



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:31 PM UTC

PDB ID : 9BJL / pdb_00009bjl
Title : Crystal structure of Influenza D virus Nucleoprotein (Oklahoma)
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2024-04-25
Resolution : 2.43 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

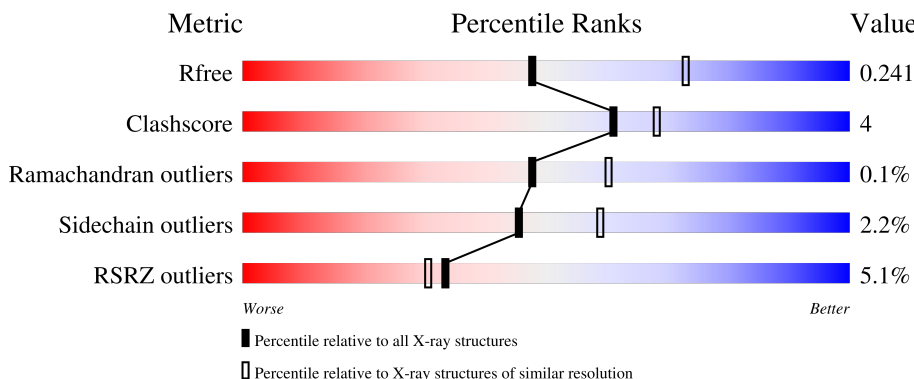
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	571	5% 74% 8% 18%
1	B	571	5% 67% 11% 20%
1	C	571	3% 73% 6% 20%
1	D	571	4% 72% 8% 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14456 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	468	Total	C	N	O	S	0	0	0
			3673	2330	634	683	26			
1	B	456	Total	C	N	O	S	0	0	0
			3580	2271	613	670	26			
1	C	455	Total	C	N	O	S	0	0	0
			3571	2263	614	668	26			
1	D	458	Total	C	N	O	S	0	0	0
			3588	2275	615	672	26			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	initiating methionine	UNP W5RBB9
A	-17	GLY	-	expression tag	UNP W5RBB9
A	-16	SER	-	expression tag	UNP W5RBB9
A	-15	SER	-	expression tag	UNP W5RBB9
A	-14	HIS	-	expression tag	UNP W5RBB9
A	-13	HIS	-	expression tag	UNP W5RBB9
A	-12	HIS	-	expression tag	UNP W5RBB9
A	-11	HIS	-	expression tag	UNP W5RBB9
A	-10	HIS	-	expression tag	UNP W5RBB9
A	-9	HIS	-	expression tag	UNP W5RBB9
A	-8	SER	-	expression tag	UNP W5RBB9
A	-7	SER	-	expression tag	UNP W5RBB9
A	-6	GLY	-	expression tag	UNP W5RBB9
A	-5	LEU	-	expression tag	UNP W5RBB9
A	-4	VAL	-	expression tag	UNP W5RBB9
A	-3	PRO	-	expression tag	UNP W5RBB9
A	-2	ARG	-	expression tag	UNP W5RBB9
A	-1	GLY	-	expression tag	UNP W5RBB9
A	0	SER	-	expression tag	UNP W5RBB9
B	-18	MET	-	initiating methionine	UNP W5RBB9
B	-17	GLY	-	expression tag	UNP W5RBB9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP W5RBB9
B	-15	SER	-	expression tag	UNP W5RBB9
B	-14	HIS	-	expression tag	UNP W5RBB9
B	-13	HIS	-	expression tag	UNP W5RBB9
B	-12	HIS	-	expression tag	UNP W5RBB9
B	-11	HIS	-	expression tag	UNP W5RBB9
B	-10	HIS	-	expression tag	UNP W5RBB9
B	-9	HIS	-	expression tag	UNP W5RBB9
B	-8	SER	-	expression tag	UNP W5RBB9
B	-7	SER	-	expression tag	UNP W5RBB9
B	-6	GLY	-	expression tag	UNP W5RBB9
B	-5	LEU	-	expression tag	UNP W5RBB9
B	-4	VAL	-	expression tag	UNP W5RBB9
B	-3	PRO	-	expression tag	UNP W5RBB9
B	-2	ARG	-	expression tag	UNP W5RBB9
B	-1	GLY	-	expression tag	UNP W5RBB9
B	0	SER	-	expression tag	UNP W5RBB9
C	-18	MET	-	initiating methionine	UNP W5RBB9
C	-17	GLY	-	expression tag	UNP W5RBB9
C	-16	SER	-	expression tag	UNP W5RBB9
C	-15	SER	-	expression tag	UNP W5RBB9
C	-14	HIS	-	expression tag	UNP W5RBB9
C	-13	HIS	-	expression tag	UNP W5RBB9
C	-12	HIS	-	expression tag	UNP W5RBB9
C	-11	HIS	-	expression tag	UNP W5RBB9
C	-10	HIS	-	expression tag	UNP W5RBB9
C	-9	HIS	-	expression tag	UNP W5RBB9
C	-8	SER	-	expression tag	UNP W5RBB9
C	-7	SER	-	expression tag	UNP W5RBB9
C	-6	GLY	-	expression tag	UNP W5RBB9
C	-5	LEU	-	expression tag	UNP W5RBB9
C	-4	VAL	-	expression tag	UNP W5RBB9
C	-3	PRO	-	expression tag	UNP W5RBB9
C	-2	ARG	-	expression tag	UNP W5RBB9
C	-1	GLY	-	expression tag	UNP W5RBB9
C	0	SER	-	expression tag	UNP W5RBB9
D	-18	MET	-	initiating methionine	UNP W5RBB9
D	-17	GLY	-	expression tag	UNP W5RBB9
D	-16	SER	-	expression tag	UNP W5RBB9
D	-15	SER	-	expression tag	UNP W5RBB9
D	-14	HIS	-	expression tag	UNP W5RBB9
D	-13	HIS	-	expression tag	UNP W5RBB9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-12	HIS	-	expression tag	UNP W5RBB9
D	-11	HIS	-	expression tag	UNP W5RBB9
D	-10	HIS	-	expression tag	UNP W5RBB9
D	-9	HIS	-	expression tag	UNP W5RBB9
D	-8	SER	-	expression tag	UNP W5RBB9
D	-7	SER	-	expression tag	UNP W5RBB9
D	-6	GLY	-	expression tag	UNP W5RBB9
D	-5	LEU	-	expression tag	UNP W5RBB9
D	-4	VAL	-	expression tag	UNP W5RBB9
D	-3	PRO	-	expression tag	UNP W5RBB9
D	-2	ARG	-	expression tag	UNP W5RBB9
D	-1	GLY	-	expression tag	UNP W5RBB9
D	0	SER	-	expression tag	UNP W5RBB9

