



Full wwPDB X-ray Structure Validation Report i

Feb 10, 2024 – 02:59 PM EST

PDB ID : 2I4L
Title : Rhodopseudomonas palustris prolyl-tRNA synthetase
Authors : Crepin, T.; Yaremcuk, A.; Tukalo, M.; Cusack, S.
Deposited on : 2006-08-22
Resolution : 2.00 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 i 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](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

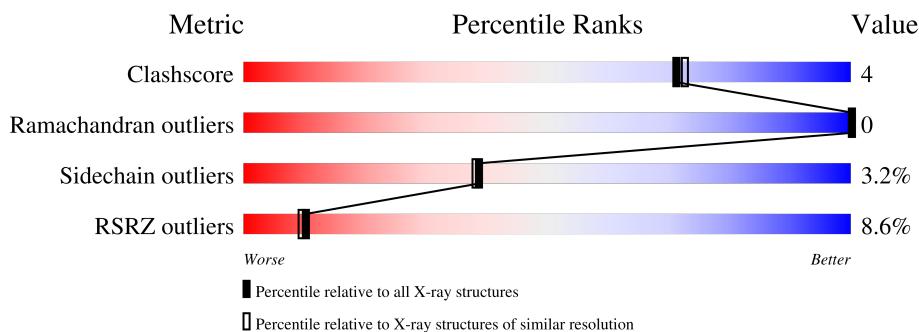
1 Overall quality at a glance [i](#)

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 $<=5\%$. 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	458	15%	86%	9%	..
1	B	458	8%	88%	7%	..
1	C	458	2%	89%	6%	..

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 11092 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 Proline-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C 3479	N 2201	O 618	S 646	14	0	0
1	B	441	Total	C 3495	N 2211	O 620	S 650	14	0	0
1	C	441	Total	C 3495	N 2211	O 620	S 650	14	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q6N5P6
A	-18	GLY	-	expression tag	UNP Q6N5P6
A	-17	SER	-	expression tag	UNP Q6N5P6
A	-16	SER	-	expression tag	UNP Q6N5P6
A	-15	HIS	-	expression tag	UNP Q6N5P6
A	-14	HIS	-	expression tag	UNP Q6N5P6
A	-13	HIS	-	expression tag	UNP Q6N5P6
A	-12	HIS	-	expression tag	UNP Q6N5P6
A	-11	HIS	-	expression tag	UNP Q6N5P6
A	-10	HIS	-	expression tag	UNP Q6N5P6
A	-9	SER	-	expression tag	UNP Q6N5P6
A	-8	SER	-	expression tag	UNP Q6N5P6
A	-7	GLY	-	expression tag	UNP Q6N5P6
A	-6	LEU	-	expression tag	UNP Q6N5P6
A	-5	VAL	-	expression tag	UNP Q6N5P6
A	-4	PRO	-	expression tag	UNP Q6N5P6
A	-3	ARG	-	expression tag	UNP Q6N5P6
A	-2	GLY	-	expression tag	UNP Q6N5P6
A	-1	SER	-	expression tag	UNP Q6N5P6
A	0	HIS	-	expression tag	UNP Q6N5P6
B	-19	MET	-	expression tag	UNP Q6N5P6
B	-18	GLY	-	expression tag	UNP Q6N5P6
B	-17	SER	-	expression tag	UNP Q6N5P6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP Q6N5P6
B	-15	HIS	-	expression tag	UNP Q6N5P6
B	-14	HIS	-	expression tag	UNP Q6N5P6
B	-13	HIS	-	expression tag	UNP Q6N5P6
B	-12	HIS	-	expression tag	UNP Q6N5P6
B	-11	HIS	-	expression tag	UNP Q6N5P6
B	-10	HIS	-	expression tag	UNP Q6N5P6
B	-9	SER	-	expression tag	UNP Q6N5P6
B	-8	SER	-	expression tag	UNP Q6N5P6
B	-7	GLY	-	expression tag	UNP Q6N5P6
B	-6	LEU	-	expression tag	UNP Q6N5P6
B	-5	VAL	-	expression tag	UNP Q6N5P6
B	-4	PRO	-	expression tag	UNP Q6N5P6
B	-3	ARG	-	expression tag	UNP Q6N5P6
B	-2	GLY	-	expression tag	UNP Q6N5P6
B	-1	SER	-	expression tag	UNP Q6N5P6
B	0	HIS	-	expression tag	UNP Q6N5P6
C	-19	MET	-	expression tag	UNP Q6N5P6
C	-18	GLY	-	expression tag	UNP Q6N5P6
C	-17	SER	-	expression tag	UNP Q6N5P6
C	-16	SER	-	expression tag	UNP Q6N5P6
C	-15	HIS	-	expression tag	UNP Q6N5P6
C	-14	HIS	-	expression tag	UNP Q6N5P6
C	-13	HIS	-	expression tag	UNP Q6N5P6
C	-12	HIS	-	expression tag	UNP Q6N5P6
C	-11	HIS	-	expression tag	UNP Q6N5P6
C	-10	HIS	-	expression tag	UNP Q6N5P6
C	-9	SER	-	expression tag	UNP Q6N5P6
C	-8	SER	-	expression tag	UNP Q6N5P6
C	-7	GLY	-	expression tag	UNP Q6N5P6
C	-6	LEU	-	expression tag	UNP Q6N5P6
C	-5	VAL	-	expression tag	UNP Q6N5P6
C	-4	PRO	-	expression tag	UNP Q6N5P6
C	-3	ARG	-	expression tag	UNP Q6N5P6
C	-2	GLY	-	expression tag	UNP Q6N5P6
C	-1	SER	-	expression tag	UNP Q6N5P6
C	0	HIS	-	expression tag	UNP Q6N5P6

