



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:42 PM UTC

PDB ID : 2I4L / pdb_00002i4l
Title : Rhodopseudomonas palustris prolyl-tRNA synthetase
Authors : Crepin, T.; Yaremchuk, 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 ⓘ 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

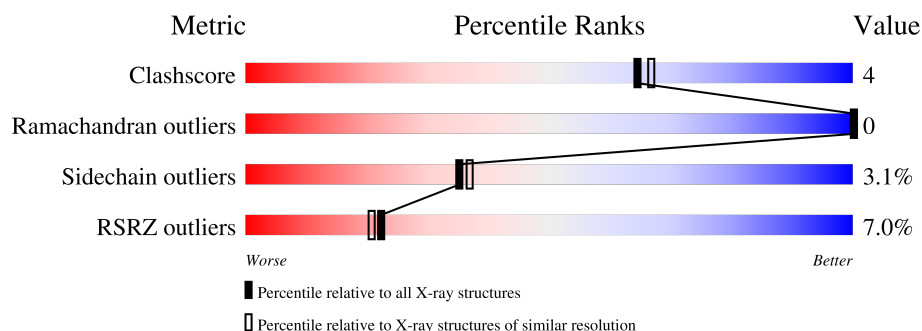
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 $\leq 5\%$. 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	458	16% 85% 10% • •
1	B	458	3% 88% 8% • •
1	C	458	2% 88% 7% • •

2 Entry composition

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	N	O	S	0	0	0
			3479	2201	618	646	14			
1	B	441	Total	C	N	O	S	0	0	0
			3495	2211	620	650	14			
1	C	441	Total	C	N	O	S	0	0	0
			3495	2211	620	650	14			

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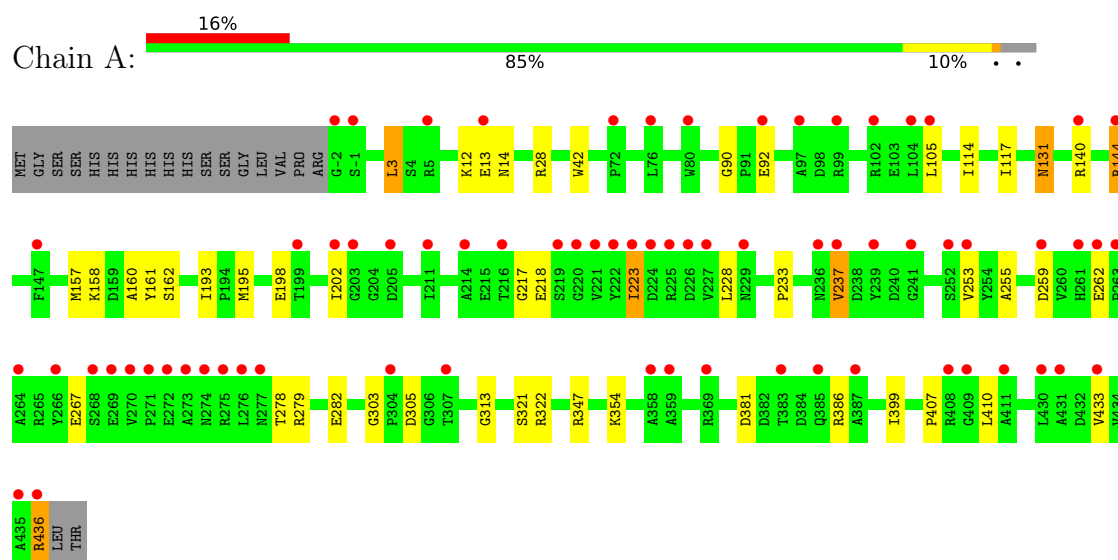
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	222	Total 222	O 222	0	0
2	C	272	Total 272	O 272	0	0

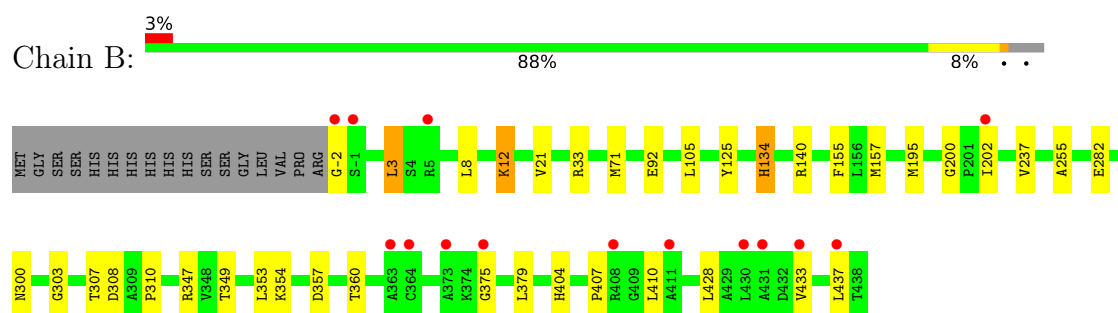
3 Residue-property plots [i](#)

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.

