



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:21 AM UTC

PDB ID : 5WVA / pdb_00005wva
Title : Serratia marcescens short-chain dehydrogenase/reductase F98Y/F202Y mutant
Authors : Liu, J.S.; Tsou, Y.; Wang, W.C.
Deposited on : 2016-12-23
Resolution : 1.47 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

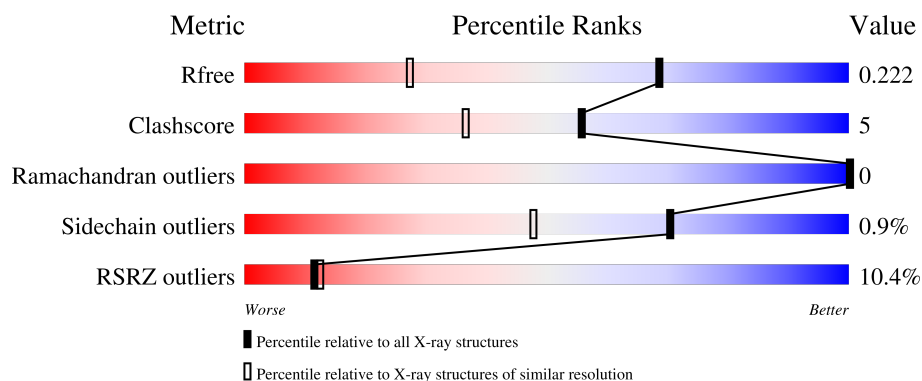
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.47 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	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	287	10% 71% 13% • 15%
1	B	287	7% 63% 10% • 24%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3666 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 Short-chain dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1760	1094	316	344	6			
1	B	218	Total	C	N	O	S	0	0	0
			1561	977	282	297	5			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-37	MET	-	expression tag	UNP A0A192ICX3
A	-36	HIS	-	expression tag	UNP A0A192ICX3
A	-35	HIS	-	expression tag	UNP A0A192ICX3
A	-34	HIS	-	expression tag	UNP A0A192ICX3
A	-33	HIS	-	expression tag	UNP A0A192ICX3
A	-32	HIS	-	expression tag	UNP A0A192ICX3
A	-31	HIS	-	expression tag	UNP A0A192ICX3
A	-30	SER	-	expression tag	UNP A0A192ICX3
A	-29	SER	-	expression tag	UNP A0A192ICX3
A	-28	GLY	-	expression tag	UNP A0A192ICX3
A	-27	LEU	-	expression tag	UNP A0A192ICX3
A	-26	VAL	-	expression tag	UNP A0A192ICX3
A	-25	PRO	-	expression tag	UNP A0A192ICX3
A	-24	ARG	-	expression tag	UNP A0A192ICX3
A	-23	GLY	-	expression tag	UNP A0A192ICX3
A	-22	SER	-	expression tag	UNP A0A192ICX3
A	-21	GLY	-	expression tag	UNP A0A192ICX3
A	-20	MET	-	expression tag	UNP A0A192ICX3
A	-19	LYS	-	expression tag	UNP A0A192ICX3
A	-18	GLU	-	expression tag	UNP A0A192ICX3
A	-17	THR	-	expression tag	UNP A0A192ICX3
A	-16	ALA	-	expression tag	UNP A0A192ICX3
A	-15	ALA	-	expression tag	UNP A0A192ICX3
A	-14	ALA	-	expression tag	UNP A0A192ICX3
A	-13	LYS	-	expression tag	UNP A0A192ICX3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	PHE	-	expression tag	UNP A0A192ICX3
A	-11	GLU	-	expression tag	UNP A0A192ICX3
A	-10	ARG	-	expression tag	UNP A0A192ICX3
A	-9	GLN	-	expression tag	UNP A0A192ICX3
A	-8	HIS	-	expression tag	UNP A0A192ICX3
A	-7	MET	-	expression tag	UNP A0A192ICX3
A	-6	ASP	-	expression tag	UNP A0A192ICX3
A	-5	SER	-	expression tag	UNP A0A192ICX3
A	-4	PRO	-	expression tag	UNP A0A192ICX3
A	-3	ASP	-	expression tag	UNP A0A192ICX3
A	-2	LEU	-	expression tag	UNP A0A192ICX3
A	-1	GLY	-	expression tag	UNP A0A192ICX3
A	0	THR	-	expression tag	UNP A0A192ICX3
A	98	TYR	PHE	engineered mutation	UNP A0A192ICX3
A	202	TYR	PHE	engineered mutation	UNP A0A192ICX3
B	-37	MET	-	expression tag	UNP A0A192ICX3
B	-36	HIS	-	expression tag	UNP A0A192ICX3
B	-35	HIS	-	expression tag	UNP A0A192ICX3
B	-34	HIS	-	expression tag	UNP A0A192ICX3
B	-33	HIS	-	expression tag	UNP A0A192ICX3
B	-32	HIS	-	expression tag	UNP A0A192ICX3
B	-31	HIS	-	expression tag	UNP A0A192ICX3
B	-30	SER	-	expression tag	UNP A0A192ICX3
B	-29	SER	-	expression tag	UNP A0A192ICX3
B	-28	GLY	-	expression tag	UNP A0A192ICX3
B	-27	LEU	-	expression tag	UNP A0A192ICX3
B	-26	VAL	-	expression tag	UNP A0A192ICX3
B	-25	PRO	-	expression tag	UNP A0A192ICX3
B	-24	ARG	-	expression tag	UNP A0A192ICX3
B	-23	GLY	-	expression tag	UNP A0A192ICX3
B	-22	SER	-	expression tag	UNP A0A192ICX3
B	-21	GLY	-	expression tag	UNP A0A192ICX3
B	-20	MET	-	expression tag	UNP A0A192ICX3
B	-19	LYS	-	expression tag	UNP A0A192ICX3
B	-18	GLU	-	expression tag	UNP A0A192ICX3
B	-17	THR	-	expression tag	UNP A0A192ICX3
B	-16	ALA	-	expression tag	UNP A0A192ICX3
B	-15	ALA	-	expression tag	UNP A0A192ICX3
B	-14	ALA	-	expression tag	UNP A0A192ICX3
B	-13	LYS	-	expression tag	UNP A0A192ICX3
B	-12	PHE	-	expression tag	UNP A0A192ICX3
B	-11	GLU	-	expression tag	UNP A0A192ICX3

