



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:59 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 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

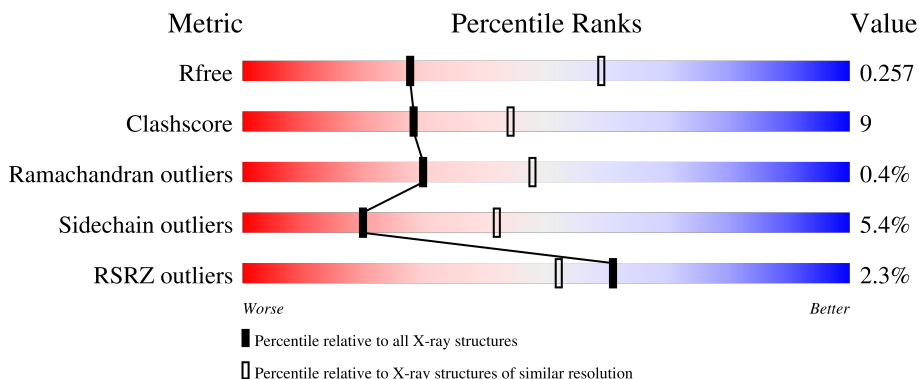
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	0% 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



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

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	0.73	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

All (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
1	D	498	ARG	NE-CZ-NH2	8.22	126.60	119.20
1	B	498	ARG	NE-CZ-NH1	-7.84	113.66	121.50
1	A	410	SER	CA-C-N	7.74	127.40	119.19
1	A	410	SER	C-N-CA	7.74	127.40	119.19
1	A	304	ARG	NE-CZ-NH1	-7.69	113.81	121.50
1	A	140	ARG	NE-CZ-NH2	-7.66	112.30	119.20
1	D	498	ARG	NE-CZ-NH1	-7.59	113.91	121.50
1	C	140	ARG	NE-CZ-NH2	7.58	126.02	119.20
1	A	304	ARG	NE-CZ-NH2	7.05	125.55	119.20
1	C	410	SER	CA-C-N	6.95	126.56	119.19
1	C	410	SER	C-N-CA	6.95	126.56	119.19
1	A	547	ILE	N-CA-C	6.81	116.70	106.42
1	B	35	GLU	CA-C-N	6.76	127.00	119.90
1	B	35	GLU	C-N-CA	6.76	127.00	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	367	ARG	NE-CZ-NH2	6.74	125.27	119.20
1	C	137	GLY	CA-C-N	6.67	126.92	119.32
1	C	137	GLY	C-N-CA	6.67	126.92	119.32
1	C	367	ARG	NE-CZ-NH1	-6.59	114.91	121.50
1	A	319	ASN	N-CA-C	6.46	119.53	109.52
1	A	35	GLU	CA-C-N	6.43	126.66	119.90
1	A	35	GLU	C-N-CA	6.43	126.66	119.90
1	D	410	SER	CA-C-N	6.40	125.97	119.19
1	D	410	SER	C-N-CA	6.40	125.97	119.19
1	B	410	SER	CA-C-N	6.33	125.90	119.19
1	B	410	SER	C-N-CA	6.33	125.90	119.19
1	A	208	SER	CA-C-N	6.27	127.62	120.85
1	A	208	SER	C-N-CA	6.27	127.62	120.85
1	B	140	ARG	NE-CZ-NH2	6.19	124.77	119.20
1	D	554	LEU	N-CA-C	6.16	117.87	111.03
1	C	140	ARG	NE-CZ-NH1	-6.16	115.34	121.50