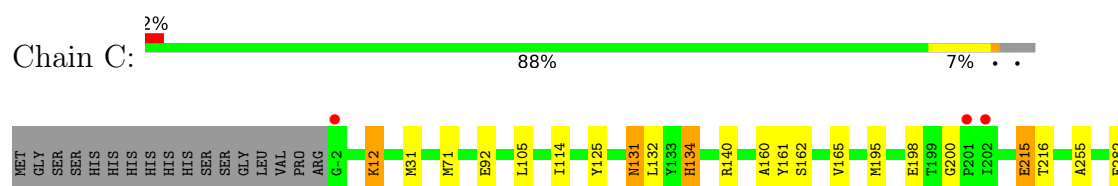
• Molecule 1: Proline-tRNA ligase



• Molecule 1: Proline-tRNA ligase



• Molecule 1: Proline-tRNA ligase





4 Data and refinement statistics

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) – 2.00 106.28 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.6 ((Not available)-2.00) 96.6 (106.28-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.35 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.79	0/3554	0.93	9/4807 (0.2%)
1	B	0.85	1/3570 (0.0%)	0.91	3/4828 (0.1%)
1	C	0.98	1/3570 (0.0%)	0.94	3/4828 (0.1%)
All	All	0.87	2/10694 (0.0%)	0.93	15/14463 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	237	VAL	CA-CB	5.38	1.60	1.54
1	C	320	VAL	CA-CB	5.05	1.60	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	200	GLY	CA-C-N	6.90	128.46	119.84
1	B	200	GLY	C-N-CA	6.90	128.46	119.84
1	C	320	VAL	N-CA-C	5.78	116.43	110.36
1	A	90	GLY	CA-C-N	5.67	125.76	119.87
1	A	90	GLY	C-N-CA	5.67	125.76	119.87
1	C	200	GLY	CA-C-N	5.61	125.08	119.24
1	C	200	GLY	C-N-CA	5.61	125.08	119.24
1	A	223	ILE	N-CA-C	5.36	117.79	108.90
1	A	202	ILE	CB-CA-C	-5.30	104.91	111.70
1	A	262	GLU	CA-C-N	5.27	126.43	119.84
1	A	262	GLU	C-N-CA	5.27	126.43	119.84
1	B	21	VAL	N-CA-C	5.19	115.40	110.42
1	A	399	ILE	CA-C-N	5.13	125.17	119.32
1	A	399	ILE	C-N-CA	5.13	125.17	119.32
1	A	433	VAL	N-CA-C	5.06	117.38	111.05

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	3479	0	3448	24	1
1	B	3495	0	3466	24	0
1	C	3495	0	3466	34	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	81	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 (81) 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:A:131:ASN:HD22	1:A:131:ASN:C	2.04	0.64
1:C:195:MET:HG2	1:C:255:ALA:HB1	1.81	0.63
1:C:131:ASN:C	1:C:131:ASN:HD22	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:31:MET:HE1	1:C:339:TRP:HZ2	1.80	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:31:MET:HE1	1:C:339:TRP:CZ2	2.51	0.46
1:A:195:MET:HE2	1:A:223:ILE:HG21	1.97	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:B:157:MET:HE3	1:B:157:MET:HB2	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:HD12	1:A:381:ASP:CG	2.44	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:A:303:GLY:C	1:A:305:ASP:H	2.29	0.41
1:A:157:MET:HE3	1:A:157:MET:HB2	1.75	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:C:131:ASN:HD22	1:C:132:LEU:N	2.18	0.41
1:A:162:SER:O	1:A:313:GLY:HA2	2.21	0.41
1:A:158:LYS:HD2	1:A:158:LYS:C	2.46	0.40
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 ⓘ

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%)	343 (96%)	16 (4%)	24	23
1	B	361/376 (96%)	353 (98%)	8 (2%)	45	50
1	C	361/376 (96%)	352 (98%)	9 (2%)	42	45
All	All	1081/1128 (96%)	1048 (97%)	33 (3%)	35	37

