



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:06 PM UTC

PDB ID : 6Y2P / pdb_00006y2p
Title : Escherichia coli RnlA-RnlB Toxin-Antitoxin System.
Authors : Garcia-Rodriguez, G.; Talavera Perez, A.; Loris, R.
Deposited on : 2020-02-17
Resolution : 2.64 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

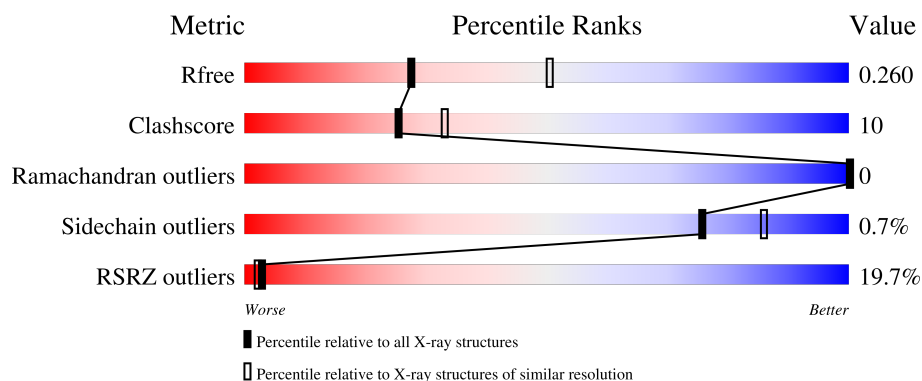
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	357	14% 74% 25% .
1	B	357	34% 78% 18% ..
2	C	134	5% 77% 13% 10%
2	D	134	7% 80% 9% 10%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7002 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 mRNA endoribonuclease toxin LS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2728	1745	466	504	13			
1	B	348	Total	C	N	O	S	0	0	0
			2468	1566	426	465	11			

- Molecule 2 is a protein called Antitoxin RnlB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	120	Total	C	N	O	S	0	0	0
			872	557	137	173	5			
2	D	120	Total	C	N	O	S	0	0	1
			907	579	147	176	5			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	124	ALA	-	expression tag	UNP P52130
C	125	ALA	-	expression tag	UNP P52130
C	126	ALA	-	expression tag	UNP P52130
C	127	LEU	-	expression tag	UNP P52130
C	128	GLU	-	expression tag	UNP P52130
C	129	HIS	-	expression tag	UNP P52130
C	130	HIS	-	expression tag	UNP P52130
C	131	HIS	-	expression tag	UNP P52130
C	132	HIS	-	expression tag	UNP P52130
C	133	HIS	-	expression tag	UNP P52130
C	134	HIS	-	expression tag	UNP P52130
D	124	ALA	-	expression tag	UNP P52130
D	125	ALA	-	expression tag	UNP P52130
D	126	ALA	-	expression tag	UNP P52130
D	127	LEU	-	expression tag	UNP P52130
D	128	GLU	-	expression tag	UNP P52130

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Chain	Residue	Modelled	Actual	Comment	Reference
D	129	HIS	-	expression tag	UNP P52130
D	130	HIS	-	expression tag	UNP P52130
D	131	HIS	-	expression tag	UNP P52130
D	132	HIS	-	expression tag	UNP P52130
D	133	HIS	-	expression tag	UNP P52130
D	134	HIS	-	expression tag	UNP P52130