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	129	Total O 129 129	0	0

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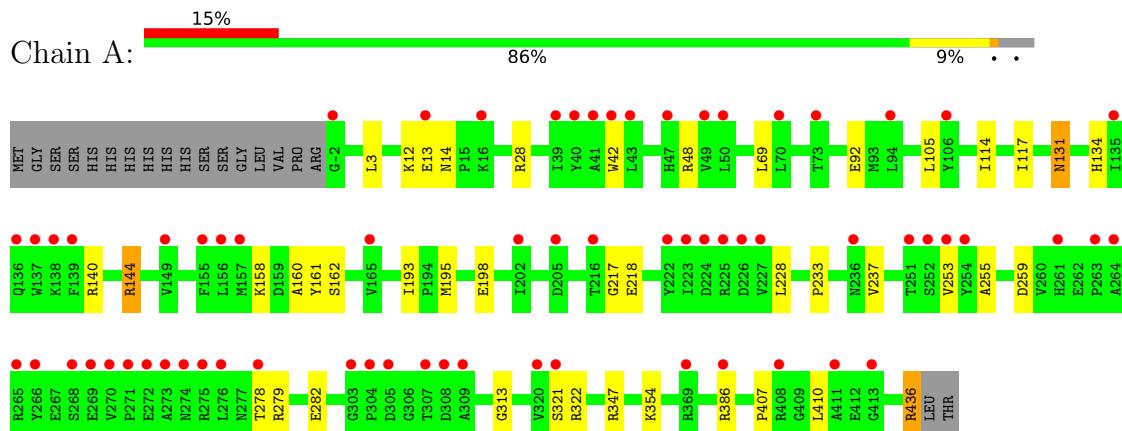
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	222	Total O 222 222	0	0
2	C	272	Total O 272 272	0	0

