



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:03 PM UTC

PDB ID : 3TJ1 / pdb_00003tj1
Title : Crystal Structure of RNA Polymerase I Transcription Initiation Factor Rrn3
Authors : Blattner, C.; Jennebach, S.; Herzog, F.; Mayer, A.; Cheung, A.C.M.; Witte, G.; Lorenzen, K.; Hopfner, K.-P.; Heck, A.J.R.; Aebersold, R.; Cramer, P.
Deposited on : 2011-08-23
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

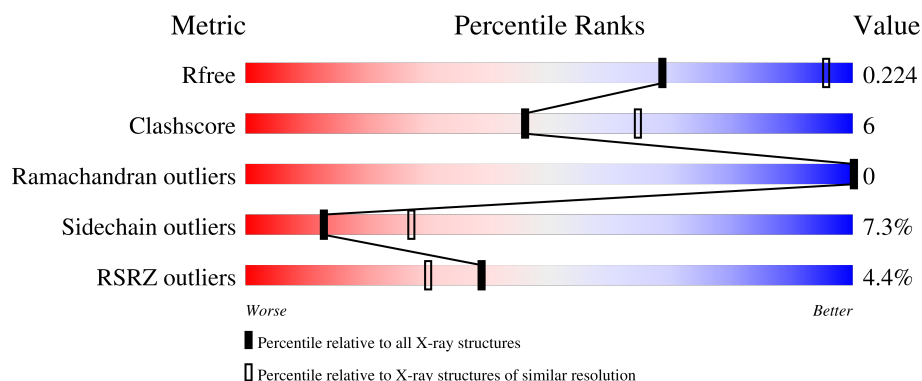
1 Overall quality at a glance

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	649	
1	B	649	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8075 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 RNA polymerase I-specific transcription initiation factor RRN3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	0
			3988	2583	654	730	21			
1	B	482	Total	C	N	O	S	0	0	0
			3984	2581	653	729	21			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP P36070
A	-20	GLY	-	expression tag	UNP P36070
A	-19	SER	-	expression tag	UNP P36070
A	-18	SER	-	expression tag	UNP P36070
A	-17	HIS	-	expression tag	UNP P36070
A	-16	HIS	-	expression tag	UNP P36070
A	-15	HIS	-	expression tag	UNP P36070
A	-14	HIS	-	expression tag	UNP P36070
A	-13	HIS	-	expression tag	UNP P36070
A	-12	HIS	-	expression tag	UNP P36070
A	-11	SER	-	expression tag	UNP P36070
A	-10	SER	-	expression tag	UNP P36070
A	-9	GLY	-	expression tag	UNP P36070
A	-8	LEU	-	expression tag	UNP P36070
A	-7	VAL	-	expression tag	UNP P36070
A	-6	PRO	-	expression tag	UNP P36070
A	-5	ARG	-	expression tag	UNP P36070
A	-4	GLY	-	expression tag	UNP P36070
A	-3	SER	-	expression tag	UNP P36070
A	-2	HIS	-	expression tag	UNP P36070
A	-1	MET	-	expression tag	UNP P36070
A	0	ALA	-	expression tag	UNP P36070
B	-21	MET	-	expression tag	UNP P36070
B	-20	GLY	-	expression tag	UNP P36070
B	-19	SER	-	expression tag	UNP P36070

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	SER	-	expression tag	UNP P36070
B	-17	HIS	-	expression tag	UNP P36070
B	-16	HIS	-	expression tag	UNP P36070
B	-15	HIS	-	expression tag	UNP P36070
B	-14	HIS	-	expression tag	UNP P36070
B	-13	HIS	-	expression tag	UNP P36070
B	-12	HIS	-	expression tag	UNP P36070
B	-11	SER	-	expression tag	UNP P36070
B	-10	SER	-	expression tag	UNP P36070
B	-9	GLY	-	expression tag	UNP P36070
B	-8	LEU	-	expression tag	UNP P36070
B	-7	VAL	-	expression tag	UNP P36070
B	-6	PRO	-	expression tag	UNP P36070
B	-5	ARG	-	expression tag	UNP P36070
B	-4	GLY	-	expression tag	UNP P36070
B	-3	SER	-	expression tag	UNP P36070
B	-2	HIS	-	expression tag	UNP P36070
B	-1	MET	-	expression tag	UNP P36070
B	0	ALA	-	expression tag	UNP P36070