1	A	140	ARG	CD-NE-CZ	6.11	132.95	124.40
1	D	137	GLY	CA-C-N	6.06	126.23	119.32
1	D	137	GLY	C-N-CA	6.06	126.23	119.32
1	D	498	ARG	CD-NE-CZ	5.97	132.76	124.40
1	A	140	ARG	NE-CZ-NH1	5.94	127.44	121.50
1	A	392	ILE	N-CA-C	5.83	116.56	110.62
1	C	393	ASP	N-CA-C	5.79	116.20	108.38
1	A	498	ARG	NE-CZ-NH2	-5.76	114.01	119.20
1	D	140	ARG	NE-CZ-NH2	-5.73	114.04	119.20
1	B	392	ILE	N-CA-C	5.71	116.45	110.62
1	B	140	ARG	NE-CZ-NH1	-5.69	115.81	121.50
1	B	498	ARG	CD-NE-CZ	5.67	132.34	124.40
1	A	347	LYS	N-CA-C	-5.64	106.25	113.02
1	B	137	GLY	CA-C-N	5.61	126.86	119.84
1	B	137	GLY	C-N-CA	5.61	126.86	119.84
1	B	554	LEU	N-CA-C	5.58	120.36	113.50
1	D	140	ARG	CD-NE-CZ	5.57	132.20	124.40
1	C	208	SER	CA-C-N	5.54	126.77	119.84
1	C	208	SER	C-N-CA	5.54	126.77	119.84
1	C	498	ARG	NE-CZ-NH2	-5.52	114.23	119.20
1	A	393	ASP	N-CA-C	5.49	115.80	108.38
1	B	393	ASP	N-CA-C	5.49	115.79	108.38
1	D	437	LYS	N-CA-C	-5.47	106.61	113.72
1	B	208	SER	CA-C-N	5.45	126.66	119.84
1	B	208	SER	C-N-CA	5.45	126.66	119.84
1	D	140	ARG	NE-CZ-NH1	5.42	126.92	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	35	GLU	CA-C-N	5.40	125.57	119.90
1	D	35	GLU	C-N-CA	5.40	125.57	119.90
1	D	539	LEU	N-CA-C	-5.40	106.53	113.01
1	A	137	GLY	CA-C-N	5.37	125.44	119.32
1	A	137	GLY	C-N-CA	5.37	125.44	119.32
1	A	367	ARG	NE-CZ-NH2	-5.33	114.41	119.20
1	A	367	ARG	CD-NE-CZ	5.31	131.83	124.40
1	D	393	ASP	N-CA-C	5.30	115.53	108.38
1	C	367	ARG	CD-NE-CZ	5.19	131.66	124.40
1	C	35	GLU	CA-C-N	5.13	125.29	119.90
1	C	35	GLU	C-N-CA	5.13	125.29	119.90
1	B	319	ASN	N-CA-C	5.12	116.62	108.79
1	D	447	GLU	N-CA-C	5.10	116.80	108.63
1	D	192	THR	N-CA-C	5.08	116.69	108.41
1	C	140	ARG	CD-NE-CZ	5.07	131.50	124.40
1	A	438	ASP	CA-C-N	5.05	124.65	119.05
1	A	438	ASP	C-N-CA	5.05	124.65	119.05
1	D	208	SER	CA-C-N	5.03	126.13	119.84
1	D	208	SER	C-N-CA	5.03	126.13	119.84

