



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:58 PM UTC

PDB ID : 3V9G / pdb_00003v9g
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

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	:	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

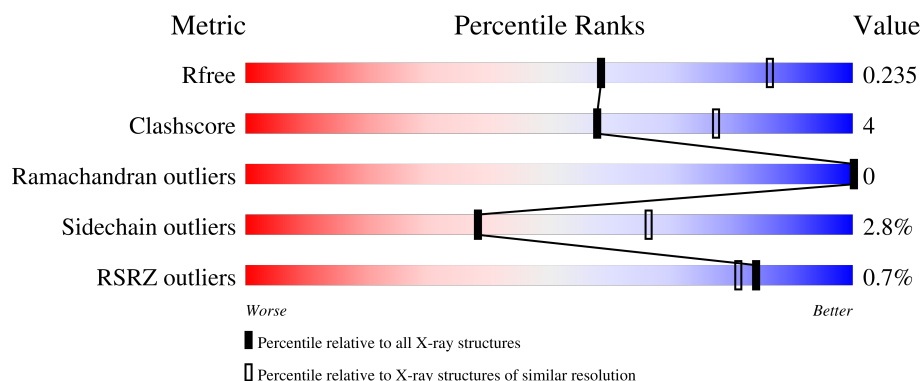
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	566	
1	B	566	
1	C	566	
1	D	566	

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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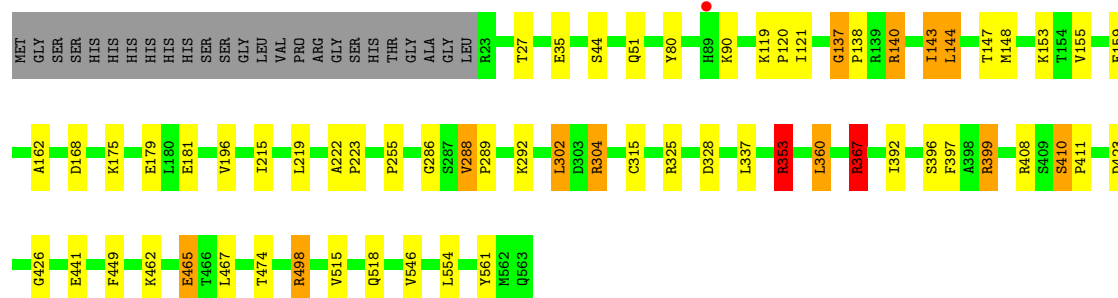
Chain	Residue	Modelled	Actual	Comment	Reference
D	1	SER	-	expression tag	UNP P30038
D	2	HIS	-	expression tag	UNP P30038
D	3	HIS	-	expression tag	UNP P30038
D	4	HIS	-	expression tag	UNP P30038
D	5	HIS	-	expression tag	UNP P30038
D	6	HIS	-	expression tag	UNP P30038
D	7	HIS	-	expression tag	UNP P30038
D	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, 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.

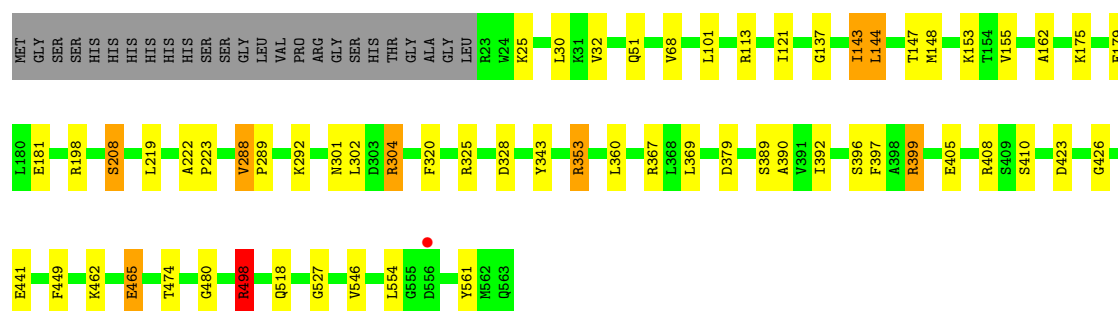
- Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial