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	60	Total O 60 60	0	0
2	B	43	Total O 43 43	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.77Å 101.77Å 162.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.55 – 2.85 48.55 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.55-2.85) 99.9 (48.55-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.99 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.208 , 0.242 (Not available) , 0.224	Depositor DCC
R_{free} test set	1900 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	1.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8075	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1769e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.89	4/4078 (0.1%)	1.48	33/5511 (0.6%)
1	B	0.87	3/4074 (0.1%)	1.45	25/5506 (0.5%)
All	All	0.88	7/8152 (0.1%)	1.47	58/11017 (0.5%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	396	MET	SD-CE	-7.40	1.61	1.79
1	A	509	MET	SD-CE	-6.67	1.62	1.79
1	B	525	MET	SD-CE	-6.48	1.63	1.79
1	B	509	MET	SD-CE	-6.00	1.64	1.79
1	A	525	MET	SD-CE	-5.28	1.66	1.79
1	A	324	GLY	C-N	5.12	1.40	1.34
1	B	385	MET	SD-CE	-5.05	1.67	1.79

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	600	LYS	N-CA-C	8.78	120.62	111.14
1	B	600	LYS	N-CA-C	7.05	118.75	111.14
1	A	324	GLY	N-CA-C	-6.65	106.60	115.32
1	B	61	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	61	ASP	CA-CB-CG	6.40	119.00	112.60
1	A	607	LYS	CA-C-N	6.36	129.43	120.28
1	A	607	LYS	C-N-CA	6.36	129.43	120.28
1	B	607	LYS	CA-C-N	6.33	129.39	120.28
1	B	607	LYS	C-N-CA	6.33	129.39	120.28
1	A	596	PRO	N-CA-C	6.06	120.74	111.11
1	A	324	GLY	CA-C-N	5.98	130.43	120.62
1	A	324	GLY	C-N-CA	5.98	130.43	120.62
1	B	596	PRO	N-CA-C	5.92	120.50	111.15
1	A	348	THR	CB-CA-C	5.90	117.75	108.84
1	B	348	THR	CB-CA-C	5.86	117.69	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	ILE	CA-C-N	5.82	128.08	120.28
1	A	428	ILE	C-N-CA	5.82	128.08	120.28
1	A	457	ARG	N-CA-C	5.80	122.19	114.12
1	B	457	ARG	N-CA-C	5.72	122.07	114.12
1	B	428	ILE	CA-C-N	5.67	127.81	120.44
1	B	428	ILE	C-N-CA	5.67	127.81	120.44
1	A	519	PHE	N-CA-C	5.66	120.35	113.38
1	B	201	LYS	CA-C-N	5.66	128.43	120.28
1	B	201	LYS	C-N-CA	5.66	128.43	120.28
1	A	350	GLU	CA-C-N	5.63	128.39	120.28
1	A	350	GLU	C-N-CA	5.63	128.39	120.28
1	A	581	THR	CA-C-N	5.63	127.76	120.44
1	A	581	THR	C-N-CA	5.63	127.76	120.44
1	B	410	VAL	N-CA-C	5.59	116.32	110.62
1	A	510	VAL	N-CA-CB	-5.54	103.54	110.47
1	A	454	VAL	N-CA-CB	5.51	117.63	110.57
1	A	493	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	493	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	515	ASN	CA-CB-CG	5.44	118.04	112.60
1	A	541	PHE	N-CA-C	5.42	118.69	111.75
1	A	430	ARG	N-CA-C	5.40	119.96	112.45
1	B	515	ASN	CA-CB-CG	5.38	117.98	112.60
1	B	578	SER	CA-C-N	5.35	128.19	120.38
1	B	578	SER	C-N-CA	5.35	128.19	120.38
1	A	410	VAL	N-CA-C	5.34	116.12	110.72
1	A	61	ASP	CA-C-N	5.32	127.41	120.28
1	A	61	ASP	C-N-CA	5.32	127.41	120.28
1	B	225	LEU	CA-C-N	5.32	125.98	120.03
1	B	225	LEU	C-N-CA	5.32	125.98	120.03
1	A	536	SER	CA-C-N	5.24	128.24	120.74
1	A	536	SER	C-N-CA	5.24	128.24	120.74
1	A	201	LYS	N-CA-C	-5.21	105.49	111.07
1	A	437	THR	CB-CA-C	5.21	119.44	110.79
1	B	541	PHE	N-CA-C	5.21	118.42	111.75
1	B	437	THR	CB-CA-C	5.18	119.39	110.79
1	A	250	GLU	CB-CG-CD	5.16	121.36	112.60
1	B	536	SER	CA-C-N	5.14	128.09	120.74
1	B	536	SER	C-N-CA	5.14	128.09	120.74
1	B	430	ARG	N-CA-C	5.11	119.64	113.41
1	A	610	TYR	N-CA-C	5.09	117.78	109.59
1	A	601	ASN	N-CA-C	5.05	116.59	111.14
1	B	69	THR	CA-C-N	5.03	127.02	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	THR	C-N-CA	5.03	127.02	120.28