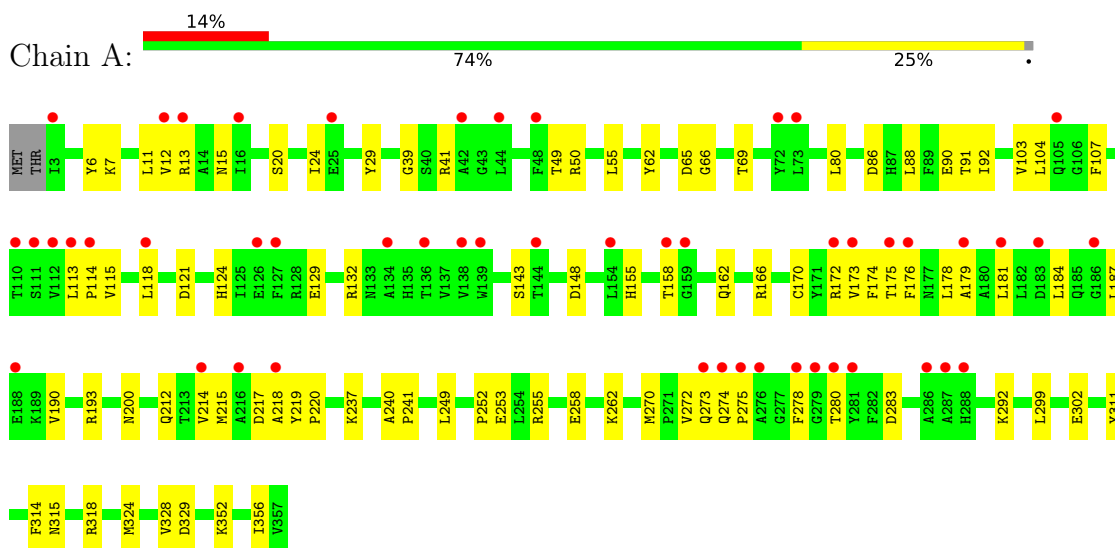
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	7	Total O 7 7	0	0
3	C	4	Total O 4 4	0	0
3	D	8	Total O 8 8	0	0

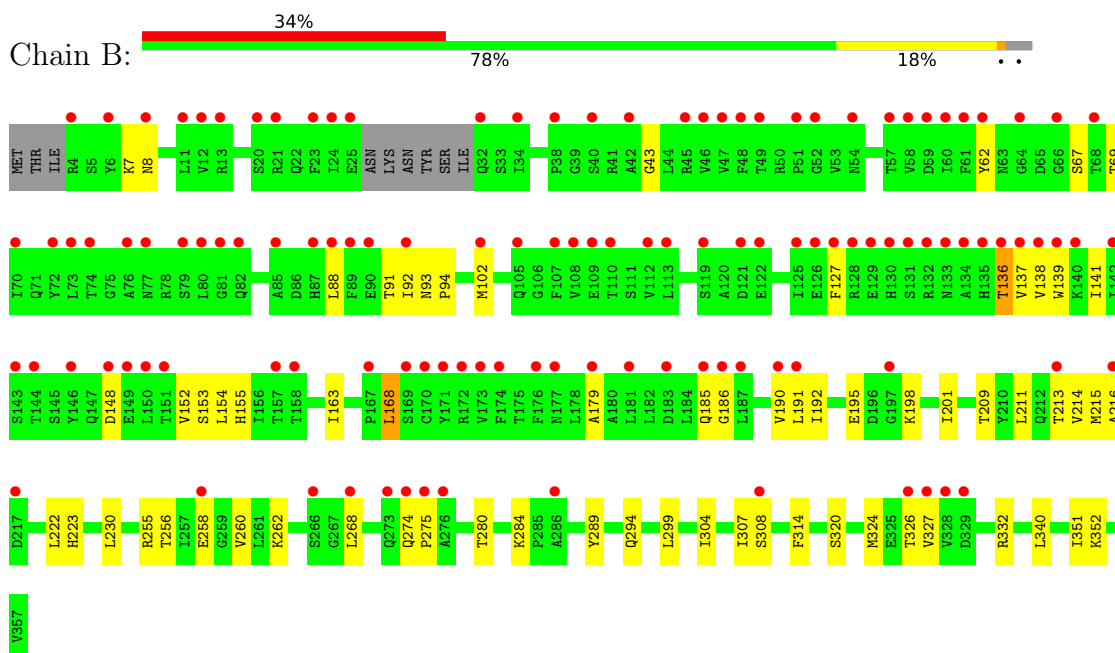
3 Residue-property plots

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.