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0

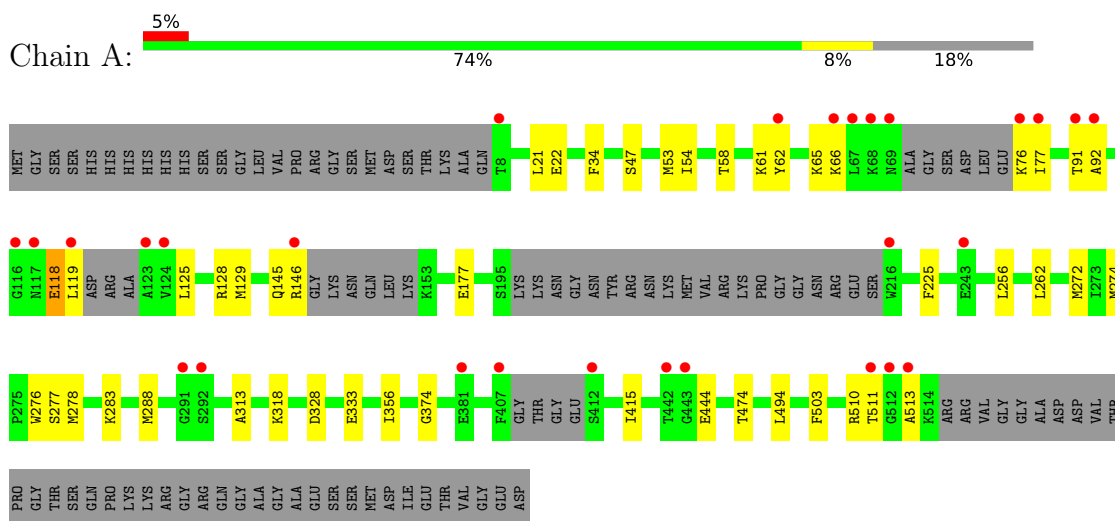
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	9	Total O 9 9	0	0
3	C	13	Total O 13 13	0	0
3	D	13	Total O 13 13	0	0