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	3988	0	3983	47	0
1	B	3984	0	3980	45	0
2	A	60	0	0	9	0
2	B	43	0	0	1	0
All	All	8075	0	7963	92	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 6.

All (92) 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:A:481:CYS:HA	2:A:670:HOH:O	1.54	1.06
1:A:480:LEU:HD22	2:A:669:HOH:O	1.60	1.00
1:B:390:GLN:HG2	1:B:396:MET:HE3	1.52	0.91
1:A:347:VAL:HG11	1:A:388:VAL:HG23	1.64	0.80
1:A:450:LEU:HD12	2:A:669:HOH:O	1.81	0.79
1:B:477:PHE:HE2	1:B:525:MET:HE1	1.52	0.74
1:A:477:PHE:HE2	1:A:525:MET:HE1	1.51	0.74
1:A:390:GLN:HG2	1:A:396:MET:HE3	1.70	0.74
1:A:400:LEU:HD21	1:A:428:ILE:HD11	1.72	0.70
1:B:400:LEU:HD21	1:B:428:ILE:HD11	1.73	0.69
1:A:517:LEU:HD23	1:A:525:MET:HE3	1.77	0.67
1:A:477:PHE:CE2	1:A:525:MET:HE1	2.29	0.66
1:A:208:LEU:O	1:A:212:THR:HG23	1.95	0.66
1:A:387:HIS:HB2	1:A:606:MET:HE1	1.78	0.65
1:B:517:LEU:HD23	1:B:525:MET:HE3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:PHE:CE2	1:B:525:MET:HE1	2.31	0.65
1:B:387:HIS:HB2	1:B:606:MET:HE1	1.79	0.64
1:B:141:LYS:HG3	1:B:175:MET:HE1	1.78	0.64
1:A:141:LYS:HG3	1:A:175:MET:HE1	1.79	0.63
1:A:449:TRP:HA	2:A:677:HOH:O	1.99	0.62
1:A:343:VAL:O	1:A:347:VAL:HG12	2.00	0.62
1:A:400:LEU:CD2	1:A:428:ILE:HD11	2.29	0.62
1:B:400:LEU:CD2	1:B:428:ILE:HD11	2.30	0.62
1:B:378:THR:OG1	1:B:382:GLN:OE1	2.18	0.61
1:A:396:MET:HE1	1:A:433:LYS:C	2.26	0.61
1:B:373:LEU:HB3	1:B:374:PRO:HD3	1.83	0.60
1:A:165:PRO:HD3	1:A:206:ARG:HH12	1.66	0.59
1:B:208:LEU:O	1:B:212:THR:HG23	2.03	0.58
1:A:348:THR:HG22	1:A:351:SER:H	1.68	0.57
1:B:376:TYR:CZ	1:B:591:TYR:HD2	2.25	0.55
1:B:390:GLN:NE2	1:B:433:LYS:H	2.05	0.55
1:B:348:THR:HG22	1:B:351:SER:H	1.72	0.55
1:B:376:TYR:CZ	1:B:591:TYR:CD2	2.94	0.54
1:B:461:VAL:HG13	1:B:467:MET:HE1	1.91	0.52
1:A:521:ASN:HD22	1:A:524:VAL:H	1.56	0.52
1:B:521:ASN:HD22	1:B:524:VAL:H	1.56	0.52
1:A:484:PHE:HB3	2:A:670:HOH:O	2.10	0.52
1:A:377:TYR:HA	1:A:591:TYR:CE1	2.45	0.52
1:A:184:PRO:HA	2:A:683:HOH:O	2.10	0.51
1:B:390:GLN:HE21	1:B:433:LYS:H	1.58	0.51
1:B:217:LYS:NZ	2:B:665:HOH:O	2.43	0.50
1:B:451:ASN:O	1:B:454:VAL:HG12	2.11	0.50
1:A:383:TYR:HB3	1:A:606:MET:HE3	1.94	0.50
1:B:370:THR:OG1	1:B:371:HIS:HD2	1.94	0.50
1:A:370:THR:OG1	1:A:371:HIS:HD2	1.95	0.50
1:B:47:PHE:HA	1:B:51:MET:HE2	1.93	0.49
1:A:386:PHE:HB2	1:A:594:TYR:CE2	2.48	0.49
