



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:48 PM UTC

PDB ID : 5N2U / pdb_00005n2u
Title : Influenza D virus nucleoprotein
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Deposited on : 2017-02-08
Resolution : 2.40 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

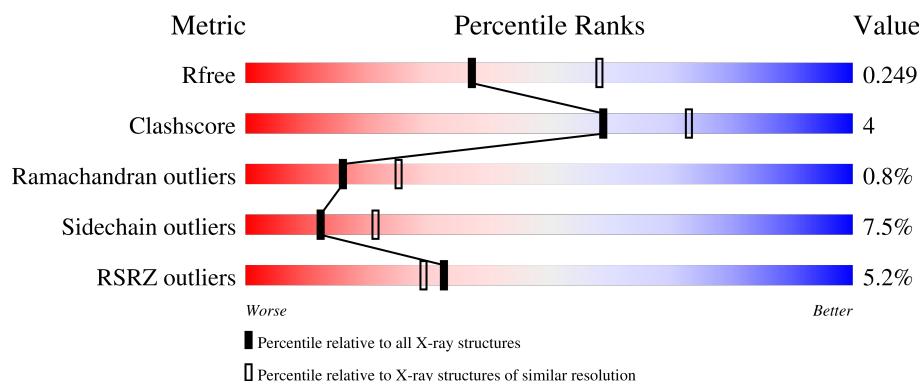
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	552	7% 65% 18% • 15%
1	B	552	4% 67% 15% • 17%
1	C	552	3% 72% 11% • 15%
1	D	552	4% 74% 11% • 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14881 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	0	0
			3674	2329	635	684	26			
1	B	460	Total	C	N	O	S	0	0	0
			3591	2279	614	672	26			
1	C	467	Total	C	N	O	S	0	0	0
			3649	2314	628	681	26			
1	D	476	Total	C	N	O	S	0	0	0
			3732	2367	647	692	26			

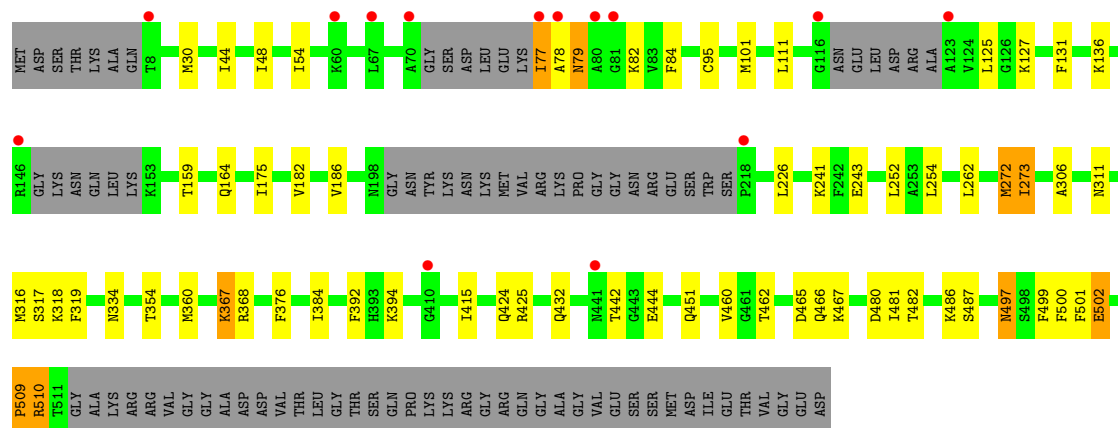
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	45	Total	O	0	0
			45	45		
2	B	56	Total	O	0	0
			56	56		
2	C	86	Total	O	0	0
			86	86		
2	D	48	Total	O	0	0
			48	48		