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	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.

All (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
1:A:470:VAL:O	1:A:474:THR:HG23	1.83	0.79
1:C:42:GLN:CB	1:C:43:GLY:HA3	2.12	0.79
1:A:439:PRO:HB3	1:A:469:LEU:HD11	1.66	0.78
1:D:470:VAL:O	1:D:474:THR:HG23	1.84	0.77
1:B:301:ASN:HB3	1:B:304:ARG:CD	2.15	0.76
1:B:470:VAL:O	1:B:474:THR:HG23	1.84	0.76
1:A:318:LYS:HE2	1:A:475:SER:H	1.54	0.72
1:D:352:LEU:HG	1:D:352:LEU:O	1.90	0.70
1:A:413:LEU:HD22	1:A:434:VAL:CG1	2.21	0.70
1:A:29:SER:O	1:C:25:LYS:N	2.22	0.68
1:B:301:ASN:HB3	1:B:304:ARG:HD3	1.75	0.67
1:B:301:ASN:HB3	1:B:304:ARG:HD2	1.77	0.66
1:C:506:ILE:HB	1:D:549:GLU:CG	2.25	0.66
1:B:416:LEU:HD11	1:B:435:GLU:HB2	1.79	0.65
1:C:416:LEU:HD11	1:C:435:GLU:HB2	1.79	0.64
1:D:351:CYS:O	1:D:353:ARG:N	2.31	0.64
1:B:329:VAL:CG2	1:B:360:LEU:HD23	2.28	0.64
1:C:423:ASP:HA	1:C:426:GLY:O	1.98	0.64
1:C:42:GLN:CB	1:C:43:GLY:CA	2.75	0.64
1:B:423:ASP:HA	1:B:426:GLY:O	1.98	0.64
1:D:354:LEU:C	1:D:354:LEU:HD23	2.24	0.63
1:C:404:LEU:O	1:C:404:LEU:HD23	1.99	0.63
1:A:549:GLU:HB2	1:B:506:ILE:HB	1.81	0.62
1:C:506:ILE:CB	1:D:549:GLU:HG3	2.30	0.61
1:A:423:ASP:HA	1:A:426:GLY:O	1.99	0.61
1:B:405:GLU:C	1:B:407:ALA:H	2.07	0.60
1:C:155:VAL:HB	1:D:561:TYR:CE2	2.37	0.60
1:A:351:CYS:HB3	1:A:448:ILE:HD13	1.84	0.59
1:C:479:THR:HG22	1:C:503:ASN:HB2	1.83	0.59
1:A:301:ASN:O	1:A:304:ARG:HG2	2.02	0.59
1:B:354:LEU:HG	1:B:356:VAL:HG23	1.84	0.59
1:A:416:LEU:HD11	1:A:435:GLU:HB2	1.85	0.59
1:A:482:VAL:HG23	1:A:504:PHE:CZ	2.37	0.59
1:A:140:ARG:HG2	1:A:144:LEU:HD22	1.85	0.58
1:D:175:LYS:HZ2	1:D:179:GLU:CD	2.11	0.58
1:D:340:ALA:HB2	1:D:352:LEU:HD23	1.86	0.58
1:D:479:THR:HG22	1:D:503:ASN:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:TYR:CD2	1:A:90:LYS:HD3	2.38	0.58
1:B:407:ALA:C	1:B:409:SER:H	2.12	0.57
1:A:412:SER:HB2	1:A:441:GLU:OE2	2.05	0.57
1:A:413:LEU:HD22	1:A:434:VAL:HG11	1.86	0.57
1:B:482:VAL:HG23	1:B:504:PHE:CZ	2.40	0.56
1:B:405:GLU:O	1:B:407:ALA:N	2.38	0.56
1:B:479:THR:HG22	1:B:503:ASN:HB2	1.88	0.56
1:D:549:GLU:OE1	1:D:551:HIS:CE1	2.58	0.56
1:B:61:MET:HB2	1:B:90:LYS:O	2.06	0.56
1:A:479:THR:HG22	1:A:503:ASN:HB2	1.88	0.56
1:A:354:LEU:HG	1:A:356:VAL:HG23	1.89	0.55
1:B:292:LYS:O	1:B:296:LYS:HG3	2.07	0.55
1:A:30:LEU:HD13	1:C:24:TRP:CD2	2.42	0.55
1:D:321:HIS:CD2	1:D:352:LEU:HD11	2.41	0.55
1:D:354:LEU:HD23	1:D:355:TYR:N	2.22	0.55
1:C:448:ILE:O	1:C:449:PHE:HB2	2.07	0.54
1:D:165:GLU:O	1:D:169:PHE:CD2	2.61	0.54
1:A:293:HIS:O	1:A:297:GLN:HG3	2.08	0.54