1:B:515:ASN:HD21	1:B:547:ASN:HD21	1.61	0.48
1:A:515:ASN:HD21	1:A:547:ASN:HD21	1.62	0.48
1:A:359:GLY:O	1:A:363:THR:HG23	2.13	0.48
1:A:372:VAL:HG13	1:A:381:ILE:HG23	1.96	0.48
1:B:355:GLY:C	1:B:357:GLY:H	2.22	0.47
1:B:386:PHE:HB2	1:B:594:TYR:CE2	2.49	0.47
1:B:400:LEU:HD21	1:B:428:ILE:CD1	2.43	0.46
1:B:392:GLN:HB2	1:B:395:LEU:HD22	1.96	0.46
1:B:356:GLU:H	1:B:356:GLU:HG3	1.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:MET:HG3	2:A:683:HOH:O	2.15	0.45
1:A:348:THR:H	1:A:351:SER:HB3	1.81	0.45
1:A:51:MET:SD	1:A:54:ARG:NH2	2.89	0.45
1:A:394:GLU:H	1:A:394:GLU:CD	2.25	0.45
1:B:467:MET:HG3	1:B:519:PHE:CZ	2.52	0.44
1:A:390:GLN:NE2	1:A:433:LYS:H	2.15	0.44
1:A:452:ARG:NE	2:A:677:HOH:O	2.50	0.44
1:B:383:TYR:HB3	1:B:606:MET:HE3	1.98	0.44
1:A:191:ASP:HA	1:A:194:LEU:HD22	2.00	0.43
1:A:392:GLN:HB2	1:A:395:LEU:HD22	2.00	0.43
1:B:597:LEU:HD21	1:B:602:TYR:CD1	2.53	0.43
1:A:400:LEU:HD21	1:A:428:ILE:CD1	2.42	0.43
1:A:450:LEU:HB3	1:A:509:MET:HE2	1.99	0.43
1:B:238:ILE:HG12	1:B:381:ILE:HG21	2.00	0.43
1:B:347:VAL:HG13	1:B:352:LEU:HD11	2.01	0.43
1:B:191:ASP:HA	1:B:194:LEU:HD22	2.01	0.43
1:B:70:GLN:HA	1:B:73:ILE:HD12	2.00	0.42
1:A:364:LEU:C	1:A:385:MET:HE3	2.43	0.42
1:B:236:LYS:O	1:B:240:ILE:HG12	2.19	0.42
1:B:396:MET:HB2	1:B:438:GLN:HE22	1.85	0.42
1:B:359:GLY:O	1:B:363:THR:HG23	2.20	0.42
1:B:158:LEU:HD11	1:B:175:MET:HG2	2.02	0.42
1:B:234:ILE:HD12	1:B:381:ILE:HD11	2.02	0.42
1:B:453:TYR:CE2	1:B:473:PHE:HB2	2.55	0.42
1:A:453:TYR:CE2	1:A:473:PHE:HB2	2.55	0.41
1:B:364:LEU:C	1:B:385:MET:HE3	2.45	0.41
1:B:158:LEU:HD22	1:B:172:HIS:HA	2.02	0.41
1:B:499:GLU:O	1:B:502:LEU:HG	2.20	0.41
1:A:105:ASN:O	1:A:108:GLU:HB2	2.20	0.41
1:A:158:LEU:HD22	1:A:172:HIS:HA	2.03	0.41
1:A:177:LYS:HG2	1:A:181:ARG:HH22	1.86	0.41
1:A:238:ILE:HG12	1:A:381:ILE:HG21	2.03	0.41
1:A:403:LEU:HB3	2:A:672:HOH:O	2.20	0.41
1:B:66:ASN:OD1	1:B:111:ARG:NH1	2.53	0.41
1:A:158:LEU:HD11	1:A:175:MET:HG2	2.03	0.40
1:A:467:MET:HG3	1:A:519:PHE:CZ	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	477/649 (74%)	453 (95%)	24 (5%)	0	100	100
1	B	476/649 (73%)	453 (95%)	23 (5%)	0	100	100
All	All	953/1298 (73%)	906 (95%)	47 (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	449/594 (76%)	414 (92%)	35 (8%)	11	25
1	B	337/594 (57%)	315 (94%)	22 (6%)	15	32
All	All	786/1188 (66%)	729 (93%)	57 (7%)	13	27