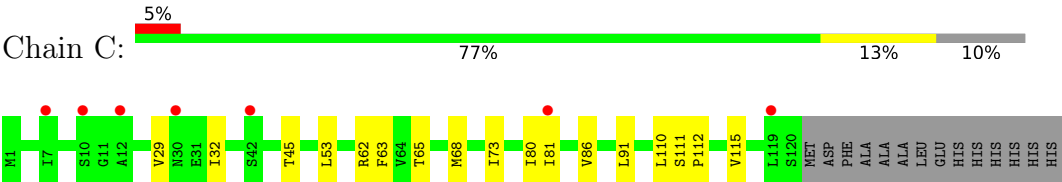
• Molecule 1: mRNA endoribonuclease toxin LS



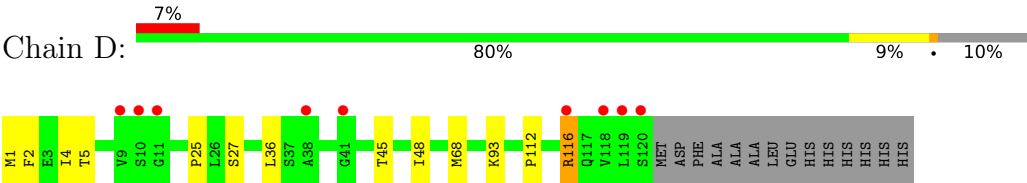
• Molecule 1: mRNA endoribonuclease toxin LS



• Molecule 2: Antitoxin RnlB



● Molecule 2: Antitoxin RnlB



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	243.32Å 133.58Å 55.64Å 90.00° 95.11° 90.00°	Depositor
Resolution (Å)	48.78 – 2.64 48.78 – 2.64	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.78-2.64) 99.3 (48.78-2.64)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.197 , 0.242 0.222 , 0.260	Depositor DCC
R_{free} test set	2584 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	76.7	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 65.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7002	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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	0.65	1/2785 (0.0%)	0.76	1/3790 (0.0%)
1	B	0.67	0/2517	0.84	3/3438 (0.1%)
2	C	0.45	0/887	0.69	0/1214
2	D	0.56	0/922	0.75	0/1256
All	All	0.62	1/7111 (0.0%)	0.78	4/9698 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	ALA	C-O	17.79	1.32	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	280	THR	CB-CA-C	-6.53	99.59	110.68
1	B	168	LEU	N-CA-C	-6.18	97.64	110.80
1	B	327	VAL	CB-CA-C	5.92	120.00	111.65
1	A	240	ALA	O-C-N	-5.36	119.06	121.53

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	2728	0	2674	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2468	0	2214	51	0
2	C	872	0	817	12	0
2	D	907	0	896	10	0
3	A	8	0	0	0	0
3	B	7	0	0	0	0
3	C	4	0	0	0	0
3	D	8	0	0	0	0
All	All	7002	0	6601	130	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 10.

