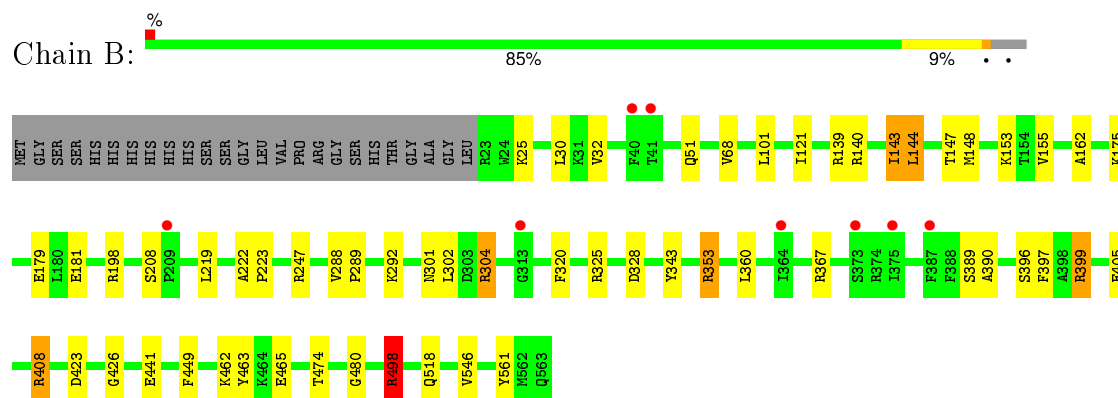
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

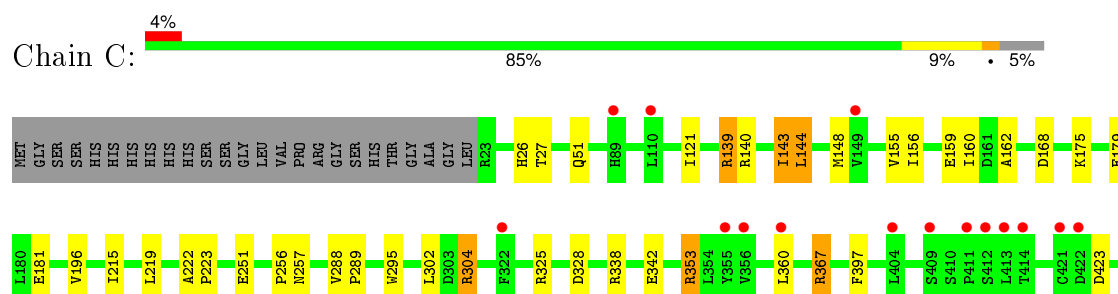
- Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial



- Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial

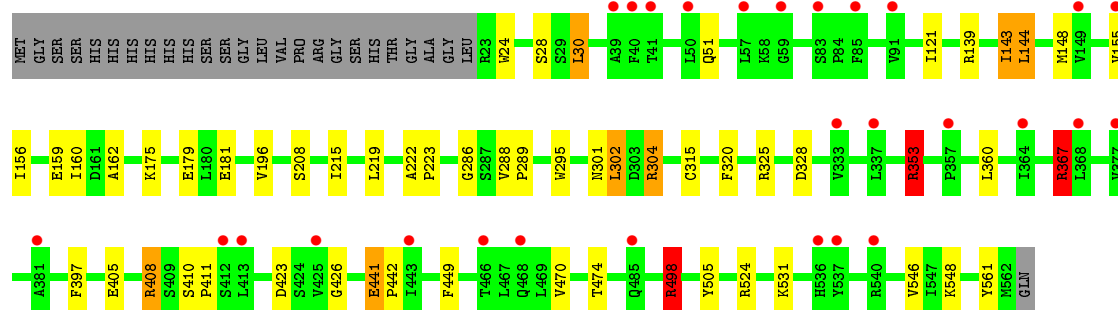
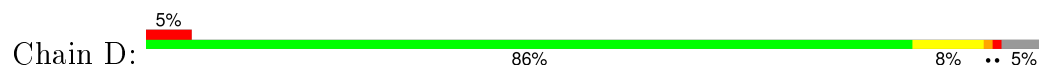


- Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial





- Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.72Å 150.72Å 191.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.66 – 2.50 47.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.66-2.50) 99.7 (47.78-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.204 , 0.238 0.195 , 0.232	Depositor DCC
$R_{free}$ test set	2002 reflections (2.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.2	EDS
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 84867 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	16032	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.47	0/4152	1.01	26/5667 (0.5%)
1	B	0.45	0/4140	0.88	22/5652 (0.4%)
1	C	0.43	0/4102	0.95	21/5607 (0.4%)
1	D	0.42	0/4064	0.79	19/5563 (0.3%)
All	All	0.44	0/16458	0.91	88/22489 (0.4%)

There are no bond length outliers.

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ARG	NE-CZ-NH2	-23.05	108.77	120.30
1	C	139	ARG	NE-CZ-NH2	-21.12	109.74	120.30
1	A	140	ARG	NE-CZ-NH1	21.00	130.80	120.30
1	C	524	ARG	NE-CZ-NH1	-17.89	111.35	120.30
1	C	139	ARG	NE-CZ-NH1	17.51	129.05	120.30
1	A	408	ARG	NE-CZ-NH1	-16.61	111.99	120.30
1	A	367	ARG	NE-CZ-NH1	16.60	128.60	120.30
1	C	367	ARG	NE-CZ-NH1	-16.41	112.09	120.30
1	B	498	ARG	NE-CZ-NH2	16.14	128.37	120.30
1	C	524	ARG	NE-CZ-NH2	16.12	128.36	120.30
1	C	498	ARG	NE-CZ-NH2	-15.98	112.31	120.30
1	C	498	ARG	NE-CZ-NH1	15.96	128.28	120.30
1	A	408	ARG	NE-CZ-NH2	15.87	128.23	120.30
1	B	367	ARG	NE-CZ-NH1	-15.75	112.42	120.30
1	C	367	ARG	NE-CZ-NH2	15.72	128.16	120.30
1	D	498	ARG	NE-CZ-NH2	15.69	128.14	120.30
1	B	367	ARG	NE-CZ-NH2	15.20	127.90	120.30
1	A	367	ARG	NE-CZ-NH2	-14.81	112.90	120.30
1	A	498	ARG	NE-CZ-NH1	14.56	127.58	120.30
1	B	304	ARG	NE-CZ-NH2	-13.27	113.67	120.30
1	D	498	ARG	NE-CZ-NH1	-13.23	113.68	120.30
1	A	399	ARG	NE-CZ-NH1	-13.07	113.76	120.30
1	B	399	ARG	NE-CZ-NH2	-13.03	113.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	498	ARG	NE-CZ-NH2	-12.90	113.85	120.30
1	C	304	ARG	NE-CZ-NH1	-12.83	113.89	120.30
1	B	304	ARG	NE-CZ-NH1	12.78	126.69	120.30
1	D	304	ARG	NE-CZ-NH2	-12.76	113.92	120.30
1	B	353	ARG	NE-CZ-NH2	12.72	126.66	120.30
1	D	367	ARG	NE-CZ-NH1	12.65	126.62	120.30
1	D	353	ARG	NE-CZ-NH1	12.64	126.62	120.30
1	A	353	ARG	NE-CZ-NH1	12.57	126.58	120.30
1	A	399	ARG	NE-CZ-NH2	12.56	126.58	120.30
1	A	304	ARG	NE-CZ-NH1	-12.53	114.03	120.30
1	B	399	ARG	NE-CZ-NH1	12.49	126.55	120.30