All (33) 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	105	LEU
1	A	131	ASN
1	A	144	ARG
1	A	198	GLU
1	A	218	GLU
1	A	237	VAL
1	A	253	VAL
1	A	267	GLU
1	A	282	GLU
1	A	322	ARG
1	A	386	ARG
1	A	410	LEU
1	A	436	ARG

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Mol	Chain	Res	Type
1	B	3	LEU
1	B	12	LYS
1	B	105	LEU
1	B	134	HIS
1	B	282	GLU
1	B	307	THR
1	B	308	ASP
1	B	410	LEU
1	C	12	LYS
1	C	105	LEU
1	C	131	ASN
1	C	134	HIS
1	C	198	GLU
1	C	215	GLU
1	C	282	GLU
1	C	408	ARG
1	C	430	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	131	ASN
1	A	229	ASN
1	A	274	ASN
1	A	277	ASN
1	B	134	HIS
1	B	300	ASN
1	C	100	HIS
1	C	131	ASN
1	C	134	HIS
1	C	249	GLN
1	C	300	ASN
1	C	402	GLN

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	439/458 (95%)	1.12	71 (16%) 4 4	20, 31, 51, 62	0
1	B	441/458 (96%)	0.09	14 (3%) 50 49	19, 27, 47, 65	0
1	C	441/458 (96%)	-0.15	7 (1%) 70 70	14, 24, 41, 55	0
All	All	1321/1374 (96%)	0.35	92 (6%) 22 21	14, 28, 47, 65	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	ILE	5.5
1	A	273	ALA	5.4
1	A	-2	GLY	5.0
1	A	271	PRO	4.7
1	A	266	TYR	4.6
1	A	276	LEU	4.2
1	A	261	HIS	4.2
1	A	253	VAL	4.0
1	A	270	VAL	3.9
1	A	252	SER	3.8
1	B	-2	GLY	3.7
1	A	214	ALA	3.6
1	A	223	ILE	3.6
1	A	369	ARG	3.5
1	A	224	ASP	3.4
1	A	269	GLU	3.2
1	C	-2	GLY	3.2
1	A	272	GLU	3.1
1	A	227	VAL	3.1
1	A	-1	SER	3.0
1	C	408	ARG	3.0
1	A	264	ALA	3.0
1	C	202	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	268	SER	2.9
1	A	203	GLY	2.9
1	B	408	ARG	2.9
1	A	220	GLY	2.9
1	B	202	ILE	2.8
1	B	411	ALA	2.8
1	A	216	THR	2.8
1	A	259	ASP	2.8
1	A	411	ALA	2.8
1	A	436	ARG	2.7
1	A	430	LEU	2.7
1	B	373	ALA	2.7
1	A	199	THR	2.7
1	A	263	PRO	2.7
1	B	431	ALA	2.6
1	B	437	LEU	2.6
1	C	307	THR	2.6
1	A	408	ARG	2.6
1	A	144	ARG	2.6
1	A	435	ALA	2.6
1	A	236	ASN	2.5
1	A	205	ASP	2.5
1	B	430	LEU	2.5
1	A	241	GLY	2.5
1	A	274	ASN	2.5
1	B	433	VAL	2.5
1	A	222	TYR	2.5
1	A	221	VAL	2.4
1	A	105	LEU	2.4
1	B	363	ALA	2.4
1	A	226	ASP	2.4
1	B	-1	SER	2.4
1	A	97	ALA	2.3
1	A	359	ALA	2.3
1	A	225	ARG	2.3
1	C	201	PRO	2.3
1	A	387	ALA	2.3
1	A	219	SER	2.3
1	A	147	PHE	2.3
1	A	140	ARG	2.3
1	B	375	GLY	2.3
1	C	431	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	72	PRO	2.2
1	A	409	GLY	2.2
1	A	92	GLU	2.2
1	A	5	ARG	2.2
1	A	80	TRP	2.2
1	A	99	ARG	2.2
1	A	76	LEU	2.2
1	A	102	ARG	2.2
1	A	275	ARG	2.2
1	A	239	TYR	2.2
1	A	304	PRO	2.1
1	A	433	VAL	2.1
1	A	307	THR	2.1
1	A	211	ILE	2.1
1	A	237	VAL	2.1
1	A	104	LEU	2.1
1	A	229	ASN	2.1
1	C	385	GLN	2.1
1	A	431	ALA	2.1
1	A	262	GLU	2.1
1	B	364	CYS	2.1
1	A	358	ALA	2.1
1	A	277	ASN	2.0
1	A	383	THR	2.0
1	A	13	GLU	2.0
1	A	385	GLN	2.0
1	B	5	ARG	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.