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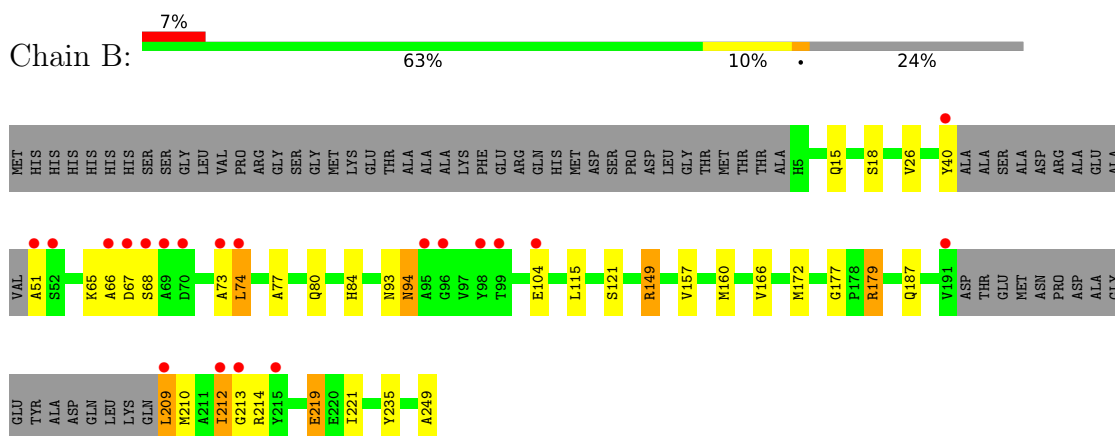
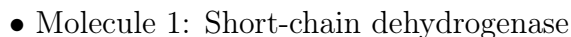
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	ARG	-	expression tag	UNP A0A192ICX3
B	-9	GLN	-	expression tag	UNP A0A192ICX3
B	-8	HIS	-	expression tag	UNP A0A192ICX3
B	-7	MET	-	expression tag	UNP A0A192ICX3
B	-6	ASP	-	expression tag	UNP A0A192ICX3
B	-5	SER	-	expression tag	UNP A0A192ICX3
B	-4	PRO	-	expression tag	UNP A0A192ICX3
B	-3	ASP	-	expression tag	UNP A0A192ICX3
B	-2	LEU	-	expression tag	UNP A0A192ICX3
B	-1	GLY	-	expression tag	UNP A0A192ICX3
B	0	THR	-	expression tag	UNP A0A192ICX3
B	98	TYR	PHE	engineered mutation	UNP A0A192ICX3
B	202	TYR	PHE	engineered mutation	UNP A0A192ICX3