1:A:448:ILE:O	1:A:449:PHE:HB2	2.07	0.54
1:B:61:MET:HE3	1:B:93:LYS:HB2	1.89	0.54
1:C:29:SER:OG	1:C:30:LEU:N	2.40	0.54
1:A:409:SER:OG	1:A:410:SER:N	2.40	0.54
1:B:226:MET:HE3	1:B:542:THR:HB	1.89	0.54
1:A:549:GLU:O	1:A:549:GLU:HG3	2.06	0.53
1:A:539:LEU:O	1:A:542:THR:HG22	2.08	0.53
1:C:337:LEU:HD22	1:C:375:ILE:HD11	1.90	0.53
1:C:77:ASP:OD1	1:C:79:GLN:NE2	2.42	0.53
1:D:448:ILE:O	1:D:449:PHE:HB2	2.08	0.53
1:A:413:LEU:HD22	1:A:434:VAL:HG12	1.89	0.52
1:B:349:SER:HA	1:B:449:PHE:CZ	2.44	0.52
1:A:292:LYS:O	1:A:296:LYS:HG3	2.09	0.52
1:A:336:THR:HG21	1:A:354:LEU:HD22	1.90	0.52
1:C:404:LEU:HD21	1:C:419:GLY:O	2.10	0.52
1:B:77:ASP:OD1	1:B:79:GLN:NE2	2.41	0.52
1:D:159:GLU:O	1:D:163:ALA:HB3	2.10	0.52
1:D:349:SER:HB3	1:D:449:PHE:CE2	2.45	0.51
1:A:330:GLU:OE2	1:A:367:ARG:HD3	2.10	0.51
1:C:116:TRP:CZ2	1:C:124:ARG:HD2	2.46	0.51
1:C:140:ARG:HG2	1:C:144:LEU:HD22	1.92	0.51
1:B:97:ALA:CB	1:B:101:LEU:HD23	2.41	0.51
1:D:232:TRP:O	1:D:234:PRO:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:LEU:HD12	1:A:353:ARG:N	2.26	0.50
1:A:509:LYS:HD2	1:A:511:THR:OG1	2.11	0.50
1:A:116:TRP:CZ2	1:A:124:ARG:HD2	2.47	0.50
1:B:486:ASP:OD1	1:B:486:ASP:C	2.55	0.50
1:D:175:LYS:O	1:D:179:GLU:HG3	2.10	0.50
1:A:508:ASP:HA	1:B:554:LEU:HD11	1.92	0.50
1:A:61:MET:HE3	1:A:93:LYS:HB2	1.93	0.50
1:B:120:PRO:O	1:B:123:ASP:HB2	2.12	0.50
1:B:448:ILE:O	1:B:449:PHE:HB2	2.11	0.49
1:A:508:ASP:OD1	1:A:509:LYS:N	2.45	0.49
1:C:35:GLU:CD	1:C:36:PRO:HD2	2.37	0.49
1:D:508:ASP:OD1	1:D:509:LYS:N	2.45	0.49
1:C:293:HIS:O	1:C:297:GLN:HG3	2.13	0.49
1:B:357:PRO:HG2	1:B:360:LEU:HB2	1.95	0.49
1:A:61:MET:HB2	1:A:90:LYS:O	2.13	0.48
1:C:549:GLU:HG3	1:C:550:THR:N	2.27	0.48
1:A:337:LEU:HD22	1:A:375:ILE:HD11	1.95	0.48
1:D:116:TRP:CZ2	1:D:124:ARG:HD2	2.49	0.48
1:B:116:TRP:CZ2	1:B:124:ARG:HD2	2.49	0.48
1:C:302:LEU:HD11	1:D:295:TRP:CD1	2.49	0.48
1:C:121:ILE:HD12	1:C:124:ARG:HH21	1.79	0.48
1:A:97:ALA:CB	1:A:101:LEU:HD23	2.44	0.48
1:A:413:LEU:HD11	1:A:444:MET:HE1	1.96	0.48
1:B:509:LYS:HD2	1:B:511:THR:OG1	2.14	0.47
1:D:439:PRO:HG3	1:D:456:TYR:CZ	2.49	0.47
1:A:324:HIS:HB3	1:A:484:SER:HB2	1.96	0.47
1:B:293:HIS:O	1:B:297:GLN:HG3	2.14	0.47
1:B:479:THR:HB	1:B:510:SER:HB2	1.96	0.47
1:A:24:TRP:HZ2	1:C:126:GLN:OE1	1.98	0.47
1:A:361:TRP:CZ2	1:A:365:LYS:HD2	2.48	0.47
1:A:505:TYR:CD1	1:A:510:SER:HA	2.50	0.47
1:A:352:LEU:HD12	1:A:353:ARG:H	1.78	0.47
1:A:367:ARG:NH2	1:A:371:GLU:OE2	2.30	0.47
1:B:401:LYS:O	1:B:404:LEU:HB2	2.15	0.47
1:B:405:GLU:C	1:B:407:ALA:N	2.72	0.47
1:B:439:PRO:HG3	1:B:456:TYR:CZ	2.49	0.47
