



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2ZNL / pdb_00002znl
Title : Crystal structure of PA-PB1 complex form influenza virus RNA polymerase
Authors : Obayashi, E.; Yoshida, H.; Kawai, F.; Shibayama, N.; Kawaguchi, A.; Nagata, K.; Tame, J.R.H.; Park, S.-Y.
Deposited on : 2008-04-28
Resolution : 2.30 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

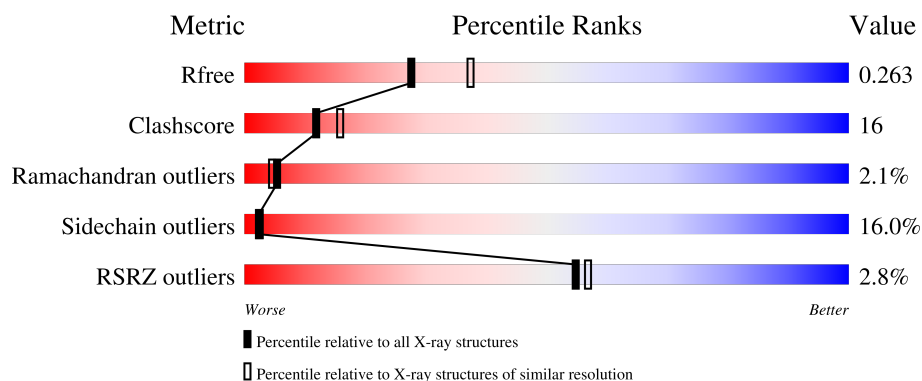
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	478	2% 48% 29% 9% 12%
2	B	81	% 6% 10% 81%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3569 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3382	2157	571	629	25			

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	15	Total	C	N	O	S	0	0	0
			117	78	18	20	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total	O	0	0
			70	70		