1	D	304	ARG	NE-CZ-NH1	12.41	126.50	120.30
1	B	498	ARG	NE-CZ-NH1	-12.20	114.20	120.30
1	C	353	ARG	NE-CZ-NH2	11.95	126.27	120.30
1	D	353	ARG	NE-CZ-NH2	-11.83	114.39	120.30
1	A	304	ARG	NE-CZ-NH2	11.78	126.19	120.30
1	C	353	ARG	NE-CZ-NH1	-11.64	114.48	120.30
1	C	304	ARG	NE-CZ-NH2	11.64	126.12	120.30
1	D	367	ARG	NE-CZ-NH2	-11.55	114.52	120.30
1	A	353	ARG	NE-CZ-NH2	-11.31	114.65	120.30
1	B	353	ARG	NE-CZ-NH1	-10.89	114.86	120.30
1	A	367	ARG	CD-NE-CZ	10.09	137.72	123.60
1	D	498	ARG	CD-NE-CZ	9.40	136.76	123.60
1	B	408	ARG	NE-CZ-NH2	-9.27	115.66	120.30
1	B	498	ARG	CD-NE-CZ	9.16	136.42	123.60
1	C	498	ARG	CD-NE-CZ	8.95	136.13	123.60
1	C	139	ARG	CD-NE-CZ	8.92	136.08	123.60
1	B	367	ARG	CD-NE-CZ	8.74	135.83	123.60
1	A	140	ARG	CD-NE-CZ	8.72	135.81	123.60
1	C	367	ARG	CD-NE-CZ	8.54	135.55	123.60
1	C	498	ARG	CG-CD-NE	-8.46	94.03	111.80
1	D	408	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	B	408	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	D	408	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	A	498	ARG	CD-NE-CZ	7.97	134.77	123.60
1	A	498	ARG	CG-CD-NE	-7.87	95.27	111.80
1	A	408	ARG	CD-NE-CZ	7.87	134.61	123.60
1	A	367	ARG	CG-CD-NE	7.82	128.21	111.80
1	C	524	ARG	CD-NE-CZ	7.71	134.39	123.60
1	D	367	ARG	CD-NE-CZ	7.59	134.23	123.60
1	A	399	ARG	CD-NE-CZ	7.14	133.59	123.60
1	B	399	ARG	CD-NE-CZ	6.92	133.28	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	367	ARG	CG-CD-NE	-6.80	97.53	111.80
1	B	498	ARG	CG-CD-NE	6.79	126.06	111.80
1	A	353	ARG	CD-NE-CZ	6.77	133.08	123.60
1	C	367	ARG	CG-CD-NE	-6.66	97.82	111.80
1	D	304	ARG	CD-NE-CZ	6.52	132.73	123.60
1	A	524	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	B	139	ARG	NE-CZ-NH2	6.41	123.51	120.30
1	B	304	ARG	CD-NE-CZ	6.38	132.53	123.60
1	D	353	ARG	CD-NE-CZ	6.27	132.38	123.60
1	B	140	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	A	139	ARG	NE-CZ-NH2	6.19	123.39	120.30
1	B	139	ARG	NE-CZ-NH1	-6.17	117.21	120.30
1	D	498	ARG	CG-CD-NE	6.17	124.77	111.80
1	D	367	ARG	CG-CD-NE	6.11	124.62	111.80
1	B	353	ARG	CD-NE-CZ	5.97	131.96	123.60
1	C	353	ARG	CD-NE-CZ	5.77	131.67	123.60
1	C	140	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	A	304	ARG	CD-NE-CZ	5.65	131.51	123.60
1	C	304	ARG	CD-NE-CZ	5.65	131.50	123.60
1	D	524	ARG	NE-CZ-NH2	-5.61	117.49	120.30
1	D	139	ARG	NE-CZ-NH1	-5.47	117.56	120.30
1	D	139	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	A	139	ARG	NE-CZ-NH1	-5.33	117.64	120.30