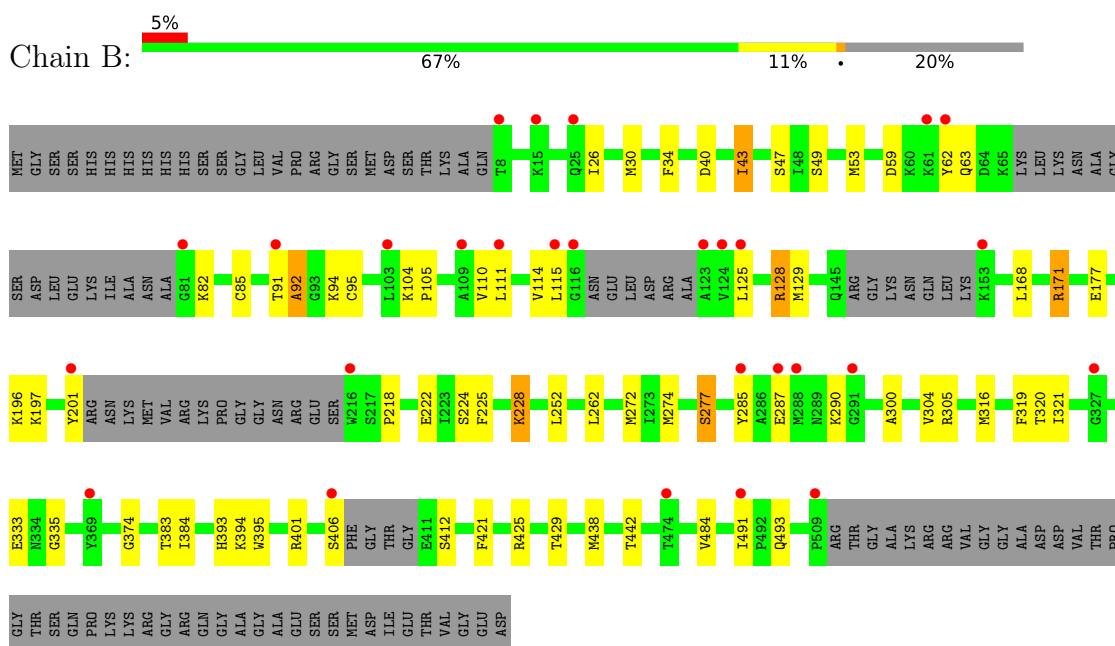
3 Residue-property plots [i](#)

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.