1:C:301:ASN:O	1:C:304:ARG:HG2	2.14	0.47
1:D:222:ALA:HB3	1:D:223:PRO:HD3	1.96	0.47
1:D:215:ILE:O	1:D:219:LEU:HG	2.14	0.47
1:C:508:ASP:OD1	1:C:509:LYS:N	2.47	0.47
1:B:329:VAL:CG2	1:B:360:LEU:CD2	2.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:MET:HE2	1:C:248:ILE:HG23	1.96	0.46
1:D:320:PHE:HA	1:D:353:ARG:O	2.16	0.46
1:B:407:ALA:C	1:B:409:SER:N	2.73	0.46
1:A:438:ASP:HB3	1:A:441:GLU:HG2	1.97	0.46
1:A:465:GLU:OE2	1:A:465:GLU:N	2.47	0.46
1:B:324:HIS:HB3	1:B:484:SER:HB2	1.97	0.46
1:A:163:ALA:O	1:A:164:ALA:C	2.58	0.46
1:B:486:ASP:OD1	1:B:488:ASP:N	2.49	0.45
1:C:91:VAL:HG11	1:C:149:VAL:HG12	1.97	0.45
1:C:549:GLU:HB2	1:D:506:ILE:HB	1.97	0.45
1:B:116:TRP:CG	1:B:258:ILE:HD12	2.51	0.45
1:D:35:GLU:CD	1:D:36:PRO:HD2	2.41	0.45
1:A:35:GLU:CD	1:A:36:PRO:HD2	2.41	0.45
1:B:479:THR:CG2	1:B:503:ASN:HB2	2.46	0.45
1:C:232:TRP:O	1:C:234:PRO:HD3	2.16	0.45
1:C:508:ASP:HB2	1:D:550:THR:OG1	2.16	0.45
1:A:393:ASP:OD1	1:A:396:SER:CB	2.64	0.45
1:B:91:VAL:HG11	1:B:149:VAL:HG12	1.98	0.45
1:C:159:GLU:O	1:C:163:ALA:HB3	2.17	0.45
1:D:134:MET:HE2	1:D:248:ILE:HG23	1.99	0.45
1:A:159:GLU:O	1:A:163:ALA:HB3	2.17	0.45
1:B:35:GLU:CD	1:B:36:PRO:HD2	2.42	0.45
1:B:407:ALA:O	1:B:409:SER:N	2.50	0.45
1:D:505:TYR:CD1	1:D:510:SER:HA	2.51	0.45
1:C:222:ALA:HB3	1:C:223:PRO:HD3	1.99	0.45
1:A:215:ILE:O	1:A:219:LEU:HG	2.17	0.44
1:A:482:VAL:CG2	1:A:504:PHE:HZ	2.29	0.44
1:B:140:ARG:HG2	1:B:144:LEU:HD22	1.98	0.44
1:C:61:MET:HB2	1:C:90:LYS:O	2.17	0.44
1:A:232:TRP:O	1:A:234:PRO:HD3	2.17	0.44
1:A:392:ILE:HG23	1:A:393:ASP:N	2.30	0.44
1:B:379:ASP:OD1	1:B:379:ASP:C	2.60	0.44
1:B:505:TYR:CD1	1:B:510:SER:HA	2.51	0.44
1:A:295:TRP:CD1	1:A:295:TRP:C	2.95	0.44
1:C:342:GLU:OE2	1:D:559:TYR:HE2	2.01	0.44
1:C:439:PRO:HG3	1:C:456:TYR:CZ	2.53	0.44
1:B:329:VAL:HG22	1:B:360:LEU:HD23	1.96	0.44
1:B:328:ASP:O	1:B:332:VAL:HG23	2.18	0.44
1:B:389:SER:OG	1:B:390:ALA:N	2.51	0.44
1:A:410:SER:HA	1:A:411:PRO:HD3	1.68	0.44
1:B:349:SER:HA	1:B:449:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:LEU:HD12	1:C:369:LEU:HA	1.74	0.44
1:C:389:SER:OG	1:C:390:ALA:N	2.50	0.44
1:B:180:LEU:C	1:B:182:GLY:H	2.26	0.43
1:B:508:ASP:OD1	1:B:509:LYS:N	2.50	0.43
1:C:392:ILE:HG23	1:C:393:ASP:N	2.33	0.43
1:D:324:HIS:HB3	1:D:484:SER:HB2	2.00	0.43
1:A:324:HIS:HD1	1:A:326:SER:H	1.66	0.43
1:A:482:VAL:CG2	1:A:504:PHE:CZ	3.01	0.43
1:B:287:SER:HB2	1:B:289:PRO:HD2	2.01	0.43
1:C:479:THR:CG2	1:C:503:ASN:HB2	2.48	0.43
1:A:180:LEU:C	1:A:182:GLY:H	2.26	0.43
1:A:222:ALA:HB3	1:A:223:PRO:HD3	2.01	0.43