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.96Å 101.96Å 115.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.30) 98.2 (20.00-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.262 0.206 , 0.263	Depositor DCC
R_{free} test set	1545 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3569	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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	1.74	41/3456 (1.2%)	1.65	54/4661 (1.2%)
2	B	1.98	3/119 (2.5%)	1.75	1/162 (0.6%)
All	All	1.75	44/3575 (1.2%)	1.65	55/4823 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	1
All	All	0	3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	615	LYS	N-CA	11.34	1.60	1.46
1	A	647	ASN	N-CA	-9.12	1.33	1.46
1	A	647	ASN	CB-CG	-8.25	1.31	1.52
1	A	458	TYR	C-O	-7.76	1.15	1.24
1	A	287	ALA	CA-CB	-7.61	1.41	1.53
1	A	466	ASN	N-CA	-7.05	1.38	1.46
1	A	671	ALA	CA-CB	-7.03	1.42	1.53
1	A	696	ASN	CB-CG	-6.84	1.34	1.52
1	A	258	GLU	CA-C	6.61	1.61	1.52
1	A	408	GLN	CD-OE1	6.46	1.35	1.23
1	A	647	ASN	CA-C	6.25	1.61	1.52
1	A	643	LYS	CA-C	6.19	1.60	1.52
1	A	452	HIS	C-O	-6.13	1.15	1.24
1	A	285	MET	C-O	-6.08	1.16	1.24
1	A	700	VAL	C-O	-6.07	1.17	1.24
2	B	3	VAL	CA-C	5.89	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	283	LEU	C-O	5.85	1.31	1.23
1	A	614	ASN	CA-C	-5.85	1.45	1.52
1	A	705	SER	CB-OG	-5.84	1.30	1.42
2	B	11	LYS	C-O	-5.84	1.14	1.23
1	A	621	ILE	CA-CB	-5.63	1.46	1.54
1	A	463	VAL	C-O	-5.57	1.17	1.24
1	A	573	ILE	N-CA	-5.48	1.39	1.46
2	B	12	VAL	N-CA	-5.48	1.41	1.46
1	A	644	SER	N-CA	-5.40	1.39	1.46
1	A	620	PRO	C-O	5.37	1.29	1.23
1	A	668	ILE	CA-C	5.37	1.59	1.52
1	A	537	TRP	N-CA	5.34	1.52	1.46
1	A	316	GLY	C-O	-5.31	1.19	1.24
1	A	587	GLN	C-O	-5.31	1.18	1.24
1	A	443	ARG	C-O	-5.26	1.18	1.24
1	A	695	ILE	CA-CB	5.26	1.60	1.55
1	A	369	ALA	CA-CB	-5.25	1.44	1.53
1	A	467	THR	N-CA	-5.25	1.39	1.46
1	A	294	ASP	CG-OD2	5.23	1.35	1.25
1	A	454	ARG	C-O	-5.21	1.18	1.24
1	A	668	ILE	CA-CB	5.20	1.60	1.54
1	A	702	LEU	N-CA	5.20	1.52	1.46
1	A	632	SER	CB-OG	5.17	1.52	1.42
1	A	638	ARG	CG-CD	5.12	1.67	1.52
1	A	450	VAL	CB-CG2	5.11	1.69	1.52
1	A	427	GLU	CA-C	-5.09	1.46	1.52
1	A	654	GLN	CG-CD	5.01	1.64	1.52
1	A	274	PRO	CA-C	5.01	1.55	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	614	ASN	CA-C-N	-12.20	98.24	121.54
1	A	614	ASN	C-N-CA	-12.20	98.24	121.54
1	A	647	ASN	CB-CA-C	9.84	128.60	109.72
1	A	646	PHE	CA-C-N	-9.22	104.91	122.06
1	A	646	PHE	C-N-CA	-9.22	104.91	122.06
1	A	614	ASN	O-C-N	-8.44	113.37	123.16
1	A	614	ASN	N-CA-C	-8.43	95.80	109.96
1	A	319	GLU	CA-C-N	8.10	128.16	119.90
1	A	319	GLU	C-N-CA	8.10	128.16	119.90
1	A	448	SER	N-CA-C	-7.94	102.85	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	695	ILE	CB-CA-C	-7.86	103.97	111.44
1	A	292	ILE	CB-CA-C	-7.79	98.51	110.50
1	A	294	ASP	CA-C-N	-7.73	111.48	119.83
1	A	294	ASP	C-N-CA	-7.73	111.48	119.83
1	A	301	GLY	N-CA-C	-7.48	104.52	114.25
1	A	685	GLY	N-CA-C	-7.44	95.54	113.18
1	A	628	VAL	N-CA-C	7.44	118.70	108.89
1	A	331	ASN	CA-C-N	-7.43	112.02	120.04
1	A	331	ASN	C-N-CA	-7.43	112.02	120.04
1	A	404	ALA	N-CA-C	-7.20	97.69	108.99
1	A	405	SER	N-CA-C	7.13	121.08	112.38
1	A	291	SER	N-CA-C	6.82	119.29	109.14
1	A	668	ILE	CB-CA-C	6.53	120.33	111.97
1	A	600	SER	N-CA-C	-6.51	105.34	113.28
1	A	292	ILE	CB-CG1-CD1	-6.32	100.54	113.80
1	A	266	ARG	NE-CZ-NH1	-6.16	115.34	121.50
1	A	658	PHE	CA-C-N	-6.14	110.98	120.31
1	A	658	PHE	C-N-CA	-6.14	110.98	120.31
1	A	639	THR	N-CA-C	6.11	117.74	111.14
1	A	668	ILE	N-CA-CB	5.74	117.27	110.55
1	A	583	ARG	CG-CD-NE	5.68	124.50	112.00
1	A	564	TYR	CA-C-N	-5.59	115.34	123.06
1	A	564	TYR	C-N-CA	-5.59	115.34	123.06
1	A	565	VAL	N-CA-C	5.49	116.39	108.48
1	A	586	LEU	CB-CA-C	-5.40	102.40	110.88
1	A	258	GLU	N-CA-C	5.40	121.74	109.81
1	A	459	ILE	N-CA-C	-5.37	105.14	110.62
1	A	408	GLN	N-CA-C	-5.33	105.64	111.82
1	A	631	SER	CA-C-N	5.32	129.86	120.87
1	A	631	SER	C-N-CA	5.32	129.86	120.87
1	A	641	LEU	CB-CA-C	-5.31	102.78	110.96
1	A	430	GLU	CA-CB-CG	5.31	124.72	114.10
1	A	460	MET	N-CA-C	-5.30	105.56	112.23
1	A	658	PHE	CA-C-O	5.26	126.13	120.55
2	B	10	LEU	N-CA-C	-5.23	106.16	112.54
1	A	497	LYS	CA-C-N	-5.20	115.40	122.93
1	A	497	LYS	C-N-CA	-5.20	115.40	122.93
1	A	361	LYS	N-CA-C	-5.15	102.29	109.96
1	A	647	ASN	N-CA-C	-5.14	107.00	113.28
1	A	347	ASP	N-CA-C	5.13	116.42	107.49
1	A	326	HIS	CA-C-N	-5.12	113.40	122.26
1	A	326	HIS	C-N-CA	-5.12	113.40	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	716	SER	CB-CA-C	5.07	119.73	110.10
1	A	616	SER	CA-C-N	-5.04	113.72	120.87
1	A	616	SER	C-N-CA	-5.04	113.72	120.87

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	258	GLU	Peptide
1	A	695	ILE	Peptide
2	B	14	ALA	Peptide

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	3382	0	3392	107	0
2	B	117	0	128	5	0
3	A	70	0	0	5	0
All	All	3569	0	3520	111	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 16.