Chain A: 



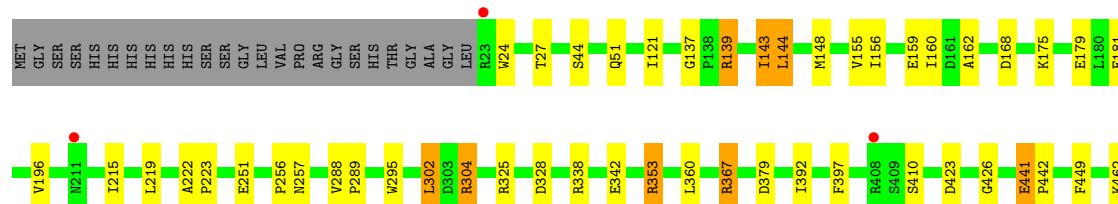
- Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial

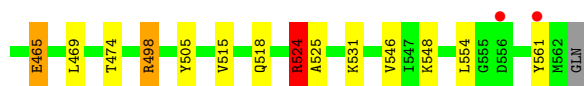
Chain B: 



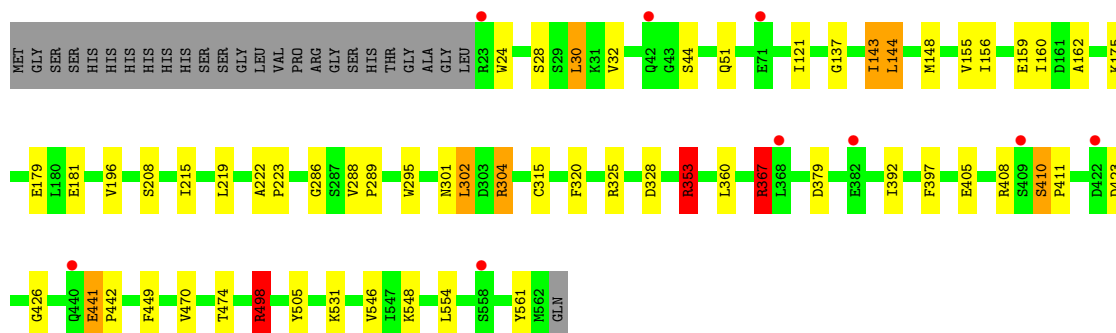
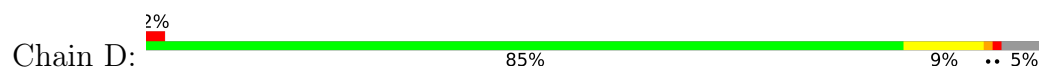
- Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial

Chain C: 





- 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, α , β , γ	150.72Å 150.72Å 191.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.66 – 2.50 38.66 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.66-2.50) 99.6 (38.66-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.7 _650	Depositor
R, R_{free}	0.204 , 0.238 0.200 , 0.235	Depositor DCC
R_{free} test set	2006 reflections (2.36%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16032	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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	0.63	0/4152	1.03	34/5667 (0.6%)
1	B	0.59	0/4140	1.00	30/5652 (0.5%)
1	C	0.54	0/4102	1.01	30/5607 (0.5%)
1	D	0.54	0/4064	0.95	24/5563 (0.4%)
All	All	0.58	0/16458	1.00	118/22489 (0.5%)

There are no bond length outliers.