GLY
ALA
ASP
ASP
VAL
THR
LEU
GLY
THR
SER
GLN
PRO
LYS
LYS
ARG
GLY
ARG
GLN
GLY
ALA
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SER
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ASP
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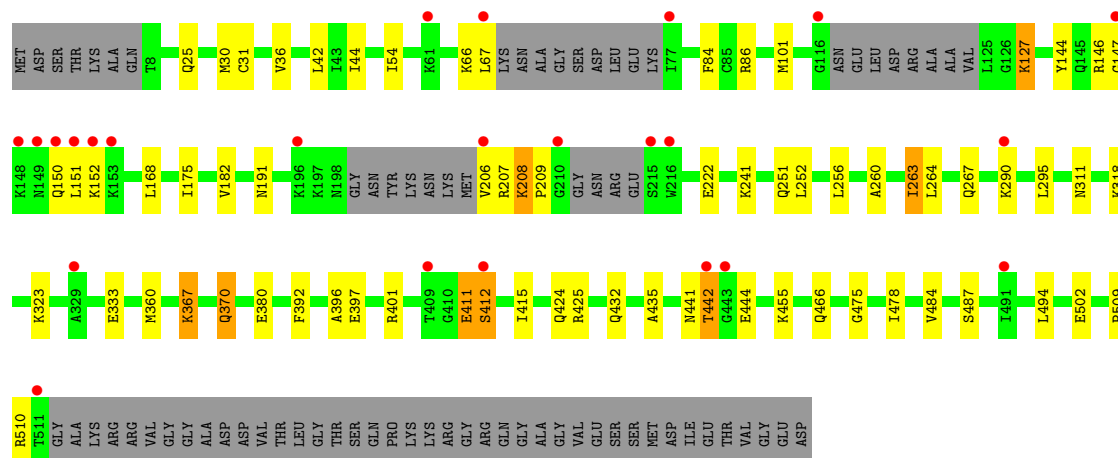
• Molecule 1: Nucleoprotein

Chain C: 3% 72% 11% 15%



• Molecule 1: Nucleoprotein

Chain D: 4% 74% 11% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.17Å 85.17Å 103.39Å 91.20° 101.94° 101.02°	Depositor
Resolution (Å)	39.71 – 2.40 39.71 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.4 (39.71-2.40) 91.4 (39.71-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.202 , 0.252 (Not available) , 0.249	Depositor DCC
R_{free} test set	4331 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14881	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% 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	0.84	3/3736 (0.1%)	1.45	22/5016 (0.4%)
1	B	0.83	3/3649 (0.1%)	1.43	15/4898 (0.3%)
1	C	0.80	0/3708	1.41	17/4976 (0.3%)
1	D	0.80	0/3793	1.38	16/5088 (0.3%)
All	All	0.82	6/14886 (0.0%)	1.42	70/19978 (0.4%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	MET	SD-CE	-7.45	1.60	1.79
1	B	278	MET	SD-CE	-6.49	1.63	1.79
1	A	53	MET	SD-CE	-5.92	1.64	1.79
1	A	278	MET	SD-CE	-5.70	1.65	1.79
1	B	360	MET	SD-CE	-5.26	1.66	1.79
1	B	274	MET	SD-CE	-5.12	1.66	1.79