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	4045	0	3842	42	0
1	B	4033	0	3827	38	0
1	C	3995	0	3765	40	0
1	D	3959	0	3706	45	0
All	All	16032	0	15140	138	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 4.

All (138) 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:396:SER:HA	1:A:399:ARG:HH11	1.27	0.98
1:B:396:SER:HA	1:B:399:ARG:NH1	1.98	0.78
1:A:325:ARG:HA	1:A:360:LEU:HD22	1.70	0.74
1:A:396:SER:HA	1:A:399:ARG:NH1	2.05	0.70
1:A:175:LYS:O	1:A:179:GLU:HG3	1.93	0.69
1:D:353:ARG:HH11	1:D:474:THR:HG21	1.58	0.68
1:D:353:ARG:HH11	1:D:474:THR:CG2	2.07	0.67
1:C:175:LYS:O	1:C:179:GLU:HG3	1.94	0.67
1:C:196:VAL:CG1	1:D:498:ARG:HH22	2.08	0.67
1:A:353:ARG:HH11	1:A:474:THR:HG21	1.61	0.66
1:B:396:SER:HA	1:B:399:ARG:HH11	1.62	0.65
1:D:175:LYS:O	1:D:179:GLU:HG3	1.98	0.64
1:D:143:ILE:HD12	1:D:162:ALA:HB1	1.80	0.63
1:A:353:ARG:HH11	1:A:474:THR:CG2	2.12	0.62
1:B:175:LYS:O	1:B:179:GLU:HG3	2.00	0.61
1:A:367:ARG:HB3	1:A:367:ARG:HH11	1.64	0.61
1:A:396:SER:CA	1:A:399:ARG:HH11	2.07	0.61
1:C:353:ARG:HH11	1:C:474:THR:CG2	2.13	0.61
1:B:143:ILE:HD12	1:B:162:ALA:HB1	1.83	0.61
1:D:353:ARG:NH1	1:D:474:THR:CG2	2.64	0.60
1:A:143:ILE:HD12	1:A:162:ALA:HB1	1.84	0.60
1:C:155:VAL:HB	1:D:561:TYR:CE2	2.37	0.60
1:D:367:ARG:HB3	1:D:367:ARG:HH11	1.66	0.59
1:B:353:ARG:HH11	1:B:474:THR:CG2	2.15	0.59
1:A:353:ARG:NH1	1:A:474:THR:CG2	2.67	0.58
1:C:498:ARG:NH2	1:D:196:VAL:CG1	2.66	0.57
1:D:144:LEU:O	1:D:148:MET:HG3	2.05	0.57
1:C:196:VAL:HG11	1:D:498:ARG:NH2	2.20	0.57
1:D:222:ALA:HB3	1:D:223:PRO:HD3	1.87	0.57
1:C:143:ILE:HD12	1:C:162:ALA:HB1	1.86	0.56
1:D:353:ARG:NH1	1:D:474:THR:HG23	2.21	0.55
1:A:80:TYR:CD2	1:A:90:LYS:HD3	2.42	0.55
1:B:423:ASP:HA	1:B:426:GLY:O	2.07	0.55
1:C:462:LYS:O	1:C:465:GLU:HG2	2.08	0.54
1:C:561:TYR:CE2	1:D:155:VAL:HB	2.43	0.53
1:B:325:ARG:HA	1:B:360:LEU:HD12	1.91	0.53
1:D:121:ILE:HG21	1:D:181:GLU:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:ASP:HA	1:D:426:GLY:O	2.09	0.53
1:A:546:VAL:HG11	1:B:518:GLN:HA	1.92	0.52
1:A:353:ARG:NH1	1:A:474:THR:HG23	2.23	0.52
1:A:423:ASP:HA	1:A:426:GLY:O	2.07	0.52