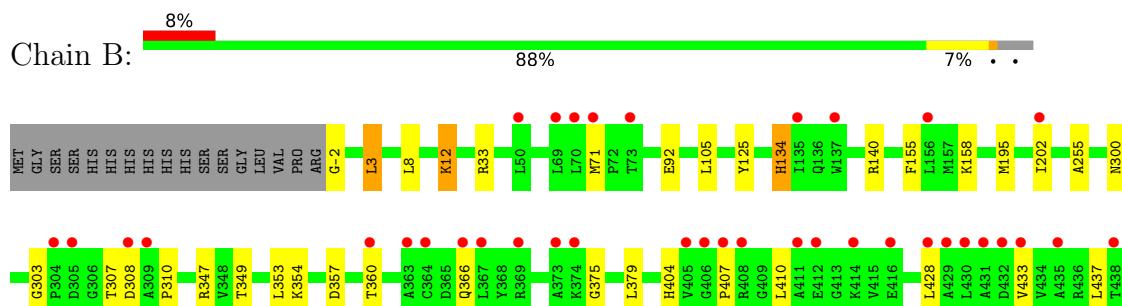
3 Residue-property plots

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.

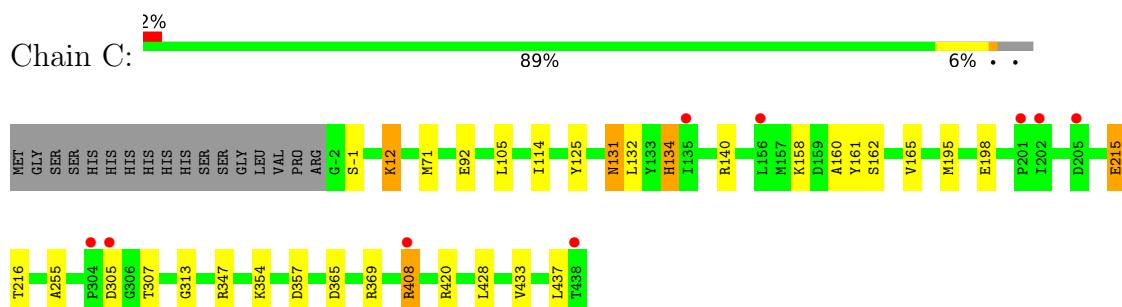
- Molecule 1: Proline-tRNA ligase



- Molecule 1: Proline-tRNA ligase



- Molecule 1: Proline-tRNA ligase



4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	110.84Å 212.56Å 150.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00 46.72 – 1.96	Depositor EDS
% Data completeness (in resolution range)	96.6 ((Not available)-2.00) 94.5 (46.72-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$< I/\sigma(I) >$ ¹	1.38 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.2.0000	Depositor
R , R_{free}	0.191 , 0.221 0.188 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.3	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.5	EDS
L-test for twinning ²	$< L > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11092	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ 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	0.64	0/3554	0.69	1/4807 (0.0%)
1	B	0.70	0/3570	0.71	0/4828
1	C	0.80	0/3570	0.75	1/4828 (0.0%)
All	All	0.72	0/10694	0.72	2/14463 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	48	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	C	420	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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	3479	0	3448	19	1
1	B	3495	0	3466	23	0
1	C	3495	0	3466	32	0
2	A	129	0	0	1	0
2	B	222	0	0	0	0
2	C	272	0	0	0	0
All	All	11092	0	10380	73	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 4.