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	190	Total	O	0	0
			190	190		
2	B	155	Total	O	0	0
			155	155		

- Molecule 1: Short-chain dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	83.92Å 83.92Å 115.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	67.55 – 1.47 67.55 – 1.47	Depositor EDS
% Data completeness (in resolution range)	98.6 (67.55-1.47) 73.5 (67.55-1.47)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	15.41 (at 1.47Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.175 , 0.207 (Not available) , 0.222	Depositor DCC
R_{free} test set	3393 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	13.2	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3666	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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	1.77	16/1784 (0.9%)	1.69	18/2416 (0.7%)
1	B	1.71	21/1581 (1.3%)	1.46	11/2137 (0.5%)
All	All	1.74	37/3365 (1.1%)	1.59	29/4553 (0.6%)

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	172	MET	SD-CE	-10.00	1.54	1.79
1	B	160	MET	SD-CE	-9.11	1.56	1.79
1	B	66	ALA	N-CA	-8.63	1.35	1.46
1	A	160	MET	SD-CE	-7.31	1.61	1.79
1	A	103	THR	N-CA	-6.88	1.38	1.46
1	A	113	ARG	CA-C	6.68	1.61	1.52
1	B	187	GLN	N-CA	6.25	1.52	1.46
1	A	97	VAL	C-O	6.09	1.30	1.24
1	A	172	MET	SD-CE	-6.05	1.64	1.79
1	B	157	VAL	C-N	-6.01	1.26	1.33
1	B	209	LEU	C-N	-5.84	1.25	1.33
1	A	109	ASP	CA-C	5.82	1.60	1.52
1	A	94	ASN	C-N	-5.74	1.25	1.33
1	B	149	ARG	CD-NE	5.58	1.54	1.46
1	A	120	ARG	C-N	-5.58	1.25	1.33
1	B	213	GLY	N-CA	5.53	1.52	1.45
1	A	30	ALA	N-CA	5.50	1.53	1.46
1	A	105	GLU	CA-CB	-5.49	1.45	1.53
1	B	73	ALA	CA-CB	-5.47	1.44	1.53
1	B	210	MET	C-N	-5.41	1.26	1.33
1	B	26	VAL	CA-CB	-5.33	1.48	1.54
1	B	94	ASN	C-N	-5.33	1.26	1.33
1	B	93	ASN	C-N	-5.31	1.25	1.34
1	B	77	ALA	CA-C	5.30	1.59	1.52
1	A	102	GLY	CA-C	-5.24	1.46	1.52
1	B	51	ALA	C-N	5.20	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	VAL	C-N	-5.19	1.27	1.33
1	B	212	ILE	N-CA	5.17	1.52	1.46
1	B	235	TYR	C-O	-5.17	1.16	1.23
1	B	221	ILE	C-O	5.15	1.30	1.24
1	A	46	ARG	C-O	-5.15	1.18	1.24
1	A	134	ASN	C-N	5.14	1.40	1.33
1	A	15	GLN	CA-CB	5.12	1.59	1.53
1	B	179	ARG	CZ-NH2	-5.11	1.26	1.33
1	B	15	GLN	CD-OE1	5.10	1.33	1.23
1	B	67	ASP	CA-C	5.04	1.59	1.52
1	A	60	LYS	N-CA	5.00	1.52	1.46