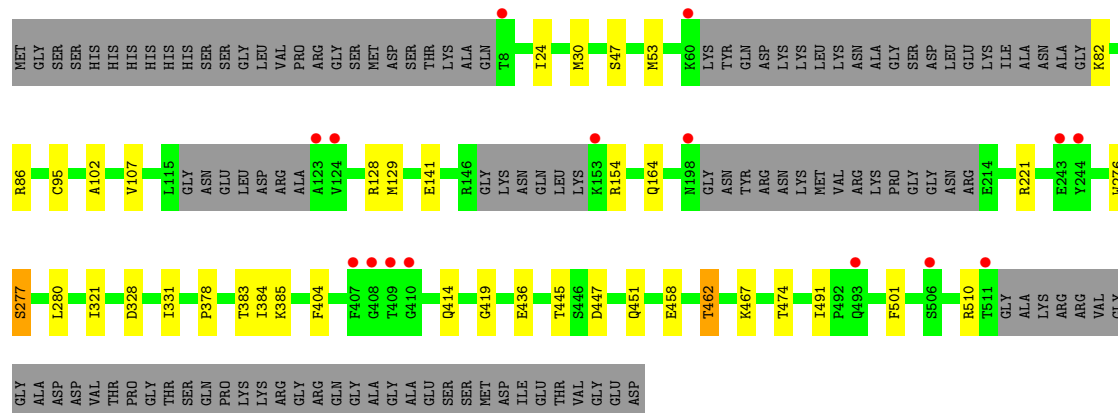
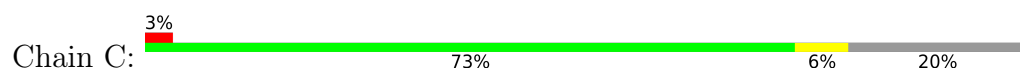
• Molecule 1: Nucleoprotein



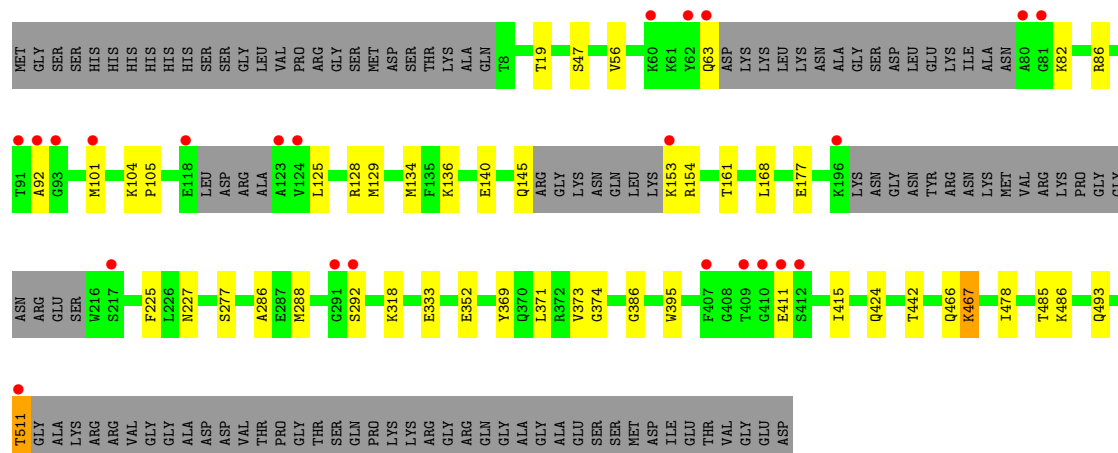
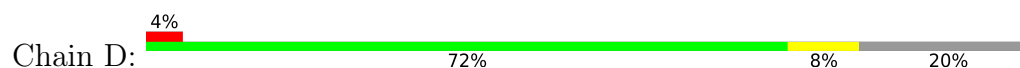
• Molecule 1: Nucleoprotein



• Molecule 1: Nucleoprotein



● Molecule 1: Nucleoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	74.46Å 84.50Å 88.73Å 102.34° 97.37° 97.14°	Depositor
Resolution (Å)	85.57 – 2.43 85.56 – 2.43	Depositor EDS
% Data completeness (in resolution range)	91.8 (85.57-2.43) 91.9 (85.56-2.43)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, R_{free}	0.203 , 0.241 0.205 , 0.241	Depositor DCC
R_{free} test set	3511 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14456	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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