All (73) 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:12:LYS:HD2	1:C:12:LYS:N	1.49	1.25
1:C:12:LYS:H	1:C:12:LYS:CD	1.52	1.13
1:C:92:GLU:OE1	1:C:140:ARG:CZ	2.16	0.93
1:A:347:ARG:HH12	1:A:436:ARG:HD3	1.34	0.92
1:C:12:LYS:HD2	1:C:12:LYS:H	0.73	0.88
1:B:12:LYS:HE3	1:B:12:LYS:H	1.41	0.82
1:C:408:ARG:HH11	1:C:408:ARG:CG	1.91	0.82
1:C:408:ARG:HH11	1:C:408:ARG:HG3	1.44	0.82
1:C:305:ASP:OD1	1:C:307:THR:HG22	1.85	0.77
1:C:131:ASN:HD21	1:C:160:ALA:HB1	1.56	0.70
1:C:347:ARG:NH1	1:C:437:LEU:O	2.23	0.68
1:C:408:ARG:H	1:C:408:ARG:HD2	1.61	0.64
1:C:195:MET:HG2	1:C:255:ALA:HB1	1.81	0.63
1:A:347:ARG:NH1	1:A:436:ARG:HD3	2.12	0.62
1:C:408:ARG:HG3	1:C:408:ARG:NH1	2.04	0.62
1:B:71:MET:H	1:B:134:HIS:HD2	1.45	0.62
1:A:354:LYS:HD3	1:A:407:PRO:HG2	1.82	0.62
1:B:92:GLU:OE1	1:B:140:ARG:NH2	2.33	0.61
1:B:354:LYS:HD2	1:B:407:PRO:HG2	1.82	0.61
1:C:92:GLU:OE1	1:C:140:ARG:NH1	2.34	0.61
1:A:195:MET:HG2	1:A:255:ALA:HB1	1.84	0.60
1:B:71:MET:H	1:B:134:HIS:CD2	2.20	0.60
1:B:354:LYS:HD2	1:B:407:PRO:CG	2.31	0.60
1:C:71:MET:H	1:C:134:HIS:HD2	1.48	0.60
1:A:131:ASN:HD22	1:A:131:ASN:C	2.04	0.60
1:B:300:ASN:HD22	1:B:310:PRO:HA	1.66	0.59
1:B:12:LYS:HE3	1:B:12:LYS:N	2.14	0.59
1:B:12:LYS:H	1:B:12:LYS:CE	2.14	0.58
1:C:131:ASN:C	1:C:131:ASN:HD22	2.07	0.58
1:C:365:ASP:O	1:C:369:ARG:HG3	2.04	0.57
1:A:92:GLU:OE1	1:A:140:ARG:NH1	2.38	0.56
1:C:71:MET:H	1:C:134:HIS:CD2	2.23	0.56
1:C:408:ARG:H	1:C:408:ARG:CD	2.18	0.56
1:A:131:ASN:HD21	1:A:160:ALA:HB1	1.72	0.54
1:C:408:ARG:CG	1:C:408:ARG:NH1	2.60	0.54
1:A:92:GLU:OE1	1:A:140:ARG:CZ	2.55	0.54
1:C:12:LYS:N	1:C:12:LYS:CD	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:LEU:HD21	1:B:8:LEU:HD23	1.91	0.52
1:C:114:ILE:HG21	1:C:161:TYR:CG	2.46	0.51
1:A:217:GLY:O	1:A:279:ARG:NH2	2.43	0.50
1:B:140:ARG:HG2	1:B:155:PHE:HE2	1.77	0.50
1:B:349:THR:HA	1:B:379:LEU:O	2.12	0.49
1:A:140:ARG:HD2	2:A:510:HOH:O	2.14	0.48
1:B:195:MET:HG2	1:B:255:ALA:HB1	1.95	0.48
1:B:202:ILE:HG22	1:B:202:ILE:O	2.14	0.47
1:C:428:LEU:HD11	1:C:433:VAL:HB	1.96	0.47
1:A:92:GLU:OE1	1:A:140:ARG:NH2	2.48	0.47
1:B:353:LEU:HD11	1:B:404:HIS:HB3	1.97	0.47
1:C:428:LEU:CD1	1:C:433:VAL:HB	2.45	0.47
1:A:233:PRO:HB3	1:A:237:VAL:HG21	1.97	0.47
1:B:347:ARG:NH1	1:B:437:LEU:O	2.49	0.46
1:C:408:ARG:HH11	1:C:408:ARG:HG2	1.80	0.45
1:A:278:THR:OG1	1:A:279:ARG:N	2.49	0.44
1:A:114:ILE:HG21	1:A:161:TYR:CG	2.52	0.44
1:C:428:LEU:HD11	1:C:433:VAL:CB	2.48	0.44
1:A:42:TRP:CH2	1:A:321:SER:HB2	2.53	0.43
1:C:92:GLU:OE1	1:C:140:ARG:NE	2.48	0.43
1:B:428:LEU:HD11	1:B:433:VAL:HA	2.01	0.43
1:A:193:ILE:HD11	1:A:228:LEU:HD23	2.00	0.42
1:B:354:LYS:HD2	1:B:407:PRO:HG3	1.99	0.42
1:B:125:TYR:HB3	1:B:303:GLY:HA2	2.00	0.42
1:C:215:GLU:HG2	1:C:216:THR:HG23	2.02	0.42
1:C:131:ASN:HD22	1:C:132:LEU:N	2.18	0.41
1:B:140:ARG:HG2	1:B:155:PHE:CE2	2.55	0.41
1:B:357:ASP:OD2	1:B:360:THR:HG23	2.20	0.41
1:C:125:TYR:HB2	1:C:165:VAL:HG21	2.02	0.41
1:C:215:GLU:HG2	1:C:216:THR:N	2.35	0.41
1:C:354:LYS:HG2	1:C:357:ASP:HB2	2.02	0.41
1:A:162:SER:O	1:A:313:GLY:HA2	2.21	0.41
1:B:-2:GLY:HA3	1:B:375:GLY:HA2	2.03	0.40
1:C:162:SER:O	1:C:313:GLY:HA2	2.21	0.40
1:A:14:ASN:OD1	1:A:28:ARG:HD2	2.20	0.40
1:A:117:ILE:HG12	1:B:33:ARG:HD3	2.03	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:A:144:ARG:NH2	1:A:259:ASP:OD1[3_555]	2.14	0.06