All (130) 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:215:MET:HE2	1:B:222:LEU:HD21	1.62	0.82
1:A:274:GLN:N	1:A:275:PRO:HD2	1.98	0.79
1:A:273:GLN:HB3	1:A:275:PRO:HD2	1.66	0.75
1:B:7:LYS:HA	1:B:69:THR:HG23	1.68	0.74
1:B:258:GLU:HB2	1:B:314:PHE:CE1	2.23	0.73
1:A:314:PHE:O	1:A:318:ARG:HB2	1.88	0.73
1:A:129:GLU:OE2	1:A:132:ARG:HD2	1.90	0.72
1:B:258:GLU:HG3	1:B:314:PHE:CZ	2.25	0.71
1:B:138:VAL:HA	1:B:153:SER:HA	1.72	0.70
1:B:191:LEU:HB3	1:B:192:ILE:HD12	1.75	0.69
1:B:216:ALA:HB3	1:B:352:LYS:HD2	1.75	0.68
1:A:115:VAL:HG22	1:A:181:LEU:HD12	1.75	0.68
2:C:45:THR:HA	2:C:68:MET:O	1.93	0.67
2:C:29:VAL:HA	2:C:32:ILE:HD12	1.77	0.67
1:A:184:LEU:HB3	1:A:187:LEU:HD13	1.77	0.65
2:C:112:PRO:HA	2:C:115:VAL:HG12	1.80	0.64
1:A:273:GLN:NE2	2:D:27:SER:O	2.31	0.64
1:A:129:GLU:CD	1:A:132:ARG:HD2	2.22	0.63
1:B:179:ALA:HB1	1:B:185:GLN:HA	1.80	0.63
1:A:103:VAL:HG22	1:A:162:GLN:HB2	1.81	0.62
1:A:274:GLN:H	1:A:275:PRO:HD2	1.64	0.62
1:A:172:ARG:O	1:A:175:THR:HG22	1.99	0.62
1:A:175:THR:HG23	1:A:176:PHE:N	2.15	0.62
1:A:274:GLN:N	1:A:275:PRO:CD	2.62	0.62
1:A:214:VAL:HG12	1:A:215:MET:HE2	1.82	0.61
1:B:43:GLY:HA2	1:B:62:TYR:HD2	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:VAL:HG23	1:A:15:ASN:HB2	1.83	0.60
2:C:86:VAL:HG13	2:C:91:LEU:HD11	1.82	0.60
1:B:195:GLU:HG2	1:B:198:LYS:HB2	1.83	0.60
1:A:193:ARG:HE	1:B:102:MET:HE2	1.66	0.60
1:B:258:GLU:HB2	1:B:314:PHE:HE1	1.66	0.59
2:C:62:ARG:HG2	2:C:63:PHE:CD2	2.36	0.59
1:A:66:GLY:HA3	1:A:148:ASP:HB3	1.84	0.59
1:A:129:GLU:OE2	1:A:132:ARG:CD	2.51	0.58
1:A:280:THR:HG22	1:A:280:THR:O	2.04	0.58
1:A:88:LEU:O	1:A:91:THR:HB	2.03	0.57
1:A:324:MET:O	1:B:262:LYS:HE3	2.03	0.57
1:A:155:HIS:HB2	1:A:158:THR:OG1	2.05	0.57
1:B:139:TRP:N	1:B:152:VAL:O	2.25	0.56
1:B:215:MET:HE1	1:B:351:ILE:HG22	1.85	0.56
1:A:13:ARG:CZ	1:A:62:TYR:HB3	2.35	0.56
1:A:190:VAL:HG11	1:B:190:VAL:HG11	1.87	0.56
1:A:252:PRO:HG2	1:A:253:GLU:OE1	2.06	0.56
1:B:136:THR:CB	1:B:155:HIS:HA	2.36	0.55
2:C:111:SER:OG	2:C:112:PRO:HD2	2.06	0.55
2:D:2:PHE:HE2	2:D:4:ILE:HD11	1.71	0.55