Bond lengths and bond angles in the following residue types are not validated in this section:
CL

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	0.29	0/3733	0.47	0/5011
1	B	0.25	0/3640	0.44	0/4888
1	C	0.24	0/3631	0.42	0/4878
1	D	0.25	0/3649	0.45	0/4903
All	All	0.26	0/14653	0.45	0/19680

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	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	171	ARG	Sidechain
1	D	86	ARG	Sidechain

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	3673	0	3721	35	0
1	B	3580	0	3608	44	0
1	C	3571	0	3604	21	0
1	D	3588	0	3614	32	0
2	A	1	0	0	0	0
3	A	8	0	0	0	0
3	B	9	0	0	0	0
3	C	13	0	0	0	0
3	D	13	0	0	0	0
All	All	14456	0	14547	122	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 (122) 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:128:ARG:HG3	1:C:129:MET:HE2	1.56	0.87
1:B:110:VAL:O	1:B:114:VAL:HG23	1.92	0.69
1:A:177:GLU:HG3	1:A:225:PHE:CG	2.33	0.64
1:A:125:LEU:CD1	1:A:129:MET:HE3	2.28	0.63
1:A:125:LEU:HD11	1:A:129:MET:HE3	1.81	0.62
1:B:285:TYR:CD1	1:B:316:MET:HE3	2.34	0.61
1:C:128:ARG:CG	1:C:129:MET:HE2	2.29	0.61
1:B:285:TYR:HD1	1:B:316:MET:HE3	1.66	0.60
1:A:58:THR:HG21	1:A:125:LEU:HD21	1.84	0.60
1:A:22:GLU:OE1	1:A:128:ARG:NH2	2.35	0.59
1:B:493:GLN:O	1:B:493:GLN:HG2	2.03	0.58
1:B:272:MET:SD	1:B:274:MET:HG3	2.44	0.57
1:C:458:GLU:O	1:C:462:THR:HG22	2.04	0.57
1:B:177:GLU:HG3	1:B:225:PHE:CG	2.40	0.56
1:D:177:GLU:HG3	1:D:225:PHE:CG	2.41	0.56
1:D:369:TYR:HD1	1:D:511:THR:HG22	1.71	0.56
1:D:125:LEU:HD11	1:D:129:MET:HE3	1.88	0.55
1:B:287:GLU:HG2	1:B:290:LYS:HZ1	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ARG:HB2	1:A:129:MET:HE2	1.89	0.55
1:A:328:ASP:OD1	1:A:510:ARG:NH2	2.39	0.55
1:D:177:GLU:HG3	1:D:225:PHE:CD2	2.43	0.54
1:B:429:THR:O	1:C:467:LYS:NZ	2.41	0.53
1:C:47:SER:HB2	1:C:277:SER:HB3	1.91	0.52
1:D:153:LYS:HG3	1:D:154:ARG:H	1.74	0.52
1:A:262:LEU:HD13	1:D:415:ILE:HD11	1.90	0.52
1:B:320:THR:HG22	1:B:384:ILE:CD1	2.39	0.52
1:C:95:CYS:HB3	1:C:384:ILE:HG13	1.91	0.52
1:A:272:MET:SD	1:A:274:MET:HG3	2.50	0.52
1:B:287:GLU:HG2	1:B:290:LYS:NZ	2.24	0.52
1:D:125:LEU:CD1	1:D:129:MET:HE3	2.41	0.51