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	437/458 (95%)	424 (97%)	13 (3%)	0	100 100
1	B	439/458 (96%)	426 (97%)	13 (3%)	0	100 100
1	C	439/458 (96%)	430 (98%)	9 (2%)	0	100 100
All	All	1315/1374 (96%)	1280 (97%)	35 (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	359/376 (96%)	342 (95%)	17 (5%)	26 22
1	B	361/376 (96%)	352 (98%)	9 (2%)	47 49
1	C	361/376 (96%)	352 (98%)	9 (2%)	47 49
All	All	1081/1128 (96%)	1046 (97%)	35 (3%)	39 38

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	12	LYS
1	A	13	GLU
1	A	69	LEU
1	A	105	LEU
1	A	131	ASN
1	A	134	HIS
1	A	144	ARG
1	A	158	LYS
1	A	198	GLU
1	A	218	GLU
1	A	253	VAL
1	A	282	GLU
1	A	322	ARG
1	A	386	ARG
1	A	410	LEU
1	A	436	ARG
1	B	3	LEU
1	B	12	LYS
1	B	105	LEU
1	B	134	HIS
1	B	158	LYS
1	B	307	THR
1	B	308	ASP
1	B	366	GLN
1	B	410	LEU
1	C	-1	SER
1	C	12	LYS
1	C	105	LEU
1	C	131	ASN
1	C	134	HIS
1	C	158	LYS
1	C	198	GLU
1	C	215	GLU
1	C	408	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	229	ASN
1	B	134	HIS
1	B	300	ASN

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Mol	Chain	Res	Type
1	C	131	ASN
1	C	134	HIS
1	C	300	ASN