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ASP	CA-C-N	22.59	150.47	120.65
1	A	112	ASP	C-N-CA	22.59	150.47	120.65
1	B	177	GLY	O-C-N	12.15	125.44	121.07
1	B	210	MET	O-C-N	-9.62	112.00	123.16
1	A	109	ASP	CA-C-O	-8.63	111.81	120.70
1	A	113	ARG	N-CA-C	8.44	120.17	110.97
1	A	28	ARG	NE-CZ-NH2	-8.06	111.94	119.20
1	A	112	ASP	O-C-N	-7.89	112.13	122.39
1	A	15	GLN	CA-C-O	-7.48	112.15	120.60
1	B	249	ALA	CA-C-O	-7.17	108.61	120.80
1	A	116	ALA	CA-C-O	-6.50	113.53	120.42
1	B	66	ALA	N-CA-C	-6.50	98.03	108.55
1	A	134	ASN	CA-C-N	-6.46	109.94	120.87
1	A	134	ASN	C-N-CA	-6.46	109.94	120.87
1	B	219	GLU	CB-CG-CD	6.23	123.19	112.60
1	A	213	GLY	N-CA-C	5.85	122.93	114.10
1	A	115	LEU	N-CA-CB	5.67	118.22	110.01
1	A	122	VAL	N-CA-C	-5.62	104.87	111.00
1	B	84	HIS	N-CA-C	5.47	117.33	111.36
1	A	28	ARG	CG-CD-NE	-5.44	100.03	112.00
1	B	166	VAL	CA-C-N	5.28	125.84	119.98
1	B	166	VAL	C-N-CA	5.28	125.84	119.98
1	A	210	MET	CA-CB-CG	-5.27	103.56	114.10
1	B	177	GLY	CA-C-O	-5.24	116.14	119.65
1	A	122	VAL	CA-C-O	-5.19	115.16	120.71
1	A	206	LEU	N-CA-C	-5.13	105.77	111.36
1	B	212	ILE	CA-CB-CG2	5.11	119.18	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	LEU	CB-CG-CD2	5.08	125.95	110.70
1	A	28	ARG	NH1-CZ-NH2	5.02	125.83	119.30

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	1760	0	1748	13	0
1	B	1561	0	1570	18	1
2	A	190	0	0	6	0
2	B	155	0	0	0	0
All	All	3666	0	3318	31	1

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 5.

All (31) 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:B:40:TYR:OH	1:B:65:LYS:HE3	1.54	1.06
1:A:196:ASN:HB2	2:A:457:HOH:O	1.56	1.05
1:B:40:TYR:CZ	1:B:65:LYS:HE3	2.09	0.87
1:B:18:SER:HB3	1:B:40:TYR:HB2	1.57	0.86
1:B:18:SER:HB3	1:B:40:TYR:CB	2.11	0.79
1:A:219:GLU:HB3	2:A:465:HOH:O	1.85	0.77
1:B:40:TYR:CZ	1:B:65:LYS:HG3	2.23	0.72
1:B:18:SER:CB	1:B:40:TYR:HB2	2.18	0.72
1:B:40:TYR:CE1	1:B:65:LYS:HG3	2.35	0.61
1:A:113:ARG:HD3	2:A:475:HOH:O	2.02	0.59
1:B:68:SER:O	1:B:121:SER:OG	2.10	0.59
1:B:40:TYR:CZ	1:B:65:LYS:CE	2.84	0.58
1:B:40:TYR:CE2	1:B:65:LYS:CE	2.88	0.56
1:B:40:TYR:CZ	1:B:65:LYS:CG	2.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:ILE:HG22	1:A:214:ARG:HG2	1.88	0.56
1:B:40:TYR:CE2	1:B:65:LYS:HE2	2.42	0.55
1:A:51:ALA:O	1:A:55:THR:HG23	2.07	0.54
1:B:94:ASN:O	1:B:94:ASN:CG	2.48	0.53
1:B:212:ILE:HD12	1:B:214:ARG:HG2	1.91	0.53
1:A:84:HIS:HE1	2:A:414:HOH:O	1.91	0.53
1:B:40:TYR:CE2	1:B:65:LYS:HE3	2.46	0.49
1:A:217:LYS:HE3	2:A:409:HOH:O	2.13	0.47
1:A:198:ASP:OD2	1:A:215:TYR:HB2	2.14	0.47
1:A:133:MET:O	1:A:179:ARG:NH2	2.50	0.45
1:B:18:SER:OG	1:B:40:TYR:HB2	2.17	0.45
1:A:94:ASN:CG	1:A:94:ASN:O	2.59	0.44
1:A:121:SER:HB2	2:A:307:HOH:O	2.18	0.42
1:A:74:LEU:CD1	1:A:121:SER:HB3	2.50	0.42
1:A:54:VAL:HG11	1:A:61:VAL:HB	2.02	0.41
1:B:149:ARG:HH21	1:B:209:LEU:HD22	1.86	0.40
1:B:115:LEU:HD23	1:B:115:LEU:HA	1.95	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:GLU:OE2	1:B:179:ARG:NH1[7_555]	1.58	0.62