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	263	ILE	N-CA-CB	7.95	118.16	111.64
1	B	113	ASP	CA-CB-CG	7.49	120.09	112.60
1	B	388	SER	CA-C-N	6.76	134.45	121.54
1	B	388	SER	C-N-CA	6.76	134.45	121.54
1	A	374	GLY	CA-C-N	6.65	130.09	120.38
1	A	374	GLY	C-N-CA	6.65	130.09	120.38
1	D	263	ILE	N-CA-C	-6.56	106.44	111.62
1	A	244	TYR	N-CA-C	-6.23	105.67	113.28
1	A	513	ALA	N-CA-C	-6.07	103.81	112.13
1	C	425	ARG	N-CA-C	5.99	113.61	108.22
1	A	441	ASN	N-CA-C	5.96	119.03	111.69
1	D	127	LYS	CA-C-N	5.95	128.26	120.28
1	D	127	LYS	C-N-CA	5.95	128.26	120.28
1	D	370	GLN	N-CA-C	-5.92	105.89	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	SER	CA-C-N	5.89	128.49	120.54
1	A	388	SER	C-N-CA	5.89	128.49	120.54
1	A	246	ASN	CA-CB-CG	5.77	118.37	112.60
1	B	43	ILE	CA-C-N	5.76	128.03	120.60
1	B	43	ILE	C-N-CA	5.76	128.03	120.60
1	A	338	LYS	CA-C-N	5.70	128.19	120.38
1	A	338	LYS	C-N-CA	5.70	128.19	120.38
1	A	439	ALA	CA-C-N	5.64	127.78	120.44
1	A	439	ALA	C-N-CA	5.64	127.78	120.44
1	C	465	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	139	LEU	CA-C-N	5.58	127.75	120.28
1	B	139	LEU	C-N-CA	5.58	127.75	120.28
1	B	225	PHE	CA-CB-CG	5.57	119.37	113.80
1	B	390	GLY	CA-C-N	5.52	128.00	120.54
1	B	390	GLY	C-N-CA	5.52	128.00	120.54
1	C	376	PHE	N-CA-C	-5.50	106.35	112.57
1	C	319	PHE	CA-CB-CG	5.46	119.25	113.80
1	D	509	PRO	CA-C-N	5.32	131.71	121.54
1	D	509	PRO	C-N-CA	5.32	131.71	121.54
1	A	289	ASN	CA-C-N	5.32	127.35	120.44
1	A	289	ASN	C-N-CA	5.32	127.35	120.44
1	C	79	ASN	CA-CB-CG	5.31	117.91	112.60
1	A	226	LEU	CA-C-N	5.29	127.37	120.28
1	A	226	LEU	C-N-CA	5.29	127.37	120.28
1	A	265	LYS	N-CA-C	5.24	115.63	109.60
1	D	484	VAL	CA-C-N	5.24	129.47	120.72
1	D	484	VAL	C-N-CA	5.24	129.47	120.72
1	C	111	LEU	CA-C-N	5.23	127.54	120.38
1	C	111	LEU	C-N-CA	5.23	127.54	120.38
1	B	483	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	435	ALA	CA-C-N	5.18	127.23	120.28
1	B	435	ALA	C-N-CA	5.18	127.23	120.28
1	C	509	PRO	CA-C-N	5.18	131.43	121.54
1	C	509	PRO	C-N-CA	5.18	131.43	121.54
1	B	123	ALA	CA-C-N	5.15	127.52	120.46
1	B	123	ALA	C-N-CA	5.15	127.52	120.46
1	C	334	ASN	CA-C-N	5.13	125.64	119.94
1	C	334	ASN	C-N-CA	5.13	125.64	119.94
1	D	435	ALA	CA-C-N	5.13	127.10	120.44
1	D	435	ALA	C-N-CA	5.13	127.10	120.44
1	D	44	ILE	CA-C-N	5.12	127.39	120.38
1	D	44	ILE	C-N-CA	5.12	127.39	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	375	ASN	N-CA-C	5.11	118.29	111.75
1	A	117	ASN	CA-C-N	5.09	131.26	121.54
1	A	117	ASN	C-N-CA	5.09	131.26	121.54
1	D	168	LEU	CA-C-N	5.09	127.94	120.71
1	D	168	LEU	C-N-CA	5.09	127.94	120.71
1	C	127	LYS	CA-C-N	5.06	127.02	120.44
1	C	127	LYS	C-N-CA	5.06	127.02	120.44
1	D	441	ASN	N-CA-C	5.05	117.68	111.82
1	C	226	LEU	CA-C-N	5.04	127.29	120.38
1	C	226	LEU	C-N-CA	5.04	127.29	120.38
1	A	512	GLY	CA-C-N	5.03	130.11	122.56
1	A	512	GLY	C-N-CA	5.03	130.11	122.56
1	C	460	VAL	CA-C-N	5.01	125.50	119.94
1	C	460	VAL	C-N-CA	5.01	125.50	119.94

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	3674	0	3715	54	0
1	B	3591	0	3631	42	0
1	C	3649	0	3701	24	0
1	D	3732	0	3789	21	0
2	A	45	0	0	0	0
2	B	56	0	0	0	0
2	C	86	0	0	0	0
2	D	48	0	0	0	0
All	All	14881	0	14836	129	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 4.