1:B:138:VAL:HG23	1:B:153:SER:OG	2.07	0.55
1:A:104:LEU:HB2	1:A:107:PHE:HE2	1.70	0.55
1:A:170:CYS:HA	1:A:173:VAL:HG12	1.89	0.54
2:D:4:ILE:HD12	2:D:4:ILE:H	1.73	0.53
1:B:320:SER:HB3	1:B:332:ARG:HB3	1.90	0.53
1:A:217:ASP:O	1:A:220:PRO:HD2	2.10	0.52
1:A:237:LYS:NZ	1:A:249:LEU:O	2.40	0.52
2:D:45:THR:HA	2:D:68:MET:O	2.10	0.52
1:A:273:GLN:HA	1:A:273:GLN:OE1	2.10	0.51
1:B:148:ASP:OD2	1:B:168:LEU:CB	2.59	0.50
1:B:268:LEU:HD12	1:B:307:ILE:HD11	1.94	0.50
1:B:137:VAL:O	1:B:154:LEU:N	2.44	0.50
1:A:184:LEU:HA	1:B:186:GLY:HA3	1.94	0.50
1:B:284:LYS:HD2	1:B:289:TYR:CZ	2.47	0.49
1:A:11:LEU:HD23	1:A:92:ILE:HD11	1.95	0.49
1:A:175:THR:CG2	1:A:176:PHE:N	2.76	0.49
1:A:200:ASN:HB3	1:B:198:LYS:NZ	2.27	0.49
1:B:88:LEU:O	1:B:91:THR:HG22	2.13	0.49
2:D:112:PRO:O	2:D:116:ARG:HG2	2.12	0.49
1:B:127:PHE:HA	1:B:141:ILE:HA	1.93	0.48
1:B:289:TYR:O	1:B:308:SER:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ASP:O	1:A:90:GLU:HG3	2.14	0.48
1:A:193:ARG:NE	1:B:102:MET:HE2	2.28	0.48
1:A:49:THR:OG1	1:A:55:LEU:HA	2.14	0.47
1:A:258:GLU:HB2	1:A:314:PHE:CE1	2.49	0.47
1:B:92:ILE:HD12	1:B:93:ASN:H	1.79	0.47
1:A:7:LYS:HA	1:A:69:THR:HG23	1.97	0.47
1:A:124:HIS:O	1:A:143:SER:HA	2.15	0.47
1:A:65:ASP:HB3	1:A:166:ARG:HH11	1.80	0.46
2:D:48:ILE:HD11	2:D:68:MET:SD	2.55	0.46
1:B:258:GLU:HG3	1:B:314:PHE:HZ	1.75	0.46
2:C:112:PRO:O	2:C:115:VAL:HG12	2.16	0.46
1:A:328:VAL:HB	1:B:223:HIS:CD2	2.50	0.46
2:D:4:ILE:HD12	2:D:4:ILE:N	2.31	0.46
1:A:179:ALA:HA	1:A:184:LEU:HB2	1.99	0.45
2:C:91:LEU:HD23	2:C:91:LEU:HA	1.66	0.45
1:A:241:PRO:HB3	1:B:201:ILE:HD12	1.99	0.45
1:A:118:LEU:O	1:A:121:ASP:HB2	2.17	0.45
1:B:268:LEU:HD23	1:B:268:LEU:HA	1.81	0.45
2:C:29:VAL:HG22	2:C:73:ILE:HD12	1.98	0.45
1:B:299:LEU:HB2	1:B:304:ILE:HD11	1.99	0.45
1:A:217:ASP:N	1:A:217:ASP:OD1	2.43	0.45
1:A:129:GLU:OE1	1:A:132:ARG:HD2	2.16	0.44
2:D:5:THR:HG23	2:D:93:LYS:HG2	1.99	0.44
1:B:215:MET:O	1:B:352:LYS:HG3	2.18	0.44
1:B:137:VAL:N	1:B:154:LEU:O	2.47	0.44
1:B:8:ASN:HA	1:B:67:SER:HB3	1.99	0.44
1:A:29:TYR:CZ	1:A:80:LEU:HD11	2.52	0.44
1:A:6:TYR:OH	1:A:86:ASP:OD1	2.24	0.44