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	VAL
1	A	51	MET
1	A	58	SER
1	A	63	LEU
1	A	78	VAL
1	A	80	LEU
1	A	83	LYS
1	A	141	LYS

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Mol	Chain	Res	Type
1	A	185	SER
1	A	194	LEU
1	A	203	ASP
1	A	204	THR
1	A	205	ARG
1	A	215	LEU
1	A	249	ASP
1	A	250	GLU
1	A	251	LEU
1	A	252	ASP
1	A	323	GLN
1	A	348	THR
1	A	356	GLU
1	A	395	LEU
1	A	410	VAL
1	A	437	THR
1	A	448	SER
1	A	454	VAL
1	A	468	GLU
1	A	490	ILE
1	A	508	ARG
1	A	510	VAL
1	A	526	LEU
1	A	550	GLU
1	A	584	GLN
1	A	599	LEU
1	A	607	LYS
1	B	46	VAL
1	B	58	SER
1	B	63	LEU
1	B	69	THR
1	B	78	VAL
1	B	80	LEU
1	B	86	GLU
1	B	141	LYS
1	B	194	LEU
1	B	203	ASP
1	B	205	ARG
1	B	323	GLN
1	B	437	THR
1	B	448	SER
1	B	468	GLU

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Mol	Chain	Res	Type
1	B	490	ILE
1	B	510	VAL
1	B	526	LEU
1	B	584	GLN
1	B	599	LEU
1	B	600	LYS
1	B	607	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	89	ASN
1	A	92	ASN
1	A	210	ASN
1	A	245	GLN
1	A	371	HIS
1	A	390	GLN
1	A	521	ASN
1	A	547	ASN
1	A	549	ASN
1	B	92	ASN
1	B	103	ASN
1	B	105	ASN
1	B	210	ASN
1	B	346	GLN
1	B	390	GLN
1	B	521	ASN
1	B	547	ASN
1	B	548	ASN
1	B	549	ASN

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	483/649 (74%)	0.29	27 (5%) 30 22	32, 58, 103, 122	0
1	B	482/649 (74%)	0.07	15 (3%) 51 43	32, 60, 98, 118	0
All	All	965/1298 (74%)	0.18	42 (4%) 39 30	32, 59, 100, 122	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	46	VAL	5.5
1	A	579	LEU	5.2
1	A	322	THR	5.2
1	B	46	VAL	4.8
1	A	324	GLY	4.7
1	A	375	THR	4.2
1	A	617	SER	3.6
1	B	575	SER	3.5
1	B	322	THR	3.4
1	A	576	SER	3.1
1	B	578	SER	3.0
1	B	576	SER	2.9
1	A	252	ASP	2.9
1	B	598	PHE	2.7
1	A	552	LEU	2.7
1	A	327	GLU	2.7
1	A	51	MET	2.6
1	A	578	SER	2.6
1	A	325	ILE	2.5
1	B	252	ASP	2.5
1	B	182	MET	2.4
1	A	356	GLU	2.4
1	A	65	LYS	2.4
1	B	326	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	329	SER	2.3
1	A	379	ARG	2.3
1	B	251	LEU	2.3
1	A	464	ARG	2.3
1	A	598	PHE	2.3
1	A	251	LEU	2.3
1	A	354	SER	2.3
1	A	201	LYS	2.2
1	B	494	THR	2.2
1	A	410	VAL	2.1
1	A	575	SER	2.1
1	B	111	ARG	2.1
1	B	325	ILE	2.1
1	A	47	PHE	2.1
1	A	206	ARG	2.1
1	B	356	GLU	2.1
1	B	579	LEU	2.1
1	A	323	GLN	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.