All (129) 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:125:LEU:HB3	1:A:128:ARG:HB2	1.64	0.78
1:B:272:MET:HE1	1:B:274:MET:HG3	1.70	0.74
1:A:82:LYS:HD2	1:A:101:MET:HE2	1.72	0.71
1:A:442:THR:HG21	1:B:256:LEU:HD13	1.73	0.70
1:B:360:MET:HA	1:B:394:LYS:HB2	1.77	0.66
1:A:25:GLN:O	1:A:29:ARG:HG2	1.97	0.65
1:D:432:GLN:HB2	1:D:466:GLN:HE22	1.61	0.64
1:B:452:LEU:O	1:B:456:ILE:HG12	1.98	0.63
1:C:272:MET:O	1:C:272:MET:HG3	2.00	0.62
1:D:144:TYR:HB2	1:D:147:GLY:HA2	1.82	0.61
1:B:55:ARG:HH11	1:B:132:THR:CG2	2.13	0.61
1:A:474:THR:HA	1:D:424:GLN:HG3	1.82	0.60
1:C:424:GLN:HE21	1:D:475:GLY:H	1.47	0.60
1:B:414:GLN:NE2	1:C:501:PHE:H	2.01	0.59
1:A:475:GLY:H	1:D:424:GLN:HE21	1.51	0.58
1:D:30:MET:HG3	1:D:54:ILE:HD11	1.87	0.57
1:B:55:ARG:HH11	1:B:132:THR:HG23	1.70	0.57
1:B:274:MET:CE	1:B:310:PHE:HA	2.35	0.57
1:B:421:PHE:CD2	1:C:360:MET:HE1	2.39	0.56
1:A:272:MET:HE1	1:A:274:MET:HG3	1.88	0.56
1:B:274:MET:HE1	1:B:310:PHE:HA	1.87	0.56
1:A:177:GLU:HG3	1:A:225:PHE:CG	2.42	0.55
1:A:448:ASN:HB3	1:A:451:GLN:HG2	1.89	0.54
1:A:121:ARG:HE	1:A:126:GLY:H	1.56	0.54
1:A:339:MET:HA	1:A:339:MET:HE2	1.91	0.53
1:B:275:PRO:HD2	1:B:278:MET:HE3	1.90	0.53
1:D:411:GLU:O	1:D:412:SER:HB2	2.08	0.52
1:D:367:LYS:HB2	1:D:370:GLN:HE21	1.74	0.52
1:B:272:MET:HE3	1:B:346:CYS:HB3	1.92	0.52
1:C:311:ASN:HD21	1:C:392:PHE:H	1.56	0.52
1:B:274:MET:HE3	1:B:310:PHE:CD1	2.44	0.51
1:D:311:ASN:HD21	1:D:392:PHE:H	1.58	0.51
1:C:442:THR:HG21	1:D:256:LEU:HD13	1.93	0.51
1:A:53:MET:HE1	1:A:107:VAL:CG1	2.40	0.51
1:D:396:ALA:HB2	1:D:478:ILE:HD13	1.92	0.50
1:B:409:THR:HG23	1:B:410:GLY:H	1.76	0.50
1:A:30:MET:HG3	1:A:54:ILE:HD11	1.93	0.50
1:D:208:LYS:N	1:D:209:PRO:HD3	2.27	0.50
1:D:84:PHE:CE1	1:D:101:MET:HG3	2.47	0.49
1:A:234:PRO:HB2	1:A:456:ILE:HG13	1.95	0.49
1:A:274:MET:HE1	1:A:313:ALA:HB3	1.95	0.48
1:D:260:ALA:HB1	1:D:264:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:THR:HG21	1:B:125:LEU:HD21	1.95	0.48
1:A:275:PRO:HD2	1:A:278:MET:HE3	1.95	0.48
1:B:55:ARG:HD3	1:B:132:THR:HG22	1.95	0.48
