



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 03:57 AM UTC

PDB ID : 3V9I / pdb_00003v9i
Title : Crystal structure of human 1-pyrroline-5-carboxylate dehydrogenase mutant S352L
Authors : Tanner, J.J.; Singh, R.K.
Deposited on : 2011-12-27
Resolution : 2.85 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	:	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

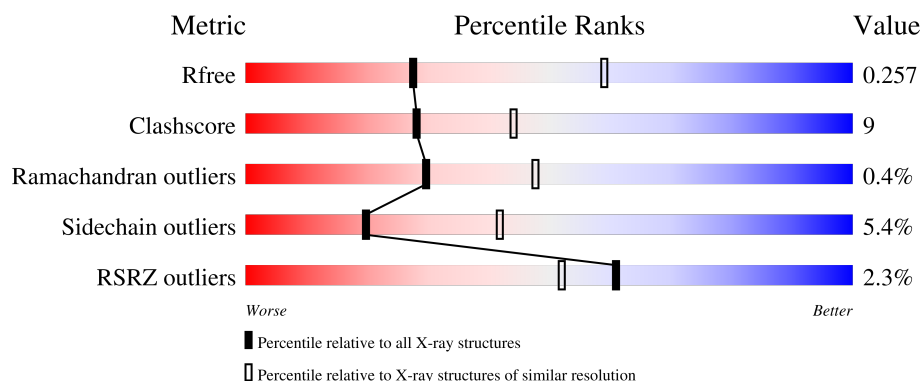
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	5% 68% 18% • 11%
1	B	566	2% 70% 16% • 11%
1	C	566	69% 15% • 13%
1	D	566	5% 72% 12% • 15%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 13924 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	506	Total	C	N	O	S	0	0	0
			3738	2414	627	682	15			
1	B	502	Total	C	N	O	S	0	0	0
			3587	2324	599	650	14			
1	C	492	Total	C	N	O	S	0	0	0
			3496	2253	588	642	13			
1	D	482	Total	C	N	O	S	0	0	0
			3103	1974	547	571	11			

There are 84 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
A	352	LEU	SER	engineered mutation	UNP P30038

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	expression tag	UNP P30038
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
B	352	LEU	SER	engineered mutation	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
C	352	LEU	SER	engineered mutation	UNP P30038

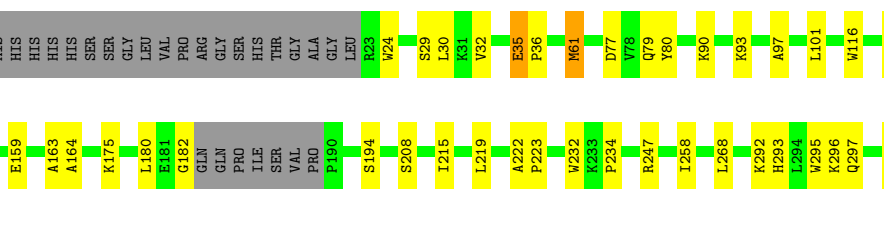
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	MET	-	expression tag	UNP P30038
D	-1	GLY	-	expression tag	UNP P30038
D	0	SER	-	expression tag	UNP P30038
D	1	SER	-	expression tag	UNP P30038
D	2	HIS	-	expression tag	UNP P30038
D	3	HIS	-	expression 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
D	352	LEU	SER	engineered mutation	UNP P30038

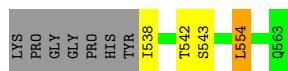
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Chain A: 