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	ARG	NE-CZ-NH2	-11.59	108.77	119.20
1	C	139	ARG	NE-CZ-NH2	-10.51	109.74	119.20
1	B	498	ARG	NE-CZ-NH2	10.19	128.37	119.20
1	C	524	ARG	NE-CZ-NH2	10.18	128.36	119.20
1	C	524	ARG	NE-CZ-NH1	-10.15	111.35	121.50
1	A	408	ARG	NE-CZ-NH2	10.04	128.23	119.20
1	C	367	ARG	NE-CZ-NH2	9.95	128.16	119.20
1	D	498	ARG	NE-CZ-NH2	9.94	128.14	119.20
1	B	367	ARG	NE-CZ-NH2	9.67	127.90	119.20
1	A	367	ARG	CD-NE-CZ	9.51	137.72	124.40
1	A	408	ARG	NE-CZ-NH1	-9.51	111.99	121.50
1	C	367	ARG	NE-CZ-NH1	-9.41	112.09	121.50
1	A	140	ARG	NE-CZ-NH1	9.30	130.80	121.50
1	B	367	ARG	NE-CZ-NH1	-9.07	112.42	121.50
1	C	137	GLY	CA-C-N	8.96	129.54	119.32
1	C	137	GLY	C-N-CA	8.96	129.54	119.32
1	D	498	ARG	CD-NE-CZ	8.83	136.76	124.40
1	B	498	ARG	CD-NE-CZ	8.59	136.42	124.40
1	C	498	ARG	CD-NE-CZ	8.38	136.13	124.40
1	C	139	ARG	CD-NE-CZ	8.35	136.08	124.40
1	B	353	ARG	NE-CZ-NH2	8.29	126.66	119.20
1	B	137	GLY	CA-C-N	8.26	128.73	119.32
1	B	137	GLY	C-N-CA	8.26	128.73	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	ARG	NE-CZ-NH2	8.20	126.58	119.20
1	B	367	ARG	CD-NE-CZ	8.17	135.83	124.40
1	C	498	ARG	CG-CD-NE	-8.17	94.03	112.00
1	A	140	ARG	CD-NE-CZ	8.15	135.81	124.40
1	C	367	ARG	CD-NE-CZ	7.97	135.55	124.40
1	C	353	ARG	NE-CZ-NH2	7.86	126.27	119.20
1	D	498	ARG	NE-CZ-NH1	-7.82	113.68	121.50
1	A	304	ARG	NE-CZ-NH2	7.77	126.19	119.20
1	A	399	ARG	NE-CZ-NH1	-7.74	113.76	121.50
1	C	304	ARG	NE-CZ-NH2	7.69	126.12	119.20
1	C	498	ARG	NE-CZ-NH2	-7.66	112.31	119.20
1	D	137	GLY	CA-C-N	7.65	128.04	119.32
1	D	137	GLY	C-N-CA	7.65	128.04	119.32
1	C	304	ARG	NE-CZ-NH1	-7.62	113.89	121.50
1	A	498	ARG	CG-CD-NE	-7.61	95.27	112.00
1	C	139	ARG	NE-CZ-NH1	7.55	129.05	121.50
1	A	304	ARG	NE-CZ-NH1	-7.46	114.03	121.50
1	A	137	GLY	CA-C-N	7.43	127.79	119.32
1	A	137	GLY	C-N-CA	7.43	127.79	119.32
1	A	498	ARG	CD-NE-CZ	7.40	134.77	124.40
1	A	367	ARG	CG-CD-NE	7.37	128.21	112.00
1	B	498	ARG	NE-CZ-NH1	-7.30	114.20	121.50
1	A	408	ARG	CD-NE-CZ	7.29	134.61	124.40
1	C	524	ARG	CD-NE-CZ	7.13	134.39	124.40
1	A	367	ARG	NE-CZ-NH1	7.10	128.60	121.50
1	D	367	ARG	CD-NE-CZ	7.02	134.23	124.40
1	C	353	ARG	NE-CZ-NH1	-7.02	114.48	121.50
1	A	367	ARG	NE-CZ-NH2	-7.00	112.90	119.20
1	C	498	ARG	NE-CZ-NH1	6.78	128.28	121.50
1	A	554	LEU	N-CA-C	6.78	118.46	111.14
1	B	353	ARG	NE-CZ-NH1	-6.64	114.86	121.50
1	B	367	ARG	CG-CD-NE	-6.58	97.53	112.00
1	A	399	ARG	CD-NE-CZ	6.57	133.59	124.40
1	A	410	SER	CA-C-N	6.55	125.99	118.85
1	A	410	SER	C-N-CA	6.55	125.99	118.85