1:A:275:PRO:HD2	1:A:278:MET:CE	2.43	0.47
1:A:103:LEU:HB3	1:A:105:PRO:HD2	1.97	0.47
1:A:177:GLU:HA	1:A:180:LEU:HD12	1.97	0.47
1:A:457:ARG:HH21	1:D:442:THR:HG22	1.80	0.47
1:C:186:VAL:HG13	1:C:254:LEU:HB3	1.97	0.47
1:B:129:MET:HE1	1:B:276:TRP:HH2	1.80	0.46
1:C:30:MET:HG3	1:C:54:ILE:HD11	1.96	0.46
1:B:502:GLU:HA	1:B:503:PHE:N	2.30	0.46
1:A:180:LEU:HD22	1:A:184:THR:HG21	1.97	0.46
1:A:30:MET:HE3	1:A:54:ILE:HD12	1.98	0.46
1:A:432:GLN:HA	1:A:466:GLN:HE22	1.79	0.46
1:A:436:GLU:HG3	1:A:463:PHE:HZ	1.80	0.46
1:A:168:LEU:HD12	1:A:180:LEU:HD21	1.98	0.46
1:A:449:PHE:O	1:A:453:VAL:HG23	2.15	0.46
1:D:207:ARG:HB3	1:D:209:PRO:HD3	1.97	0.46
1:A:361:ILE:HG22	1:A:363:GLN:O	2.16	0.45
1:A:472:GLU:HB2	1:D:425:ARG:HD2	1.98	0.45
1:B:30:MET:HE3	1:B:54:ILE:HG12	1.98	0.45
1:B:339:MET:HE2	1:B:339:MET:HA	1.99	0.45
1:B:341:ILE:HG13	1:B:373:VAL:HG11	1.99	0.45
1:A:312:THR:HA	1:A:315:TYR:CD2	2.52	0.45
1:B:138:ASN:O	1:B:142:VAL:HG23	2.17	0.45
1:A:127:LYS:O	1:A:131:PHE:HD2	2.00	0.45
1:A:53:MET:HE1	1:A:107:VAL:HG11	1.99	0.45
1:C:272:MET:HG2	1:C:306:ALA:HB1	1.99	0.45
1:C:77:ILE:HB	1:C:78:ALA:H	1.56	0.44
1:C:432:GLN:HB3	1:C:466:GLN:HE22	1.81	0.44
1:C:354:THR:HG21	1:C:367:LYS:CE	2.48	0.44
1:A:274:MET:HE1	1:A:313:ALA:CB	2.47	0.44
1:A:415:ILE:HD11	1:A:433:ARG:CZ	2.47	0.44
1:B:275:PRO:HD2	1:B:278:MET:CE	2.47	0.44
1:D:42:LEU:HB2	1:D:318:LYS:HE2	2.00	0.44
1:A:339:MET:HE1	1:A:387:THR:HG22	1.98	0.44
1:B:55:ARG:NH1	1:B:132:THR:HG23	2.32	0.44
1:B:434:LEU:HG	1:B:438:MET:HE2	2.00	0.44
1:D:267:GLN:HE21	1:D:401:ARG:HA	1.81	0.44
1:B:8:THR:HA	1:B:11:GLU:HB2	2.00	0.44
1:C:159:THR:HG22	1:C:262:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:MET:HE3	1:A:310:PHE:CD1	2.53	0.43
1:C:44:ILE:HG12	1:C:318:LYS:O	2.18	0.43
1:A:274:MET:CE	1:A:310:PHE:HA	2.48	0.43
1:B:30:MET:HG3	1:B:54:ILE:HD11	2.00	0.43
1:A:53:MET:CE	1:A:107:VAL:HG11	2.49	0.43
1:B:341:ILE:HD11	1:B:371:LEU:HD13	2.00	0.43
1:A:511:THR:C	1:A:513:ALA:H	2.27	0.43
1:B:170:ALA:HA	1:B:173:ARG:HG2	2.01	0.42