All (111) 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:476:ALA:HB1	1:A:479:ASP:HB2	1.27	1.13
1:A:462:GLY:HA3	1:A:581:MET:CE	1.79	1.12
1:A:463:VAL:O	1:A:467:THR:HG23	1.65	0.96
1:A:467:THR:HG22	1:A:579:MET:HG2	1.51	0.92
1:A:647:ASN:C	1:A:647:ASN:HD22	1.74	0.91
1:A:326:HIS:H	1:A:331:ASN:HD21	1.20	0.90
1:A:462:GLY:HA3	1:A:581:MET:HE1	1.55	0.87
1:A:576:LYS:HE2	1:A:580:GLU:OE1	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:ASN:HB2	1:A:655:LEU:HD11	1.55	0.87
1:A:506:LYS:HD2	1:A:507:GLY:O	1.77	0.83
1:A:512:ARG:HH11	1:A:512:ARG:HB2	1.42	0.83
1:A:289:LYS:HG2	1:A:499:ASN:HB3	1.64	0.80
1:A:442:ARG:HH12	1:A:597:GLU:HG2	1.47	0.80
1:A:472:ALA:CB	1:A:483:ILE:HD11	2.11	0.79
1:A:476:ALA:CB	1:A:479:ASP:HB2	2.11	0.77
1:A:365:GLN:H	1:A:365:GLN:NE2	1.83	0.77
1:A:344:GLU:HB3	1:A:358:LYS:HE3	1.65	0.76
1:A:326:HIS:N	1:A:331:ASN:HD21	1.83	0.76
1:A:336:LEU:CB	1:A:365:GLN:HG3	2.15	0.76
1:A:286:ASP:OD1	1:A:528:THR:HG21	1.89	0.72
1:A:326:HIS:H	1:A:331:ASN:ND2	1.90	0.70
3:A:4:HOH:O	2:B:6:THR:HG21	1.91	0.70
1:A:324:LYS:HG3	1:A:324:LYS:O	1.91	0.69
1:A:279:ARG:NH1	3:A:64:HOH:O	2.26	0.68
1:A:635:LYS:O	1:A:639:THR:HG23	1.93	0.68
1:A:647:ASN:CB	1:A:699:TRP:HE1	2.06	0.67
2:B:15:GLN:HA	2:B:15:GLN:OE1	1.93	0.67
1:A:479:ASP:O	1:A:506:LYS:HE2	1.95	0.67
1:A:472:ALA:HB3	1:A:483:ILE:HD11	1.77	0.66
1:A:336:LEU:HB3	1:A:365:GLN:HG3	1.75	0.66
1:A:647:ASN:HB3	1:A:699:TRP:HE1	1.60	0.65
1:A:443:ARG:HH21	1:A:444:ASN:HD21	1.42	0.65
1:A:462:GLY:HA3	1:A:581:MET:HE3	1.73	0.65
1:A:442:ARG:NH1	1:A:597:GLU:HG2	2.11	0.64
1:A:336:LEU:HB2	1:A:365:GLN:HG3	1.79	0.64
1:A:434:PRO:O	1:A:435:ILE:HG13	1.98	0.64
1:A:295:PRO:HG3	1:A:498:THR:HG23	1.83	0.60
1:A:346:GLN:C	1:A:347:ASP:OD1	2.44	0.60
1:A:528:THR:HG22	3:A:49:HOH:O	2.01	0.59
1:A:330:ILE:HG22	1:A:332:PRO:HD2	1.83	0.59
1:A:695:ILE:HD13	1:A:695:ILE:N	2.18	0.58
1:A:257:ILE:C	1:A:259:PRO:HD2	2.29	0.58
1:A:668:ILE:C	1:A:668:ILE:HD13	2.30	0.57
1:A:344:GLU:HB3	1:A:358:LYS:CE	2.35	0.57
1:A:635:LYS:O	1:A:639:THR:CG2	2.53	0.57
1:A:574:LYS:O	1:A:577:TRP:HB3	2.05	0.57
1:A:258:GLU:N	1:A:258:GLU:OE2	2.38	0.56
1:A:576:LYS:HE2	1:A:580:GLU:CD	2.30	0.56
1:A:289:LYS:CG	1:A:499:ASN:HB3	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LEU:O	1:A:346:GLN:OE1	2.25	0.55
1:A:436:GLU:HG2	1:A:437:HIS:N	2.22	0.55
1:A:512:ARG:HB2	1:A:512:ARG:NH1	2.18	0.54
1:A:589:LEU:HD22	1:A:593:GLU:HG3	1.89	0.54
1:A:647:ASN:HB3	1:A:699:TRP:NE1	2.23	0.54
1:A:348:ILE:HG22	1:A:348:ILE:O	2.06	0.54
1:A:291:SER:HB3	1:A:498:THR:O	2.07	0.54