1:C:196:VAL:CG1	1:D:498:ARG:NH2	2.72	0.52
1:C:423:ASP:HA	1:C:426:GLY:O	2.08	0.52
1:A:328:ASP:C	1:A:328:ASP:OD1	2.49	0.51
1:C:353:ARG:HH11	1:C:474:THR:HG21	1.75	0.51
1:A:121:ILE:HG21	1:A:181:GLU:HG3	1.93	0.51
1:D:301:ASN:O	1:D:304:ARG:HG2	2.11	0.51
1:D:405:GLU:HA	1:D:408:ARG:HH11	1.76	0.50
1:B:121:ILE:HG21	1:B:181:GLU:HG3	1.93	0.50
1:C:139:ARG:NH2	1:C:251:GLU:OE1	2.44	0.50
1:C:144:LEU:O	1:C:148:MET:HG3	2.12	0.50
1:C:222:ALA:HB3	1:C:223:PRO:HD3	1.93	0.50
1:B:462:LYS:O	1:B:465:GLU:HG2	2.13	0.49
1:C:328:ASP:C	1:C:328:ASP:OD1	2.51	0.49
1:A:196:VAL:CG1	1:B:498:ARG:HH22	2.26	0.49
1:B:328:ASP:OD1	1:B:328:ASP:C	2.51	0.49
1:B:32:VAL:HG12	1:D:24:TRP:HB3	1.95	0.48
1:D:367:ARG:HB3	1:D:367:ARG:NH1	2.27	0.48
1:A:292:LYS:HG2	1:B:302:LEU:HD13	1.96	0.48
1:A:498:ARG:HH21	1:B:198:ARG:HG2	1.77	0.48
1:B:353:ARG:HH11	1:B:474:THR:HG21	1.79	0.48
1:D:325:ARG:HA	1:D:360:LEU:HD12	1.96	0.48
1:A:518:GLN:HA	1:B:546:VAL:HG11	1.96	0.48
1:A:144:LEU:O	1:A:148:MET:HG3	2.14	0.47
1:D:397:PHE:CZ	1:D:423:ASP:HB3	2.49	0.47
1:A:462:LYS:O	1:A:465:GLU:HG2	2.14	0.47
1:B:288:VAL:HB	1:B:289:PRO:HD3	1.95	0.47
1:C:121:ILE:HG21	1:C:181:GLU:HG3	1.95	0.47
1:D:441:GLU:CD	1:D:442:PRO:HD2	2.35	0.47
1:B:301:ASN:O	1:B:304:ARG:HG2	2.14	0.47
1:C:288:VAL:HB	1:C:289:PRO:HD3	1.95	0.47
1:C:196:VAL:HG11	1:D:498:ARG:HH22	1.76	0.47
1:D:328:ASP:C	1:D:328:ASP:OD1	2.53	0.47
1:A:367:ARG:NH1	1:A:367:ARG:HB3	2.29	0.46
1:B:405:GLU:HA	1:B:408:ARG:HH11	1.79	0.46
1:A:144:LEU:HD11	1:A:159:GLU:HA	1.97	0.46
1:D:208:SER:HB3	1:D:219:LEU:HD12	1.98	0.46
1:B:25:LYS:O	1:D:30:LEU:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:PHE:CZ	1:B:480:GLY:HA3	2.52	0.45
1:C:295:TRP:CG	1:D:302:LEU:HD11	2.52	0.45
1:A:410:SER:HA	1:A:411:PRO:HD3	1.70	0.45
1:D:410:SER:HA	1:D:411:PRO:HD3	1.72	0.45
1:B:208:SER:HB3	1:B:219:LEU:HD12	1.99	0.45
1:D:156:ILE:O	1:D:160:ILE:HG23	2.17	0.45
1:D:144:LEU:HD11	1:D:159:GLU:HA	1.99	0.44
1:C:302:LEU:HD11	1:D:295:TRP:CG	2.52	0.44
1:C:498:ARG:NH2	1:D:196:VAL:HG11	2.31	0.44
1:B:397:PHE:CZ	1:B:423:ASP:HB3	2.52	0.44
1:B:222:ALA:HB3	1:B:223:PRO:HD3	2.00	0.44