1:C:302:LEU:HD11	1:D:295:TRP:CE2	2.54	0.43
1:D:348:CYS:HB3	1:D:478:LEU:HD23	2.00	0.43
1:D:410:SER:HA	1:D:411:PRO:HD3	1.72	0.43
1:B:97:ALA:HB1	1:B:101:LEU:HD23	2.01	0.43
1:B:410:SER:HA	1:B:411:PRO:HD3	1.71	0.43
1:A:120:PRO:O	1:A:123:ASP:HB2	2.18	0.43
1:B:153:LYS:HG2	1:B:343:TYR:CE1	2.54	0.43
1:B:465:GLU:CD	1:B:465:GLU:H	2.20	0.43
1:A:318:LYS:CE	1:A:475:SER:H	2.28	0.42
1:D:116:TRP:CG	1:D:258:ILE:HD12	2.55	0.42
1:A:413:LEU:HA	1:A:413:LEU:HD23	1.84	0.42
1:D:292:LYS:O	1:D:296:LYS:HG3	2.18	0.42
1:D:479:THR:HB	1:D:510:SER:HB2	2.02	0.42
1:B:409:SER:O	1:B:410:SER:C	2.63	0.42
1:C:144:LEU:HD12	1:C:144:LEU:HA	1.87	0.42
1:C:348:CYS:O	1:C:449:PHE:CD1	2.73	0.42
1:C:505:TYR:HA	1:D:548:LYS:O	2.20	0.42
1:B:159:GLU:O	1:B:163:ALA:HB3	2.18	0.42
1:C:119:LYS:HA	1:C:120:PRO:HD3	1.94	0.42
1:A:378:GLY:H	1:A:386:THR:HG23	1.83	0.42
1:B:392:ILE:HG23	1:B:393:ASP:N	2.35	0.41
1:B:482:VAL:CG2	1:B:504:PHE:HZ	2.33	0.41
1:B:482:VAL:CG2	1:B:504:PHE:CZ	3.02	0.41
1:C:97:ALA:CB	1:C:101:LEU:HD23	2.51	0.41
1:C:185:PRO:HD2	1:C:194:SER:HA	2.01	0.41
1:A:80:TYR:CE2	1:A:93:LYS:HG3	2.55	0.41
1:A:119:LYS:HA	1:A:120:PRO:HD3	1.97	0.41
1:B:461:ASP:OD2	1:B:462:LYS:HG3	2.20	0.41
1:C:153:LYS:HG2	1:C:343:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:TRP:O	1:B:234:PRO:HD3	2.21	0.41
1:C:505:TYR:CD1	1:C:510:SER:HA	2.55	0.41
1:D:295:TRP:CD1	1:D:295:TRP:C	2.99	0.41
1:B:462:LYS:O	1:B:465:GLU:HG2	2.20	0.41
1:C:265:ASP:CG	1:C:267:PRO:HD2	2.46	0.41
1:C:328:ASP:O	1:C:332:VAL:HG23	2.21	0.41
1:C:185:PRO:HG2	1:C:193:ASN:C	2.45	0.41
1:A:479:THR:HB	1:A:510:SER:HB2	2.02	0.41
1:B:163:ALA:O	1:B:164:ALA:C	2.64	0.41
1:B:288:VAL:HB	1:B:289:PRO:HD3	2.03	0.41
1:C:120:PRO:O	1:C:123:ASP:HB2	2.21	0.41
1:C:410:SER:HA	1:C:411:PRO:HD3	1.70	0.41
1:A:116:TRP:CG	1:A:258:ILE:HD12	2.55	0.41
1:C:354:LEU:HB2	1:C:453:LEU:HD11	2.02	0.41
1:C:163:ALA:O	1:C:164:ALA:C	2.64	0.40
1:D:148:MET:HG2	1:D:153:LYS:O	2.21	0.40
1:C:191:SER:HA	1:C:549:GLU:O	2.21	0.40
1:C:379:ASP:OD1	1:C:379:ASP:C	2.64	0.40
1:D:409:SER:O	1:D:410:SER:C	2.63	0.40
1:A:61:MET:O	1:A:61:MET:CG	2.68	0.40
1:A:77:ASP:OD1	1:A:79:GLN:NE2	2.54	0.40
1:A:465:GLU:CD	1:A:465:GLU:H	2.23	0.40
1:C:337:LEU:CD2	1:C:375:ILE:HD11	2.51	0.40
1:C:393:ASP:OD1	1:C:396:SER:CB	2.70	0.40
1:A:361:TRP:HB3	1:A:362:PRO:HD3	2.04	0.40
1:A:375:ILE:HG21	1:A:375:ILE:HD13	1.81	0.40
1:A:431:PRO:HA	1:A:451:PRO:HB2	2.04	0.40
1:D:180:LEU:C	1:D:182:GLY:H	2.29	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	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