1:A:337:SER:O	1:A:341:VAL:HG12	2.09	0.53
1:A:587:GLN:NE2	1:A:644:SER:OG	2.42	0.53
1:A:264:THR:HB	1:A:265:PRO:CD	2.39	0.52
1:A:536:LYS:HD3	1:A:537:TRP:CZ2	2.45	0.51
1:A:692:GLU:O	1:A:695:ILE:HD11	2.11	0.51
1:A:572:LYS:HA	1:A:575:MET:HE3	1.93	0.51
1:A:511:LEU:HD21	1:A:518:VAL:HG22	1.93	0.50
1:A:320:PRO:HB2	1:A:335:LEU:HD22	1.93	0.50
1:A:436:GLU:HG2	1:A:437:HIS:H	1.77	0.50
1:A:624:SER:HB2	1:A:625:PRO:HD2	1.93	0.50
1:A:338:TRP:O	1:A:341:VAL:HG13	2.12	0.49
1:A:257:ILE:C	1:A:258:GLU:OE2	2.56	0.49
1:A:370:LEU:CD2	1:A:521:VAL:HG23	2.42	0.49
1:A:421:SER:HB3	1:A:452:HIS:CE1	2.47	0.49
1:A:293:GLU:O	1:A:294:ASP:C	2.55	0.49
1:A:365:GLN:NE2	1:A:365:GLN:N	2.56	0.48
1:A:472:ALA:CB	1:A:483:ILE:CD1	2.90	0.48
1:A:304:LEU:HB2	3:A:36:HOH:O	2.14	0.47
1:A:325:PRO:HB2	1:A:331:ASN:OD1	2.15	0.47
1:A:624:SER:HB2	1:A:625:PRO:CD	2.45	0.47
1:A:629:GLU:HB3	2:B:1:MET:HE2	1.97	0.47
1:A:370:LEU:HD21	1:A:521:VAL:HG23	1.96	0.47
1:A:654:GLN:HE22	1:A:697:ASP:H	1.63	0.47
1:A:270:LEU:HB3	1:A:271:PRO:HD2	1.97	0.46
1:A:563:LEU:HD13	1:A:565:VAL:HG12	1.98	0.45
1:A:490:ARG:HA	1:A:495:ARG:O	2.16	0.45
1:A:472:ALA:HB3	1:A:483:ILE:CD1	2.46	0.45
2:B:4:ASN:OD1	2:B:4:ASN:C	2.59	0.45
1:A:549:LEU:CD2	1:A:558:SER:HB2	2.47	0.45
1:A:365:GLN:H	1:A:365:GLN:CD	2.24	0.44
1:A:409:ASN:ND2	3:A:58:HOH:O	2.50	0.44
1:A:594:SER:O	1:A:595:MET:C	2.56	0.44
1:A:362:LYS:O	1:A:367:LYS:HE3	2.18	0.44
1:A:441:MET:HE3	1:A:606:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:LEU:HD23	1:A:549:LEU:HA	1.46	0.44
1:A:654:GLN:HE22	1:A:696:ASN:H	1.65	0.44
1:A:614:ASN:HD22	1:A:614:ASN:N	2.16	0.43
1:A:274:PRO:O	1:A:401:ARG:CG	2.67	0.43
1:A:526:SER:OG	1:A:528:THR:HG23	2.19	0.43
1:A:647:ASN:C	1:A:647:ASN:ND2	2.57	0.43
1:A:294:ASP:O	1:A:295:PRO:C	2.59	0.42
1:A:647:ASN:CB	1:A:699:TRP:NE1	2.79	0.42
1:A:354:ILE:N	1:A:355:PRO:HD3	2.34	0.42
1:A:707:PHE:CE2	1:A:711:LEU:HD21	2.55	0.42
1:A:257:ILE:HG22	1:A:257:ILE:O	2.19	0.42
1:A:354:ILE:N	1:A:355:PRO:CD	2.83	0.42
1:A:647:ASN:HB2	1:A:699:TRP:HE1	1.82	0.41
1:A:694:LEU:C	1:A:695:ILE:HD13	2.45	0.41
1:A:314:PHE:CE2	1:A:548:MET:HG2	2.54	0.41
1:A:513:ASN:HB2	1:A:516:ASP:OD1	2.21	0.41
1:A:476:ALA:O	1:A:477:MET:HG2	2.20	0.41
1:A:264:THR:HB	1:A:265:PRO:HD2	2.01	0.41
1:A:573:ILE:HD13	1:A:573:ILE:HA	1.72	0.40
1:A:664:LYS:O	1:A:668:ILE:HG22	2.21	0.40
2:B:4:ASN:CG	2:B:7:LEU:HG	2.47	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	413/478 (86%)	379 (92%)	25 (6%)	9 (2%)	5	4
2	B	13/81 (16%)	11 (85%)	2 (15%)	0	100	100
All	All	426/559 (76%)	390 (92%)	27 (6%)	9 (2%)	5	4