1:D:353:ARG:HH21	1:D:470:VAL:HG13	1.83	0.44
1:A:325:ARG:HA	1:A:360:LEU:CD2	2.43	0.43
1:D:405:GLU:HA	1:D:408:ARG:NH1	2.33	0.43
1:C:367:ARG:HE	1:C:367:ARG:HB3	1.31	0.43
1:C:518:GLN:HA	1:D:546:VAL:HG11	2.00	0.43
1:C:144:LEU:HD11	1:C:159:GLU:HA	2.01	0.43
1:D:215:ILE:O	1:D:219:LEU:HG	2.19	0.43
1:C:156:ILE:O	1:C:160:ILE:HG23	2.18	0.43
1:B:343:TYR:O	1:B:343:TYR:CG	2.71	0.43
1:A:222:ALA:HB3	1:A:223:PRO:HD3	2.01	0.43
1:C:256:PRO:O	1:C:257:ASN:HB2	2.19	0.43
1:C:397:PHE:CZ	1:C:423:ASP:HB3	2.54	0.43
1:A:196:VAL:HG11	1:B:498:ARG:NH2	2.35	0.42
1:C:441:GLU:CD	1:C:442:PRO:HD2	2.39	0.42
1:B:30:LEU:HD23	1:B:175:LYS:HA	2.02	0.42
1:A:137:GLY:HA3	1:A:138:PRO:HD3	1.89	0.42
1:B:144:LEU:O	1:B:148:MET:HG3	2.19	0.42
1:B:389:SER:OG	1:B:390:ALA:N	2.52	0.42
1:A:215:ILE:O	1:A:219:LEU:HG	2.19	0.42
1:A:196:VAL:HG11	1:B:498:ARG:HH22	1.83	0.42
1:A:561:TYR:CE2	1:B:155:VAL:HB	2.54	0.42
1:C:338:ARG:O	1:C:342:GLU:HG3	2.20	0.42
1:A:302:LEU:HD13	1:B:292:LYS:HG2	2.01	0.42
1:C:546:VAL:HG23	1:D:531:LYS:HE3	2.02	0.42
1:C:325:ARG:HA	1:C:360:LEU:HD12	2.01	0.42
1:D:286:GLY:O	1:D:315:CYS:HA	2.19	0.42
1:B:68:VAL:HG21	1:B:101:LEU:HD11	2.02	0.41
1:C:469:LEU:HD23	1:C:469:LEU:HA	1.86	0.41
1:C:302:LEU:HD23	1:C:302:LEU:HA	1.88	0.41
1:C:524:ARG:HB3	1:C:525:ALA:H	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:VAL:HB	1:B:561:TYR:CE2	2.54	0.41
1:B:302:LEU:HA	1:B:302:LEU:HD23	1.89	0.41
1:A:168:ASP:HB3	1:A:515:VAL:HB	2.01	0.41
1:B:405:GLU:HA	1:B:408:ARG:NH1	2.35	0.41
1:C:505:TYR:CD2	1:D:548:LYS:HD3	2.56	0.41
1:C:168:ASP:HB3	1:C:515:VAL:HB	2.03	0.41
1:A:119:LYS:HE2	1:A:119:LYS:HB2	1.71	0.41
1:D:320:PHE:HA	1:D:353:ARG:O	2.21	0.41
1:C:531:LYS:HE3	1:D:546:VAL:HG23	2.03	0.41
1:C:548:LYS:HD3	1:D:505:TYR:CD2	2.56	0.41
1:A:147:THR:HG22	1:A:153:LYS:HD2	2.03	0.40
1:A:119:LYS:HA	1:A:120:PRO:HD3	1.96	0.40
1:B:147:THR:HG22	1:B:153:LYS:HD2	2.03	0.40
1:D:288:VAL:HB	1:D:289:PRO:HD3	2.04	0.40
1:A:35:GLU:OE2	1:A:140:ARG:NH2	2.53	0.40
1:A:286:GLY:O	1:A:315:CYS:HA	2.22	0.40
1:A:397:PHE:CZ	1:A:423:ASP:HB3	2.57	0.40
1:C:215:ILE:O	1:C:219:LEU:HG	2.21	0.40
1:A:288:VAL:HB	1:A:289:PRO:HD3	2.02	0.40