All (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
1	B	181	GLU
1	C	404	LEU
1	A	540	ARG

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

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	61	MET
1	A	143	ILE

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Mol	Chain	Res	Type
1	A	144	LEU
1	A	175	LYS
1	A	194	SER
1	A	247	ARG
1	A	268	LEU
1	A	337	LEU
1	A	360	LEU
1	A	369	LEU
1	A	425	VAL
1	A	440	GLN
1	A	463	TYR
1	A	465	GLU
1	A	467	LEU
1	A	469	LEU
1	A	473	THR
1	A	479	THR
1	A	549	GLU
1	A	550	THR
1	B	27	THR
1	B	32	VAL
1	B	61	MET
1	B	143	ILE
1	B	144	LEU
1	B	194	SER
1	B	268	LEU
1	B	360	LEU
1	B	369	LEU
1	B	425	VAL
1	B	463	TYR
1	B	465	GLU
1	B	469	LEU
1	B	479	THR
1	B	538	ILE
1	C	27	THR
1	C	32	VAL
1	C	61	MET
1	C	121	ILE
1	C	143	ILE
1	C	144	LEU
1	C	165	GLU
1	C	175	LYS
1	C	194	SER

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Mol	Chain	Res	Type
1	C	268	LEU
1	C	302	LEU
1	C	337	LEU
1	C	354	LEU
1	C	369	LEU
1	C	425	VAL
1	C	463	TYR
1	C	479	THR
1	C	543	SER
1	C	549	GLU
1	D	32	VAL
1	D	143	ILE
1	D	175	LYS
1	D	268	LEU
1	D	321	HIS
1	D	454	SER
1	D	479	THR
1	D	549	GLU
1	D	550	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	278	HIS
1	A	297	GLN
1	B	151	GLN
1	B	278	HIS
1	B	297	GLN
1	C	151	GLN
1	C	278	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

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, 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

All (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
1	D	42	GLN	3.4
1	C	412	SER	3.3
1	D	427	TYR	3.0
1	D	424	SER	3.0
1	B	75	THR	2.9
1	D	399	ARG	2.9
1	D	440	GLN	2.9
1	D	422	ASP	2.9
1	D	88	GLY	2.8
1	D	417	ALA	2.8
1	B	190	PRO	2.8
1	D	412	SER	2.7
1	D	377	VAL	2.7
1	D	486	ASP	2.7
1	D	86	ASN	2.6
1	D	84	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	502	GLY	2.5
1	D	404	LEU	2.5
1	B	409	SER	2.5
1	B	475	SER	2.5
1	D	393	ASP	2.4
1	A	560	ALA	2.4
1	D	403	TRP	2.3
1	D	75	THR	2.3
1	D	182	GLY	2.3
1	D	416	LEU	2.3
1	A	461	ASP	2.2
1	D	406	HIS	2.2
1	D	428	PHE	2.2
1	D	420	LYS	2.2
1	D	409	SER	2.2
1	D	269	PHE	2.1
1	D	396	SER	2.1
1	D	392	ILE	2.1
1	B	411	PRO	2.1
1	B	488	ASP	2.1
1	B	364	ILE	2.1
1	C	370	GLU	2.0
1	B	412	SER	2.0
1	D	321	HIS	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.