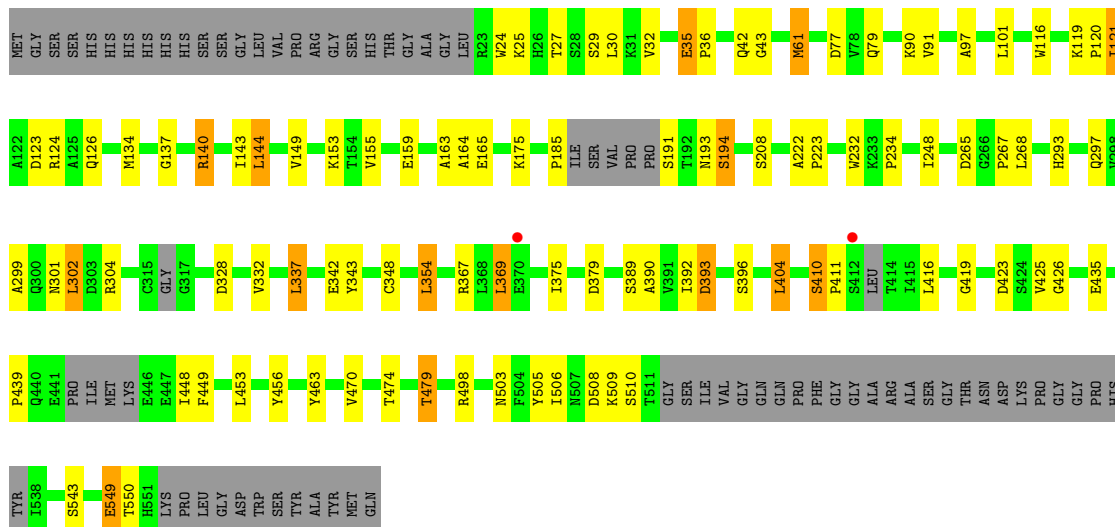
Residue	State	Percentage
GLY	68%	
THR	68%	
ASN	68%	
ASP	68%	
LYS	68%	
PRO	68%	
GLY	68%	
GLY	68%	
PRO	68%	
HIS	68%	
TYR	68%	
LEU	68%	
LEU	68%	
VAL	68%	
PRO	68%	
GLY	68%	
SER	68%	
THR	68%	
GLY	68%	
ALA	68%	
GLY	68%	
LEU	68%	
LEU	68%	
W24	68%	
S29	68%	
L30	68%	
K31	68%	
V32	68%	
E35	68%	
P36	68%	
M61	68%	
D77	68%	
V78	68%	
Q79	68%	
Y80	68%	
K90	68%	
K93	68%	
A97	68%	
L101	68%	
W116	68%	
K119	68%	
P120	68%	
D123	68%	
R124	68%	
C137	68%	
K140	68%	
I143	68%	
L144	68%	
E159	68%	
A163	68%	
A164	68%	
K175	68%	
L180	68%	
E181	68%	
G182	68%	
GLN	68%	
PRO	68%	
I18	68%	
SER	68%	
VAL	68%	
PRO	68%	
P190	68%	
S194	68%	
S208	68%	
I215	68%	
L219	68%	
A222	68%	
P223	68%	
W232	68%	
K233	68%	
P234	68%	
R247	68%	
I258	68%	
L268	68%	
S409	68%	
S410	68%	
P411	68%	
S412	68%	
L413	68%	
L416	68%	
D423	68%	
S424	68%	
V425	68%	
G426	68%	
P431	68%	
C315	68%	
GLY	68%	
C317	68%	
K318	68%	
H319	68%	
E435	68%	
D438	68%	
P439	68%	
Q440	68%	
E441	68%	
M444	68%	
L448	68%	
F449	68%	
G450	68%	
P451	68%	
D461	68%	
K462	68%	
Y463	68%	
K464	68%	
E465	68%	
T466	68%	
L467	68%	
Q468	68%	
L469	68%	
V470	68%	
T473	68%	
T474	68%	
S475	68%	
T479	68%	
V482	68%	
F483	68%	
S484	68%	
R498	68%	
N503	68%	
F504	68%	
Y505	68%	
D508	68%	
K509	68%	
S510	68%	
T511	68%	
GLY	68%	
SER	68%	
ILE	68%	
VAL	68%	
GLY	68%	
GLN	68%	
PRO	68%	
PHE	68%	
GLY	68%	
GLY	68%	
ALA	68%	
ARG	68%	
SER	68%	
GLY	68%	
THR	68%	
ASP	68%	
PRO	68%	
GLY	68%	
LEU	68%	
VAL	68%	
PRO	68%	
GLY	68%	
LEU	68%	
VAL	68%	
PRO	68%	
GLY	68%	
SER	68%	
THR	68%	
GLY	68%	
ALA	68%	
GLY	68%	
LEU	68%	
LEU	68%	
W24	68%	
S29	68%	
L30	68%	
K31	68%	
V32	68%	
E35	68%	
P36	68%	</