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 monosaccharides 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	439/458 (95%)	0.82	67 (15%) 2 1	20, 31, 51, 62	0
1	B	441/458 (96%)	0.41	37 (8%) 11 10	19, 27, 47, 65	0
1	C	441/458 (96%)	-0.05	9 (2%) 65 63	14, 24, 41, 55	0
All	All	1321/1374 (96%)	0.39	113 (8%) 10 9	14, 28, 47, 65	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273	ALA	8.1
1	B	430	LEU	7.1
1	A	202	ILE	6.7
1	A	271	PRO	6.7
1	A	270	VAL	6.5
1	A	268	SER	6.1
1	B	202	ILE	5.9
1	A	266	TYR	5.8
1	A	276	LEU	5.6
1	A	253	VAL	5.4
1	A	272	GLU	5.1
1	A	269	GLU	4.8
1	A	274	ASN	4.7
1	B	408	ARG	4.4
1	C	202	ILE	4.4
1	A	252	SER	4.2
1	B	438	THR	4.2
1	A	408	ARG	4.2
1	A	224	ASP	4.0
1	A	275	ARG	4.0
1	A	411	ALA	4.0
1	B	360	THR	4.0
1	A	223	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	137	TRP	3.9
1	A	261	HIS	3.8
1	A	156	LEU	3.8
1	B	411	ALA	3.8
1	B	433	VAL	3.7
1	A	225	ARG	3.5
1	B	70	LEU	3.4
1	B	432	ASP	3.4
1	B	366	GLN	3.4
1	A	320	VAL	3.4
1	A	50	LEU	3.4
1	B	405	VAL	3.3
1	B	429	ALA	3.2
1	B	135	ILE	3.2
1	A	155	PHE	3.2
1	B	373	ALA	3.2
1	A	305	ASP	3.1
1	B	431	ALA	3.1
1	A	-2	GLY	3.0
1	A	205	ASP	3.0
1	A	42	TRP	3.0
1	B	363	ALA	2.8
1	B	308	ASP	2.8
1	B	367	LEU	2.8
1	A	139	PHE	2.8
1	A	226	ASP	2.7
1	C	438	THR	2.7
1	A	39	ILE	2.7
1	B	156	LEU	2.7
1	A	135	ILE	2.7
1	A	304	PRO	2.7
1	A	309	ALA	2.7
1	A	43	LEU	2.7
1	B	428	LEU	2.7
1	A	308	ASP	2.6
1	A	307	THR	2.6
1	B	416	GLU	2.6
1	A	251	THR	2.6
1	A	227	VAL	2.5
1	A	263	PRO	2.5
1	B	69	LEU	2.5
1	A	149	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	369	ARG	2.5
1	C	408	ARG	2.5
1	B	73	THR	2.5
1	A	157	MET	2.5
1	B	414	LYS	2.5
1	A	47	HIS	2.4
1	B	374	LYS	2.3
1	A	236	ASN	2.3
1	B	435	ALA	2.3
1	A	222	TYR	2.3
1	B	50	LEU	2.3
1	B	406	GLY	2.3
1	A	73	THR	2.3
1	B	407	PRO	2.3
1	A	41	ALA	2.2
1	A	106	TYR	2.2
1	A	254	TYR	2.2
1	A	264	ALA	2.2
1	B	137	TRP	2.2
1	A	303	GLY	2.2
1	B	412	GLU	2.2
1	B	364	CYS	2.2
1	A	70	LEU	2.2
1	A	40	TYR	2.2
1	A	136	GLN	2.1
1	A	369	ARG	2.2
1	A	49	VAL	2.1
1	A	165	VAL	2.1
1	C	156	LEU	2.1
1	A	413	GLY	2.1
1	B	304	PRO	2.1
1	C	135	ILE	2.1
1	B	309	ALA	2.1
1	C	201	PRO	2.1
1	A	386	ARG	2.1
1	B	71	MET	2.1
1	A	265	ARG	2.1
1	A	16	LYS	2.1
1	A	94	LEU	2.0
1	C	304	PRO	2.0
1	A	216	THR	2.0
1	A	278	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	305	ASP	2.0
1	C	305	ASP	2.0
1	A	13	GLU	2.0
1	A	321	SER	2.0
1	A	138	LYS	2.0
1	C	205	ASP	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 monosaccharides 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.