1	C	367	ARG	CG-CD-NE	-6.44	97.82	112.00
1	B	498	ARG	CG-CD-NE	6.39	126.06	112.00
1	B	399	ARG	CD-NE-CZ	6.34	133.28	124.40
1	A	353	ARG	CD-NE-CZ	6.20	133.08	124.40
1	B	304	ARG	NE-CZ-NH2	-6.15	113.67	119.20
1	B	554	LEU	N-CA-C	6.15	117.78	111.14
1	B	410	SER	CA-C-N	6.14	125.54	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	410	SER	C-N-CA	6.14	125.54	118.85
1	A	498	ARG	NE-CZ-NH1	6.08	127.58	121.50
1	B	399	ARG	NE-CZ-NH2	-6.01	113.79	119.20
1	D	410	SER	CA-C-N	5.96	125.35	118.85
1	D	410	SER	C-N-CA	5.96	125.35	118.85
1	D	304	ARG	CD-NE-CZ	5.95	132.73	124.40
1	A	498	ARG	NE-CZ-NH2	-5.94	113.85	119.20
1	B	392	ILE	N-CA-C	5.90	116.64	110.62
1	D	392	ILE	N-CA-C	5.88	116.62	110.62
1	B	379	ASP	CA-C-N	5.87	125.57	119.64
1	B	379	ASP	C-N-CA	5.87	125.57	119.64
1	D	304	ARG	NE-CZ-NH2	-5.87	113.92	119.20
1	B	304	ARG	CD-NE-CZ	5.81	132.53	124.40
1	D	498	ARG	CG-CD-NE	5.80	124.77	112.00
1	D	367	ARG	CG-CD-NE	5.74	124.62	112.00
1	C	392	ILE	N-CA-C	5.72	115.91	110.42
1	D	353	ARG	CD-NE-CZ	5.70	132.38	124.40
1	B	113	ARG	N-CA-C	5.63	117.09	111.07
1	C	410	SER	CA-C-N	5.60	124.96	118.85
1	C	410	SER	C-N-CA	5.60	124.96	118.85
1	A	44	SER	CA-C-N	5.48	125.13	119.05
1	A	44	SER	C-N-CA	5.48	125.13	119.05
1	A	288	VAL	CB-CA-C	-5.46	108.52	113.70
1	C	379	ASP	CA-C-N	5.44	125.13	119.64
1	C	379	ASP	C-N-CA	5.44	125.13	119.64
1	D	379	ASP	CA-C-N	5.41	125.11	119.64
1	D	379	ASP	C-N-CA	5.41	125.11	119.64
1	B	353	ARG	CD-NE-CZ	5.40	131.96	124.40
1	C	44	SER	CA-C-N	5.38	125.02	119.05
1	C	44	SER	C-N-CA	5.38	125.02	119.05
1	C	554	LEU	N-CA-C	5.38	116.95	111.14
1	D	353	ARG	NE-CZ-NH2	-5.35	114.39	119.20
1	D	554	LEU	N-CA-C	5.22	116.77	111.14
1	C	353	ARG	CD-NE-CZ	5.20	131.67	124.40
1	D	367	ARG	NE-CZ-NH2	-5.20	114.52	119.20
1	B	304	ARG	NE-CZ-NH1	5.19	126.69	121.50
1	A	392	ILE	N-CA-C	5.14	115.91	110.72
1	D	367	ARG	NE-CZ-NH1	5.12	126.62	121.50
1	D	353	ARG	NE-CZ-NH1	5.12	126.62	121.50
1	B	208	SER	CA-C-N	5.12	126.23	119.84
1	B	208	SER	C-N-CA	5.12	126.23	119.84
1	A	255	PRO	CA-C-N	5.11	125.04	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	PRO	C-N-CA	5.11	125.04	119.78
1	A	353	ARG	NE-CZ-NH1	5.08	126.58	121.50
1	A	304	ARG	CD-NE-CZ	5.08	131.51	124.40
1	C	304	ARG	CD-NE-CZ	5.08	131.50	124.40
1	A	353	ARG	NE-CZ-NH2	-5.06	114.65	119.20
1	B	399	ARG	NE-CZ-NH1	5.04	126.55	121.50
1	B	527	GLY	N-CA-C	5.01	117.91	110.60
1	D	304	ARG	NE-CZ-NH1	5.00	126.50	121.50
1	B	288	VAL	CB-CA-C	-5.00	108.95	113.70
1	D	44	SER	CA-C-N	5.00	124.60	119.05
1	D	44	SER	C-N-CA	5.00	124.60	119.05