1:B:267:GLN:HG3	1:B:401:ARG:C	2.44	0.42
1:A:40:ASP:OD1	1:A:90:SER:HB3	2.19	0.42
1:A:263:ILE:HG23	1:A:264:LEU:HD22	2.01	0.42
1:A:300:ALA:HB3	1:A:305:ARG:HB2	2.01	0.42
1:C:95:CYS:HB3	1:C:384:ILE:HG12	2.01	0.42
1:C:367:LYS:HG2	1:C:502:GLU:HG3	2.01	0.42
1:C:360:MET:HA	1:C:394:LYS:HB2	2.02	0.42
1:A:241:LYS:O	1:A:244:TYR:HB2	2.20	0.42
1:A:272:MET:HE2	1:A:346:CYS:HB3	2.02	0.42
1:B:272:MET:HE1	1:B:274:MET:CG	2.44	0.42
1:B:368:ARG:HA	1:B:371:LEU:HD12	2.01	0.42
1:C:44:ILE:O	1:C:48:ILE:HG12	2.20	0.42
1:C:84:PHE:CE1	1:C:101:MET:HG3	2.55	0.42
1:A:353:ASP:HB3	1:A:356:ILE:HG12	2.01	0.42
1:A:420:VAL:HG23	1:B:352:GLU:HB2	2.02	0.42
1:B:341:ILE:HG13	1:B:373:VAL:HG21	2.02	0.42
1:A:361:ILE:HG13	1:A:391:TYR:CE2	2.54	0.42
1:A:424:GLN:HG3	1:B:474:THR:HA	2.02	0.42
1:B:141:GLU:O	1:B:501:PHE:HZ	2.03	0.41
1:B:396:ALA:HB2	1:B:478:ILE:HD13	2.02	0.41
1:C:131:PHE:HD1	1:C:273:ILE:HD12	1.85	0.41
1:C:509:PRO:O	1:C:510:ARG:HB2	2.20	0.41
1:A:31:CYS:HB3	1:A:36:VAL:HB	2.01	0.41
1:A:53:MET:HE1	1:A:107:VAL:HG13	2.02	0.41
1:A:146:ARG:HH21	1:A:153:LYS:HA	1.84	0.41
1:A:481:ILE:H	1:A:481:ILE:HG13	1.67	0.41
1:B:55:ARG:HH11	1:B:132:THR:HG22	1.85	0.41
1:B:227:ASN:HD22	1:B:239:CYS:HB3	1.86	0.41
1:B:234:PRO:HB2	1:B:456:ILE:HD13	2.03	0.41
1:C:497:ASN:ND2	1:C:499:PHE:H	2.19	0.41
1:A:26:ILE:HD12	1:A:111:LEU:HD23	2.03	0.40
1:B:444:GLU:HG2	1:C:252:LEU:HD21	2.03	0.40
1:A:86:ARG:HH22	1:A:380:GLU:HG2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LYS:HB3	1:B:101:MET:HE3	2.03	0.40
1:C:368:ARG:HD3	1:C:500:PHE:CE2	2.57	0.40
1:D:31:CYS:HB3	1:D:36:VAL:HB	2.03	0.40
1:D:86:ARG:HH22	1:D:380:GLU:HG2	1.86	0.40
1:A:155:ASN:HB3	1:A:258:LEU:HD21	2.04	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	461/552 (84%)	429 (93%)	27 (6%)	5 (1%)	11	18
1	B	448/552 (81%)	412 (92%)	32 (7%)	4 (1%)	14	22
1	C	457/552 (83%)	440 (96%)	14 (3%)	3 (1%)	18	28
1	D	465/552 (84%)	440 (95%)	22 (5%)	3 (1%)	21	32
All	All	1831/2208 (83%)	1721 (94%)	95 (5%)	15 (1%)	16	25