1:A:174:PHE:CZ	1:A:178:LEU:HD12	2.53	0.44
1:A:39:GLY:C	1:A:41:ARG:H	2.25	0.44
1:B:268:LEU:HD13	1:B:299:LEU:HD22	2.00	0.43
1:A:329:ASP:HB3	2:C:80:ILE:HD11	2.01	0.43
1:A:20:SER:O	1:A:24:ILE:HD12	2.17	0.43
1:A:278:PHE:HB3	1:A:311:TYR:CZ	2.53	0.43
1:A:212:GLN:HG3	1:A:219:TYR:CD2	2.53	0.43
1:A:302:GLU:H	1:A:302:GLU:CD	2.26	0.43
1:B:256:THR:O	1:B:260:VAL:HG23	2.19	0.43
2:D:36:LEU:HD23	2:D:36:LEU:HA	1.79	0.43
1:B:152:VAL:HG13	1:B:163:ILE:HG22	2.01	0.42
1:A:272:VAL:HG21	1:A:278:PHE:CE1	2.54	0.42
1:A:324:MET:HG3	1:B:255:ARG:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:53:LEU:HD21	2:C:110:LEU:HD11	2.00	0.42
1:A:262:LYS:HG3	1:A:278:PHE:HZ	1.84	0.42
1:A:218:ALA:CB	1:A:352:LYS:HG3	2.50	0.42
2:C:65:THR:HG21	2:C:81:ILE:HD11	2.00	0.42
1:A:24:ILE:HG23	1:A:29:TYR:HB2	2.02	0.42
1:A:49:THR:HG22	1:A:50:ARG:O	2.19	0.42
1:A:113:LEU:N	1:A:114:PRO:HD2	2.35	0.42
1:A:283:ASP:OD1	1:A:292:LYS:NZ	2.53	0.42
1:B:211:LEU:HA	1:B:214:VAL:HG12	2.01	0.41
1:A:12:VAL:HG23	1:A:12:VAL:O	2.20	0.41
1:B:230:LEU:HD23	1:B:230:LEU:HA	1.73	0.41
1:A:270:MET:HE1	1:A:299:LEU:HD11	2.03	0.41
1:B:209:THR:O	1:B:213:THR:HG23	2.20	0.41
1:A:352:LYS:O	1:A:356:ILE:HB	2.20	0.41
1:B:268:LEU:HD13	1:B:299:LEU:CD2	2.50	0.41
2:D:1:MET:CE	2:D:25:PRO:HA	2.51	0.41
1:A:274:GLN:H	1:A:275:PRO:CD	2.30	0.40
1:A:255:ARG:HG2	1:B:324:MET:HG3	2.02	0.40
1:B:93:ASN:HA	1:B:94:PRO:HD3	1.93	0.40
1:B:340:LEU:HD13	1:B:340:LEU:C	2.47	0.40
1:A:193:ARG:HE	1:B:102:MET:CE	2.31	0.40
1:B:274:GLN:N	1:B:275:PRO:CD	2.84	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	353/357 (99%)	336 (95%)	17 (5%)	0	100	100
1	B	344/357 (96%)	320 (93%)	24 (7%)	0	100	100
2	C	118/134 (88%)	114 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	118/134 (88%)	115 (98%)	3 (2%)	0	100	100
All	All	933/982 (95%)	885 (95%)	48 (5%)	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	286/309 (93%)	285 (100%)	1 (0%)	86	93
1	B	217/309 (70%)	214 (99%)	3 (1%)	59	75
2	C	88/117 (75%)	88 (100%)	0	100	100
2	D	98/117 (84%)	97 (99%)	1 (1%)	68	80
All	All	689/852 (81%)	684 (99%)	5 (1%)	76	86