- Chain B:
-
- | Token | Count/Value |
|-------|-------------|
| GLU | 1 |
| E447 | 1 |
| I448 | 1 |
| F449 | 1 |
| Y456 | 1 |
| D461 | 1 |
| K462 | 1 |
| Y463 | 1 |
| K464 | 1 |
| E465 | 1 |
| L469 | 1 |
| V470 | 1 |
| T474 | 1 |
| S475 | 1 |
| T479 | 1 |
| V482 | 1 |
| F483 | 1 |
| S484 | 1 |
| Q485 | 1 |
| D486 | 1 |
| K487 | 1 |
| D488 | 1 |
| R498 | 1 |
| G502 | 1 |
| N503 | 1 |
| F504 | 1 |
| Y505 | 1 |
| I506 | 1 |
| N507 | 1 |
| D508 | 1 |
| K509 | 1 |
| S510 | 1 |
| T511 | 1 |
| GLY | 1 |
| SER | 1 |
| ILE | 1 |
| VAL | 1 |
| GLY | 1 |
| GLN | 1 |
| GLN | 1 |
| PRO | 1 |
| PHE | 1 |
| GLY | 1 |
| GLY | 1 |
| ALA | 1 |
| ARG | 1 |
| ALA | 1 |
| SER | 1 |
| GLY | 1 |
| THR | 1 |
| ASN | 1 |
| ASP | 1 |
| H324 | 1 |
| D328 | 1 |
| V329 | 1 |
| V332 | 1 |
| Y343 | 1 |
| S349 | 1 |
| L354 | 1 |
| Y355 | 1 |
| V356 | 1 |
| P357 | 1 |
| L360 | 1 |
| I364 | 1 |
| L369 | 1 |
| E370 | 1 |
| E371 | 1 |
| D379 | 1 |
| S389 | 1 |
| A390 | 1 |
| V391 | 1 |
| I392 | 1 |
| D393 | 1 |
| K401 | 1 |
| L404 | 1 |
| E405 | 1 |
| H406 | 1 |
| A407 | 1 |
| R408 | 1 |
| S409 | 1 |
| S410 | 1 |
| P411 | 1 |
| S412 | 1 |
| L416 | 1 |
| D423 | 1 |
| S424 | 1 |
| V425 | 1 |
| G426 | 1 |
| E435 | 1 |
| P439 | 1 |
| Q440 | 1 |
| E441 | 1 |
| PRO | 1 |
| ILE | 1 |
| ILE | 1 |
| ASP | 1 |
| R140 | 1 |
| T143 | 1 |
| L144 | 1 |
| V149 | 1 |
| K153 | 1 |
| E159 | 1 |
| A163 | 1 |
| A164 | 1 |
| L180 | 1 |
| E181 | 1 |
| G182 | 1 |
| GLN | 1 |
| GLN | 1 |
| PRO | 1 |
| ILE | 1 |
| SER | 1 |
| VAL | 1 |
| PRO | 1 |
| P190 | 1 |
| S194 | 1 |
| S208 | 1 |
| H226 | 1 |
| W232 | 1 |
| K233 | 1 |
| P234 | 1 |
| I258 | 1 |
| T275 | 1 |
| S276 | 1 |
| D277 | 1 |
| W278 | 1 |
| Q279 | 1 |
| V288 | 1 |
| P289 | 1 |
| K292 | 1 |
| H293 | 1 |
| K296 | 1 |
| Q297 | 1 |
| N301 | 1 |
| R304 | 1 |
| C315 | 1 |
| GLY | 1 |
| K317 | 1 |
| THR | 1 |
| ASN | 1 |
| ASP | 1 |
| MET | 1 |
| GLY | 1 |
| SER | 1 |
| HIS | 1 |
| HIS | 1 |
| HIS | 1 |
| HIS | 1 |
| HIS | 1 |
| SER | 1 |
| SER | 1 |
| GLY | 1 |
| LEU | 1 |
| VAL | 1 |
| PRO | 1 |
| ARG | 1 |
| GLY | 1 |
| SER | 1 |
| HIS | 1 |
| THR | 1 |
| ALA | 1 |
| GLY | 1 |
| LEU | 1 |
| R23 | 1 |
| T27 | 1 |
| V32 | 1 |
| E35 | 1 |
| P36 | 1 |
| H61 | 1 |
| T75 | 1 |
| S76 | 1 |
| D77 | 1 |
| W78 | 1 |
| Q79 | 1 |
| K90 | 1 |
| V91 | 1 |
| A92 | 1 |
| K93 | 1 |
| A97 | 1 |
| L101 | 1 |
| W116 | 1 |
| P120 | 1 |
| D123 | 1 |
| R124 | 1 |
| G137 | 1 |