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	4045	0	3842	42	0
1	B	4033	0	3827	38	0
1	C	3995	0	3765	41	0
1	D	3959	0	3706	45	0
All	All	16032	0	15140	139	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 (139) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH11	1:A:367:ARG:HB3	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:A:328:ASP:OD1	1:A:328:ASP:C	2.49	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:328:ASP:OD1	1:C:328:ASP:C	2.51	0.53
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:B:328:ASP:OD1	1:B:328:ASP:C	2.51	0.53
1:D:121:ILE:HG21	1:D:181:GLU:HG3	1.91	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:441:GLU:CD	1:D:442:PRO:HD2	2.35	0.52
1:D:328:ASP:C	1:D:328:ASP:OD1	2.53	0.51
1:A:121:ILE:HG21	1:A:181:GLU:HG3	1.93	0.51
1:C:353:ARG:HH11	1:C:474:THR:HG21	1.75	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:A:196:VAL:CG1	1:B:498:ARG:HH22	2.26	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:A:518:GLN:HA	1:B:546:VAL:HG11	1.96	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:144:LEU:O	1:A:148:MET:HG3	2.14	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:D:397:PHE:CZ	1:D:423:ASP:HB3	2.49	0.47
1:C:121:ILE:HG21	1:C:181:GLU:HG3	1.95	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:C:441:GLU:CD	1:C:442:PRO:HD2	2.39	0.47
1:A:367:ARG:HB3	1:A:367:ARG:NH1	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
1:B:320:PHE:CZ	1:B:480:GLY:HA3	2.52	0.45
1:A:410:SER:HA	1:A:411:PRO:HD3	1.70	0.45
1:C:295:TRP:CG	1:D:302:LEU:HD11	2.52	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:C:302:LEU:HD11	1:D:295:TRP:CG	2.52	0.44
1:D:144:LEU:HD11	1:D:159:GLU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:PHE:CZ	1:B:423:ASP:HB3	2.52	0.44
1:C:498:ARG:NH2	1:D:196:VAL:HG11	2.31	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:B:343:TYR:O	1:B:343:TYR:CG	2.71	0.43
1:C:144:LEU:HD11	1:C:159:GLU:HA	2.01	0.43
1:C:156:ILE:O	1:C:160:ILE:HG23	2.18	0.43
1:D:215:ILE:O	1:D:219:LEU:HG	2.19	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:A:137:GLY:HA3	1:A:138:PRO:HD3	1.89	0.42
1:A:215:ILE:O	1:A:219:LEU:HG	2.19	0.42
1:B:30:LEU:HD23	1:B:175:LYS:HA	2.02	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: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:A:302:LEU:HD13	1:B:292:LYS:HG2	2.01	0.42
1:C:338:ARG:O	1:C:342:GLU:HG3	2.20	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:C:24:TRP:CD1	1:C:24:TRP:H	2.38	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:A:155:VAL:HB	1:B:561:TYR:CE2	2.54	0.41
1:C:524:ARG:HB3	1:C:525:ALA:H	1.73	0.41
1:A:168:ASP:HB3	1:A:515:VAL:HB	2.01	0.41
1:B:302:LEU:HD23	1:B:302:LEU:HA	1.89	0.41
1:B:405:GLU:HA	1:B:408:ARG:NH1	2.35	0.41
1:A:119:LYS:HB2	1:A:119:LYS:HE2	1.71	0.41
1:C:168:ASP:HB3	1:C:515:VAL:HB	2.03	0.41
1:C:505:TYR:CD2	1:D:548:LYS:HD3	2.56	0.41
1:C:531:LYS:HE3	1:D:546:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:548:LYS:HD3	1:D:505:TYR:CD2	2.56	0.41
1:D:320:PHE:HA	1:D:353:ARG:O	2.21	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: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:D:288:VAL:HB	1:D:289:PRO:HD3	2.04	0.40
1:A:288:VAL:HB	1:A:289:PRO:HD3	2.02	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