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	218/287 (76%)	213 (98%)	5 (2%)	0	100	100
1	B	194/287 (68%)	189 (97%)	5 (3%)	0	100	100
All	All	412/574 (72%)	402 (98%)	10 (2%)	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	171/205 (83%)	171 (100%)	0	100	100
1	B	152/205 (74%)	149 (98%)	3 (2%)	48	19
All	All	323/410 (79%)	320 (99%)	3 (1%)	70	48

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	74	LEU
1	B	80	GLN
1	B	219	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	76	GLN
1	A	84	HIS
1	A	87	ASN
1	A	93	ASN
1	A	134	ASN
1	B	8	GLN
1	B	15	GLN
1	B	84	HIS
1	B	87	ASN
1	B	94	ASN

5.3.3 RNA ⓘ

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

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	245/287 (85%)	0.61	28 (11%) 10 10	8, 14, 27, 46	0
1	B	218/287 (75%)	0.54	20 (9%) 14 15	8, 13, 28, 52	0
All	All	463/574 (80%)	0.58	48 (10%) 11 12	8, 14, 28, 52	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	66	ALA	6.1
1	A	110	ASP	4.5
1	B	69	ALA	4.4
1	A	109	ASP	4.2
1	A	111	LEU	4.0
1	B	40	TYR	3.9
1	A	97	VAL	3.7
1	B	212	ILE	3.7
1	A	100	LEU	3.5
1	A	212	ILE	3.5
1	B	67	ASP	3.5
1	A	235	TYR	3.3
1	A	107	ALA	3.3
1	A	112	ASP	3.2
1	B	51	ALA	3.2
1	B	68	SER	3.1
1	A	117	VAL	3.0
1	B	96	GLY	3.0
1	A	56	THR	2.9
1	A	96	GLY	2.9
1	A	69	ALA	2.8
1	B	191	VAL	2.8
1	B	215	TYR	2.8
1	A	113	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	115	LEU	2.7
1	B	98	TYR	2.6
1	B	95	ALA	2.6
1	A	202	TYR	2.6
1	B	213	GLY	2.6
1	A	108	LEU	2.5
1	A	99	THR	2.5
1	A	213	GLY	2.5
1	B	70	ASP	2.5
1	A	98	TYR	2.4
1	A	199	ALA	2.4
1	B	73	ALA	2.4
1	B	99	THR	2.4
1	A	121	SER	2.4
1	B	209	LEU	2.3
1	A	53	ALA	2.1
1	A	55	THR	2.1
1	B	52	SER	2.1
1	A	54	VAL	2.0
1	B	74	LEU	2.0
1	B	104	GLU	2.0
1	A	135	ASP	2.0
1	A	120	ARG	2.0
1	A	116	ALA	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.