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	GLY
1	A	467	LYS
1	D	412	SER
1	A	59	ASP
1	B	409	THR
1	B	495	GLY
1	D	510	ARG
1	A	118	GLU
1	C	467	LYS
1	C	486	LYS

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Mol	Chain	Res	Type
1	C	510	ARG
1	B	93	GLY
1	B	399	GLY
1	D	208	LYS
1	A	124	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	395/462 (86%)	366 (93%)	29 (7%)	13	22
1	B	388/462 (84%)	355 (92%)	33 (8%)	10	16
1	C	394/462 (85%)	369 (94%)	25 (6%)	16	29
1	D	403/462 (87%)	371 (92%)	32 (8%)	11	19
All	All	1580/1848 (86%)	1461 (92%)	119 (8%)	12	21

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	26	ILE
1	A	38	GLU
1	A	47	SER
1	A	53	MET
1	A	117	ASN
1	A	119	LEU
1	A	120	ASP
1	A	125	LEU
1	A	128	ARG
1	A	136	LYS
1	A	151	LEU
1	A	169	GLU
1	A	191	ASN
1	A	224	SER
1	A	227	ASN

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Mol	Chain	Res	Type
1	A	241	LYS
1	A	264	LEU
1	A	298	LEU
1	A	323	LYS
1	A	330	GLU
1	A	361	ILE
1	A	375	ASN
1	A	442	THR
1	A	445	THR
1	A	455	LYS
1	A	481	ILE
1	A	494	LEU
1	A	502	GLU
1	B	8	THR
1	B	12	GLN
1	B	13	ARG
1	B	18	LYS
1	B	29	ARG
1	B	38	GLU
1	B	53	MET
1	B	94	LYS
1	B	101	MET
1	B	132	THR
1	B	144	TYR
1	B	152	LYS
1	B	182	VAL
1	B	230	LEU
1	B	237	GLN
1	B	239	CYS
1	B	257	MET
1	B	272	MET
1	B	274	MET
1	B	278	MET
1	B	287	GLU
1	B	290	LYS
1	B	296	GLU
1	B	317	SER
1	B	325	ILE
1	B	330	GLU
1	B	362	SER
1	B	383	THR
1	B	415	ILE

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Mol	Chain	Res	Type
1	B	441	ASN
1	B	458	GLU
1	B	482	THR
1	B	487	SER
1	C	77	ILE
1	C	79	ASN
1	C	82	LYS
1	C	125	LEU
1	C	136	LYS
1	C	164	GLN
1	C	175	ILE
1	C	182	VAL
1	C	241	LYS
1	C	243	GLU
1	C	272	MET
1	C	273	ILE
1	C	316	MET
1	C	317	SER
1	C	367	LYS
1	C	415	ILE
1	C	444	GLU
1	C	451	GLN
1	C	462	THR
1	C	480	ASP
1	C	481	ILE
1	C	482	THR
1	C	487	SER
1	C	497	ASN
1	C	502	GLU
1	D	25	GLN
1	D	66	LYS
1	D	67	LEU
1	D	127	LYS
1	D	146	ARG
1	D	150	GLN
1	D	151	LEU
1	D	152	LYS
1	D	175	ILE
1	D	182	VAL
1	D	191	ASN
1	D	206	VAL
1	D	222	GLU

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Mol	Chain	Res	Type
1	D	241	LYS
1	D	251	GLN
1	D	252	LEU
1	D	263	ILE
1	D	290	LYS
1	D	295	LEU
1	D	323	LYS
1	D	333	GLU
1	D	360	MET
1	D	367	LYS
1	D	397	GLU
1	D	411	GLU
1	D	415	ILE
1	D	442	THR
1	D	444	GLU
1	D	455	LYS
1	D	487	SER
1	D	494	LEU
1	D	502	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	ASN
1	A	251	GLN
1	A	375	ASN
1	A	417	ASN
1	A	432	GLN
1	A	451	GLN
1	A	459	GLN
1	B	16	ASN
1	B	227	ASN
1	B	255	ASN
1	B	334	ASN
1	B	414	GLN
1	B	441	ASN
1	B	454	GLN
1	C	69	ASN
1	C	106	ASN
1	C	145	GLN
1	C	311	ASN
1	C	340	GLN

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Mol	Chain	Res	Type
1	C	414	GLN
1	C	424	GLN
1	C	459	GLN
1	C	466	GLN
1	D	25	GLN
1	D	63	GLN
1	D	227	ASN
1	D	237	GLN
1	D	267	GLN
1	D	289	ASN
1	D	311	ASN
1	D	370	GLN
1	D	377	ASN
1	D	393	HIS
1	D	405	ASN
1	D	424	GLN
1	D	459	GLN
1	D	466	GLN
1	D	488	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	197:LYS	C	198:ASN	N	4.81
1	B	502:GLU	C	503:PHE	N	3.25
1	A	392:PHE	C	393:HIS	N	2.99