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	GLU
1	A	297	HIS
1	A	433	ALA
1	A	346	GLN
1	A	684	GLY
1	A	362	LYS
1	A	259	PRO
1	A	621	ILE
1	A	602	VAL

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	379/429 (88%)	318 (84%)	61 (16%)	2	2
2	B	14/70 (20%)	12 (86%)	2 (14%)	3	3
All	All	393/499 (79%)	330 (84%)	63 (16%)	2	2

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	ILE
1	A	258	GLU
1	A	262	LYS
1	A	263	THR
1	A	270	LEU
1	A	291	SER
1	A	292	ILE
1	A	302	ILE
1	A	304	LEU
1	A	321	ASN
1	A	323	VAL
1	A	324	LYS
1	A	328	LYS
1	A	330	ILE

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Mol	Chain	Res	Type
1	A	341	VAL
1	A	354	ILE
1	A	364	SER
1	A	365	GLN
1	A	366	LEU
1	A	401	ARG
1	A	405	SER
1	A	432	VAL
1	A	467	THR
1	A	469	LEU
1	A	470	LEU
1	A	488	LYS
1	A	493	GLU
1	A	498	THR
1	A	506	LYS
1	A	512	ARG
1	A	515	THR
1	A	528	THR
1	A	538	GLU
1	A	548	MET
1	A	549	LEU
1	A	559	ARG
1	A	563	LEU
1	A	565	VAL
1	A	567	THR
1	A	573	ILE
1	A	586	LEU
1	A	589	LEU
1	A	601	SER
1	A	605	LYS
1	A	626	LYS
1	A	628	VAL
1	A	633	ILE
1	A	635	LYS
1	A	639	THR
1	A	641	LEU
1	A	647	ASN
1	A	649	LEU
1	A	655	LEU
1	A	659	SER
1	A	665	LEU
1	A	666	LEU

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Mol	Chain	Res	Type
1	A	668	ILE
1	A	677	GLU
1	A	692	GLU
1	A	695	ILE
1	A	716	SER
2	B	6	THR
2	B	15	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	331	ASN
1	A	333	ASN
1	A	340	GLN
1	A	365	GLN
1	A	409	ASN
1	A	444	ASN
1	A	452	HIS
1	A	481	GLN
1	A	587	GLN
1	A	614	ASN
1	A	647	ASN
1	A	703	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	421/478 (88%)	-0.08	11 (2%) 57 59	29, 48, 77, 93	0
2	B	15/81 (18%)	-0.23	1 (6%) 24 26	32, 39, 64, 73	0
All	All	436/559 (77%)	-0.09	12 (2%) 55 57	29, 48, 77, 93	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	354	ILE	6.3
1	A	348	ILE	6.1
1	A	676	LEU	5.5
1	A	257	ILE	4.3
1	A	434	PRO	3.8
1	A	432	VAL	3.3
1	A	371	GLY	2.6
1	A	476	ALA	2.5
2	B	15	GLN	2.3
1	A	477	MET	2.1
1	A	398	PRO	2.0
1	A	433	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.