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
1	B	136	THR
1	B	294	GLN
1	B	326	THR
2	D	116	ARG

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	8	ASN
1	A	63	ASN
1	A	194	GLN
1	A	200	ASN
1	B	164	GLN
1	B	315	ASN

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Mol	Chain	Res	Type
1	B	319	HIS
2	C	8	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 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	355/357 (99%)	0.84	50 (14%) 6 5	47, 90, 152, 188	0
1	B	348/357 (97%)	1.45	120 (34%) 1 0	42, 101, 197, 235	0
2	C	120/134 (89%)	0.60	7 (5%) 29 24	56, 94, 141, 170	0
2	D	120/134 (89%)	0.50	9 (7%) 20 16	47, 73, 116, 143	0
All	All	943/982 (96%)	0.99	186 (19%) 3 2	42, 89, 175, 235	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	120	SER	9.5
1	A	274	GLN	8.2
1	B	62	TYR	7.5
1	A	3	ILE	7.3
1	B	273	GLN	6.1
1	B	138	VAL	5.7
1	B	54	ASN	5.5
1	A	280	THR	5.3
1	B	122	GLU	5.3
1	B	24	ILE	5.2
1	A	218	ALA	5.1
1	B	183	ASP	5.0
1	B	136	THR	5.0
1	B	173	VAL	5.0
1	B	89	PHE	4.9
1	B	51	PRO	4.9
1	B	185	GLN	4.8
1	B	40	SER	4.8
1	B	72	TYR	4.7
1	B	137	VAL	4.5
1	A	273	GLN	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	279	GLY	4.4
1	B	34	ILE	4.4
1	A	25	GLU	4.3
2	C	42	SER	4.3
1	A	287	ALA	4.2
1	B	12	VAL	4.2
1	A	186	GLY	4.2
1	B	171	TYR	4.1
1	B	48	PHE	4.1
1	A	134	ALA	4.1
1	B	92	ILE	4.1
1	B	327	VAL	4.1
1	B	216	ALA	4.1
1	B	25	GLU	4.0
1	A	176	PHE	4.0
1	A	278	PHE	4.0
1	B	170	CYS	4.0
1	B	130	HIS	3.8
1	B	190	VAL	3.8
1	B	32	GLN	3.8
1	B	57	THR	3.7
1	B	74	THR	3.7
1	A	281	TYR	3.7
1	A	276	ALA	3.7
1	B	85	ALA	3.7
1	B	127	PHE	3.6
1	B	60	ILE	3.6
1	A	112	VAL	3.6
1	B	258	GLU	3.6
1	B	135	HIS	3.5
1	B	125	ILE	3.5
1	A	175	THR	3.5
1	A	216	ALA	3.5
1	B	274	GLN	3.5
1	A	172	ARG	3.5
1	B	151	THR	3.5
1	B	80	LEU	3.5
1	B	23	PHE	3.5
1	B	108	VAL	3.5
1	B	132	ARG	3.5
1	B	11	LEU	3.4
1	B	76	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	139	TRP	3.4
1	B	77	ASN	3.4
1	B	174	PHE	3.4
1	B	142	ILE	3.3
1	A	275	PRO	3.3
1	A	286	ALA	3.3
1	B	329	ASP	3.3
1	B	275	PRO	3.3
1	B	61	PHE	3.3
1	B	197	GLY	3.2
1	B	121	ASP	3.2
1	B	42	ALA	3.2
1	B	87	HIS	3.2
1	A	158	THR	3.2
1	B	158	THR	3.1
2	D	38	ALA	3.1
1	B	150	LEU	3.1
1	B	105	GLN	3.1
1	A	110	THR	3.1
1	B	68	THR	3.1
1	B	52	GLY	3.1
2	C	10	SER	3.1
1	A	139	TRP	3.1
1	B	46	VAL	3.1
1	A	113	LEU	3.0
1	A	105	GLN	3.0
2	D	10	SER	2.9
1	B	133	ASN	2.9
1	B	73	LEU	2.9
1	B	146	TYR	2.9
1	B	191	LEU	2.9
1	B	109	GLU	2.9
1	B	126	GLU	2.9
1	A	111	SER	2.9
1	B	66	GLY	2.9
1	B	134	ALA	2.9
1	B	79	SER	2.8
1	B	131	SER	2.8
1	B	38	PRO	2.8
2	D	11	GLY	2.8
1	B	326	THR	2.8
1	A	183	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	167	PRO	2.8
1	B	172	ARG	2.8
1	B	176	PHE	2.8
1	A	44	LEU	2.7
1	B	90	GLU	2.7
1	B	20	SER	2.7
1	B	112	VAL	2.7
1	B	328	VAL	2.7
1	B	82	GLN	2.7
1	A	288	HIS	2.7
1	B	217	ASP	2.7
1	A	12	VAL	2.6
1	B	157	THR	2.6
1	A	126	GLU	2.6
2	D	119	LEU	2.6
1	A	114	PRO	2.6
1	B	47	VAL	2.5
1	A	144	THR	2.5
1	B	268	LEU	2.5
1	A	136	THR	2.5
1	B	119	SER	2.5
1	B	187	LEU	2.5
1	B	286	ALA	2.5
1	B	144	THR	2.5
1	A	138	VAL	2.4
1	B	140	LYS	2.4
1	A	42	ALA	2.4
1	A	118	LEU	2.4
2	C	119	LEU	2.4
1	B	59	ASP	2.4
1	B	179	ALA	2.4
1	A	214	VAL	2.4
1	B	4	ARG	2.4
1	B	88	LEU	2.4
1	B	129	GLU	2.4
1	A	154	LEU	2.3
1	B	177	ASN	2.3
1	B	13	ARG	2.3
1	B	58	VAL	2.3
2	D	41	GLY	2.3
1	B	181	LEU	2.3
1	B	149	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	116	ARG	2.3
1	B	64	GLY	2.3
1	B	110	THR	2.3
1	B	8	ASN	2.3
1	A	127	PHE	2.3
1	B	49	THR	2.2
2	C	30	ASN	2.2
1	B	266	SER	2.2
1	A	73	LEU	2.2
2	C	81	ILE	2.2
1	B	186	GLY	2.2
2	C	12	ALA	2.2
1	A	181	LEU	2.2
1	A	179	ALA	2.2
1	B	213	THR	2.2
2	D	118	VAL	2.2
1	B	81	GLY	2.1
1	A	16	ILE	2.1
1	B	21	ARG	2.1
1	A	72	TYR	2.1
1	B	113	LEU	2.1
1	B	308	SER	2.1
1	A	188	GLU	2.1
1	B	45	ARG	2.1
2	D	9	VAL	2.1
1	B	107	PHE	2.1
1	A	13	ARG	2.1
1	B	102	MET	2.1
1	B	70	ILE	2.1
1	A	48	PHE	2.1
1	B	148	ASP	2.0
1	A	159	GLY	2.0
2	C	7	ILE	2.0
1	B	6	TYR	2.0
1	B	128	ARG	2.0
1	B	276	ALA	2.0
1	B	143	SER	2.0
1	B	169	SER	2.0
1	A	173	VAL	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.