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	469/552 (84%)	0.66	37 (7%) 18 15	36, 55, 91, 114	0
1	B	460/552 (83%)	0.49	22 (4%) 35 32	35, 51, 81, 108	0
1	C	467/552 (84%)	0.35	14 (2%) 52 48	32, 49, 77, 103	0
1	D	476/552 (86%)	0.48	24 (5%) 34 30	33, 52, 84, 109	0
All	All	1872/2208 (84%)	0.49	97 (5%) 33 29	32, 52, 84, 114	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	VAL	7.1
1	A	123	ALA	6.5
1	A	122	ALA	6.2
1	A	147	GLY	5.7
1	D	215	SER	5.4
1	A	513	ALA	4.4
1	A	151	LEU	4.4
1	A	125	LEU	4.2
1	D	210	GLY	4.1
1	B	407	PHE	4.1
1	B	195	SER	4.0
1	D	151	LEU	4.0
1	C	77	ILE	3.9
1	B	152	LYS	3.7
1	D	511	THR	3.7
1	D	77	ILE	3.6
1	D	148	LYS	3.3
1	B	409	THR	3.3
1	C	123	ALA	3.3
1	D	147	GLY	3.1
1	C	218	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	405	ASN	3.1
1	A	244	TYR	3.1
1	A	215	SER	3.1
1	D	206	VAL	3.0
1	B	383	THR	3.0
1	B	77	ILE	3.0
1	C	70	ALA	3.0
1	B	124	VAL	2.9
1	B	80	ALA	2.8
1	A	514	LYS	2.8
1	C	80	ALA	2.8
1	B	81	GLY	2.7
1	A	467	LYS	2.7
1	A	150	GLN	2.7
1	D	152	LYS	2.7
1	A	9	PRO	2.7
1	A	481	ILE	2.7
1	B	8	THR	2.7
1	B	123	ALA	2.7
1	A	126	GLY	2.6
1	D	149	ASN	2.6
1	C	8	THR	2.6
1	B	494	LEU	2.6
1	D	491	ILE	2.6
1	A	409	THR	2.6
1	A	491	ILE	2.5
1	C	410	GLY	2.5
1	C	67	LEU	2.5
1	D	196	LYS	2.5
1	A	149	ASN	2.5
1	A	389	ALA	2.5
1	D	409	THR	2.5
1	B	509	PRO	2.4
1	A	119	LEU	2.4
1	A	286	ALA	2.4
1	A	120	ASP	2.4
1	C	81	GLY	2.4
1	A	407	PHE	2.4
1	A	441	ASN	2.4
1	D	329	ALA	2.4
1	D	216	TRP	2.4
1	D	116	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	246	ASN	2.3
1	B	78	ALA	2.3
1	C	116	GLY	2.2
1	A	406	SER	2.2
1	D	290	LYS	2.2
1	A	411	GLU	2.2
1	A	442	THR	2.2
1	A	116	GLY	2.2
1	B	508	VAL	2.2
1	B	18	LYS	2.2
1	A	192	ILE	2.2
1	B	216	TRP	2.2
1	C	60	LYS	2.2
1	B	125	LEU	2.2
1	D	412	SER	2.2
1	A	121	ARG	2.2
1	D	61	LYS	2.2
1	A	194	ALA	2.1
1	C	78	ALA	2.1
1	A	512	GLY	2.1
1	A	216	TRP	2.1
1	A	443	GLY	2.1
1	D	443	GLY	2.1
1	C	146	ARG	2.1
1	D	153	LYS	2.1
1	D	150	GLN	2.1
1	B	320	THR	2.1
1	C	441	ASN	2.0
1	D	67	LEU	2.0
1	B	390	GLY	2.0
1	A	445	THR	2.0
1	D	442	THR	2.0
1	B	406	SER	2.0
1	A	10	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.