There are no symmetry-related clashes.

## 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	539/566 (95%)	524 (97%)	15 (3%)	0	100	100
1	B	539/566 (95%)	525 (97%)	14 (3%)	0	100	100
1	C	538/566 (95%)	525 (98%)	13 (2%)	0	100	100
1	D	538/566 (95%)	523 (97%)	15 (3%)	0	100	100
All	All	2154/2264 (95%)	2097 (97%)	57 (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	408/464 (88%)	394 (97%)	14 (3%)	44	72
1	B	404/464 (87%)	396 (98%)	8 (2%)	63	86
1	C	395/464 (85%)	386 (98%)	9 (2%)	58	83
1	D	389/464 (84%)	378 (97%)	11 (3%)	51	78
All	All	1596/1856 (86%)	1554 (97%)	42 (3%)	54	81

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	51	GLN
1	A	143	ILE
1	A	144	LEU
1	A	302	LEU
1	A	304	ARG
1	A	337	LEU
1	A	353	ARG
1	A	360	LEU
1	A	367	ARG
1	A	441	GLU
1	A	449	PHE
1	A	463	TYR
1	A	467	LEU
1	B	51	GLN
1	B	143	ILE
1	B	144	LEU
1	B	247	ARG
1	B	441	GLU
1	B	449	PHE
1	B	463	TYR
1	B	498	ARG

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Mol	Chain	Res	Type
1	C	26	HIS
1	C	27	THR
1	C	51	GLN
1	C	143	ILE
1	C	144	LEU
1	C	304	ARG
1	C	441	GLU
1	C	449	PHE
1	C	463	TYR
1	D	28	SER
1	D	30	LEU
1	D	51	GLN
1	D	143	ILE
1	D	144	LEU
1	D	302	LEU
1	D	353	ARG
1	D	367	ARG
1	D	441	GLU
1	D	449	PHE
1	D	498	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	86	ASN
1	A	103	ASN
1	A	173	ASN
1	A	218	ASN
1	B	51	GLN
1	B	86	ASN
1	B	103	ASN
1	B	173	ASN
1	B	218	ASN
1	C	51	GLN
1	C	86	ASN
1	C	103	ASN
1	C	173	ASN
1	C	218	ASN
1	D	51	GLN
1	D	86	ASN
1	D	103	ASN

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Mol	Chain	Res	Type
1	D	173	ASN
1	D	218	ASN
1	D	363	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 ⓘ

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	541/566 (95%)	-0.17	4 (0%) 89 90	30, 49, 72, 92	0
1	B	541/566 (95%)	0.04	8 (1%) 76 79	31, 56, 80, 97	0
1	C	540/566 (95%)	0.25	24 (4%) 38 43	43, 68, 89, 113	0
1	D	540/566 (95%)	0.31	28 (5%) 31 35	51, 78, 98, 122	0
All	All	2162/2264 (95%)	0.11	64 (2%) 54 59	30, 63, 91, 122	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	360	LEU	5.0
1	C	412	SER	4.9
1	D	155	VAL	4.7
1	D	368	LEU	4.4
1	D	149	VAL	4.1
1	D	425	VAL	4.0
1	C	413	LEU	4.0
1	D	50	LEU	3.8
1	D	41	THR	3.8
1	D	40	PHE	3.7
1	C	463	TYR	3.6
1	D	412	SER	3.6
1	C	356	VAL	3.6
1	C	456	TYR	3.5
1	D	537	TYR	3.1
1	A	557	TRP	3.1
1	C	322	PHE	3.0
1	C	561	TYR	3.0
1	D	413	LEU	3.0
1	A	561	TYR	3.0
1	C	557	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	333	VAL	2.9
1	D	83	SER	2.9
1	D	485	GLN	2.9
1	D	57	LEU	2.8
1	D	337	LEU	2.8
1	D	59	GLY	2.8
1	C	559	TYR	2.8
1	D	381	ALA	2.7
1	D	85	PHE	2.7
1	A	560	ALA	2.7
1	D	468	GLN	2.7
1	B	41	THR	2.7
1	B	313	GLY	2.7
1	D	357	PRO	2.6
1	C	466	THR	2.6
1	D	364	ILE	2.6
1	C	89	HIS	2.6
1	C	421	CYS	2.6
1	D	540	ARG	2.5
1	D	91	VAL	2.4
1	A	559	TYR	2.4
1	D	536	HIS	2.4
1	B	387	PHE	2.4
1	C	543	SER	2.4
1	C	149	VAL	2.3
1	B	40	PHE	2.3
1	D	466	THR	2.3
1	B	373	SER	2.3
1	D	377	VAL	2.3
1	C	409	SER	2.3
1	C	404	LEU	2.2
1	C	422	ASP	2.1
1	D	39	ALA	2.1
1	C	411	PRO	2.1
1	C	414	THR	2.1
1	B	209	PRO	2.1
1	B	375	ILE	2.1
1	C	110	LEU	2.1
1	C	355	TYR	2.0
1	C	542	THR	2.0
1	C	562	MET	2.0
1	D	443	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	364	ILE	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 carbohydrates 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.