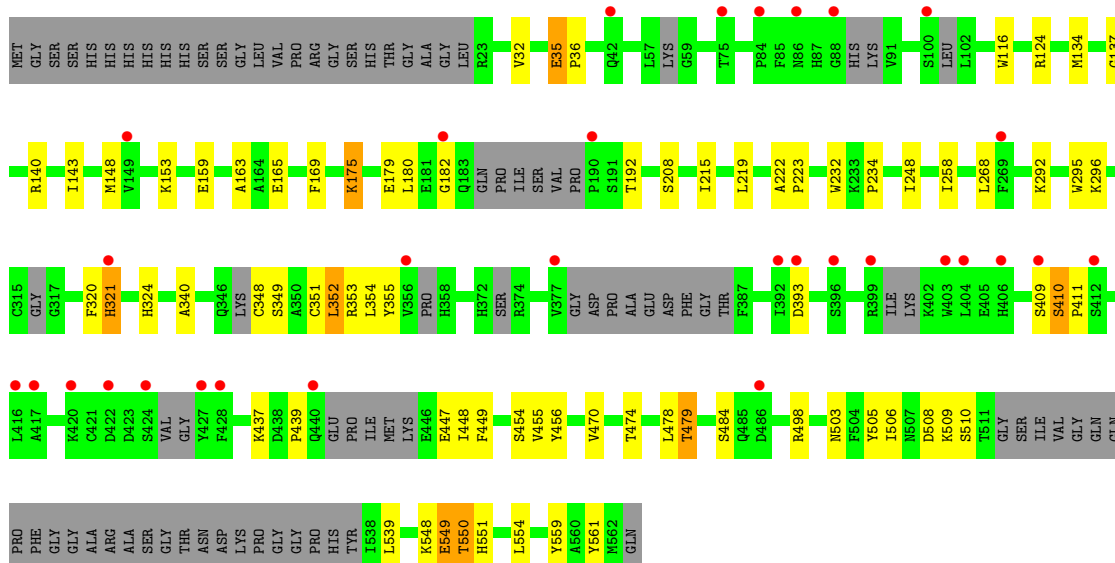
- Molecule 1: Delta-1-pyrroline-5-carboxylate dehydrogenase, mitochondrial