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	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 [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	408/464 (88%)	394 (97%)	14 (3%)	32	60
1	B	404/464 (87%)	396 (98%)	8 (2%)	48	75
1	C	395/464 (85%)	385 (98%)	10 (2%)	42	69
1	D	389/464 (84%)	377 (97%)	12 (3%)	35	62
All	All	1596/1856 (86%)	1552 (97%)	44 (3%)	38	66

All (44) 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	465	GLU
1	A	467	LEU
1	B	51	GLN
1	B	143	ILE
1	B	144	LEU
1	B	369	LEU
1	B	441	GLU
1	B	449	PHE
1	B	465	GLU
1	B	498	ARG
1	C	27	THR
1	C	51	GLN
1	C	143	ILE
1	C	144	LEU
1	C	302	LEU
1	C	304	ARG
1	C	441	GLU
1	C	449	PHE

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Mol	Chain	Res	Type
1	C	465	GLU
1	C	524	ARG
1	D	28	SER
1	D	30	LEU
1	D	32	VAL
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	86	ASN
1	A	103	ASN
1	A	126	GLN
1	A	173	ASN
1	A	218	ASN
1	A	297	GLN
1	B	51	GLN
1	B	86	ASN
1	B	173	ASN
1	B	218	ASN
1	B	297	GLN
1	C	51	GLN
1	C	86	ASN
1	C	103	ASN
1	C	173	ASN
1	C	218	ASN
1	C	297	GLN
1	C	529	ASN
1	D	51	GLN
1	D	86	ASN
1	D	103	ASN
1	D	126	GLN
1	D	173	ASN

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Mol	Chain	Res	Type
1	D	218	ASN
1	D	297	GLN
1	D	363	GLN
1	D	517	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 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	541/566 (95%)	-0.32	1 (0%) 91 89	30, 49, 72, 92	0
1	B	541/566 (95%)	-0.21	1 (0%) 91 89	31, 56, 80, 97	0
1	C	540/566 (95%)	0.14	5 (0%) 81 78	43, 68, 89, 113	0
1	D	540/566 (95%)	0.28	9 (1%) 69 65	51, 78, 98, 122	0
All	All	2162/2264 (95%)	-0.03	16 (0%) 84 81	30, 63, 91, 122	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	409	SER	3.7
1	C	556	ASP	3.2
1	D	23	ARG	2.8
1	D	440	GLN	2.6
1	A	89	HIS	2.4
1	C	211	ASN	2.4
1	C	408	ARG	2.4
1	D	71	GLU	2.4
1	D	42	GLN	2.3
1	B	556	ASP	2.2
1	D	368	LEU	2.1
1	C	23	ARG	2.1
1	D	382	GLU	2.1
1	C	561	TYR	2.1
1	D	422	ASP	2.1
1	D	558	SER	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.