Chain C: 69% 15% 13%



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

Chain D: 5% 72% 12% 15%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	150.38Å 150.38Å 192.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.83 – 2.85 43.83 – 2.85	Depositor EDS
% Data completeness (in resolution range)	97.2 (43.83-2.85) 97.1 (43.83-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.209 , 0.264 0.209 , 0.257	Depositor DCC
R_{free} test set	1338 reflections (2.39%)	wwPDB-VP
Wilson B-factor (Å ²)	61.1	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 73.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13924	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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 [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	0.73	0/3834	1.05	25/5239 (0.5%)
1	B	0.73	1/3677 (0.0%)	1.01	19/5038 (0.4%)
1	C	0.65	0/3579	0.97	16/4898 (0.3%)
1	D	0.58	0/3164	0.98	20/4343 (0.5%)
All	All	0.68	1/14254 (0.0%)	1.00	80/19518 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	371	GLU	CD-OE1	5.23	1.35	1.25

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	543	SER	CA-C-N	11.34	132.08	119.83
1	A	543	SER	C-N-CA	11.34	132.08	119.83
1	B	543	SER	CA-C-N	10.49	130.56	119.76
1	B	543	SER	C-N-CA	10.49	130.56	119.76
1	B	498	ARG	NE-CZ-NH2	8.23	126.61	119.20

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	3738	0	3492	73	0
1	B	3587	0	3236	67	0
1	C	3496	0	3151	63	0
1	D	3103	0	2428	46	0
All	All	13924	0	12307	234	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 9.

The worst 5 of 234 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:C:506:ILE:HB	1:D:549:GLU:HG3	1.52	0.91
1:B:439:PRO:HB3	1:B:469:LEU:HD11	1.58	0.86
1:D:354:LEU:HD22	1:D:455:VAL:HG13	1.59	0.82
1:C:299:ALA:HA	1:C:302:LEU:HD12	1.62	0.82
1:C:470:VAL:O	1:C:474:THR:HG23	1.82	0.79

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	498/566 (88%)	477 (96%)	20 (4%)	1 (0%)	43	62
1	B	492/566 (87%)	462 (94%)	25 (5%)	5 (1%)	12	25
1	C	480/566 (85%)	459 (96%)	20 (4%)	1 (0%)	43	62
1	D	454/566 (80%)	431 (95%)	22 (5%)	1 (0%)	43	62
All	All	1924/2264 (85%)	1829 (95%)	87 (4%)	8 (0%)	30	48

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	406	HIS
1	D	352	LEU
1	B	408	ARG
1	B	405	GLU
1	B	164	ALA

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	357/464 (77%)	336 (94%)	21 (6%)	18	37
1	B	315/464 (68%)	300 (95%)	15 (5%)	23	46
1	C	311/464 (67%)	292 (94%)	19 (6%)	17	35
1	D	201/464 (43%)	192 (96%)	9 (4%)	24	48
All	All	1184/1856 (64%)	1120 (95%)	64 (5%)	20	42

5 of 64 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	175	LYS
1	D	321	HIS
1	B	143	ILE
1	B	61	MET
1	D	454	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	278	HIS
1	C	151	GLN
1	B	278	HIS
1	B	151	GLN
1	B	297	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	506/566 (89%)	-0.21	3 (0%) 85 82	26, 47, 77, 115	0
1	B	502/566 (88%)	-0.16	9 (1%) 67 61	25, 52, 81, 117	0
1	C	492/566 (86%)	-0.16	2 (0%) 88 87	28, 56, 82, 113	0
1	D	482/566 (85%)	0.48	31 (6%) 25 19	24, 67, 104, 136	0
All	All	1982/2264 (87%)	-0.02	45 (2%) 61 52	24, 55, 90, 136	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	149	VAL	3.8
1	D	356	VAL	3.7
1	D	190	PRO	3.6
1	D	100	SER	3.5
1	A	409	SER	3.4

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.