1:D:136:LYS:NZ	1:D:140:GLU:OE2	2.40	0.51
1:C:82:LYS:N	1:C:102:ALA:O	2.43	0.51
1:A:129:MET:HE1	1:A:276:TRP:CH2	2.45	0.51
1:A:256:LEU:HD13	1:D:442:THR:HG21	1.93	0.51
1:B:91:THR:CG2	1:B:94:LYS:HE3	2.41	0.50
1:A:177:GLU:HG3	1:A:225:PHE:CD2	2.46	0.50
1:D:177:GLU:HG3	1:D:225:PHE:CD1	2.47	0.50
1:B:104:LYS:HB3	1:B:105:PRO:HD3	1.94	0.50
1:D:153:LYS:HG3	1:D:154:ARG:N	2.28	0.49
1:D:56:VAL:HG12	1:D:63:GLN:HB2	1.95	0.48
1:A:34:PHE:CE2	1:A:53:MET:HE2	2.48	0.48
1:A:62:TYR:CE2	1:A:66:LYS:HD2	2.48	0.48
1:A:129:MET:HE1	1:A:276:TRP:HH2	1.77	0.48
1:C:30:MET:HE1	1:C:107:VAL:HG13	1.95	0.48
1:B:125:LEU:HD12	1:B:129:MET:HE3	1.96	0.48
1:A:415:ILE:HD11	1:B:262:LEU:HD13	1.97	0.47
1:B:26:ILE:HD11	1:B:115:LEU:HD21	1.95	0.47
1:B:177:GLU:HG3	1:B:225:PHE:CD1	2.49	0.47
1:D:47:SER:HB2	1:D:277:SER:HB3	1.97	0.47
1:A:91:THR:O	1:A:92:ALA:HB3	2.14	0.47
1:A:177:GLU:HG3	1:A:225:PHE:CD1	2.49	0.47
1:D:318:LYS:HD3	1:D:386:GLY:HA2	1.96	0.47
1:B:300:ALA:HB3	1:B:305:ARG:HB2	1.97	0.47
1:B:47:SER:HB2	1:B:277:SER:HB3	1.96	0.47
1:D:395:TRP:HH2	1:D:486:LYS:HE3	1.79	0.46
1:C:321:ILE:HB	1:C:383:THR:HG23	1.97	0.46
1:A:21:LEU:CD2	1:A:283:LYS:HE3	2.46	0.46
1:A:503:PHE:CD2	1:D:411:GLU:O	2.69	0.46
1:C:129:MET:HE1	1:C:276:TRP:HH2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:CYS:HB3	1:B:384:ILE:HG12	1.98	0.46
1:D:371:LEU:HB3	1:D:373:VAL:HG23	1.98	0.46
1:A:54:ILE:O	1:A:58:THR:HG23	2.16	0.46
1:A:356:ILE:HD13	1:A:494:LEU:HD21	1.98	0.46
1:B:34:PHE:CE2	1:B:53:MET:HE2	2.50	0.46
1:C:141:GLU:OE2	1:C:164:GLN:HA	2.16	0.45
1:D:19:THR:HG23	1:D:128:ARG:NH2	2.31	0.45
1:D:466:GLN:O	1:D:467:LYS:C	2.60	0.45
1:B:224:SER:O	1:B:228:LYS:HG3	2.16	0.45
1:B:421:PHE:O	1:B:425:ARG:NH2	2.50	0.45
1:A:125:LEU:HD12	1:A:129:MET:HE3	1.98	0.45
1:B:30:MET:CE	1:B:111:LEU:HG	2.46	0.44
1:B:201:TYR:C	1:B:201:TYR:CD1	2.96	0.44
1:A:274:MET:HE1	1:A:313:ALA:HB3	1.99	0.44
1:B:94:LYS:HG2	1:B:95:CYS:H	1.82	0.44
1:B:321:ILE:HD11	1:B:335:GLY:HA2	1.99	0.44
1:C:419:GLY:HA2	1:D:352:GLU:OE1	2.17	0.44
1:B:438:MET:O	1:B:442:THR:OG1	2.31	0.44
1:D:128:ARG:HG3	1:D:129:MET:HE2	1.99	0.44
1:B:320:THR:HG22	1:B:384:ILE:HD13	1.99	0.43
1:A:274:MET:CE	1:A:278:MET:HE2	2.48	0.43
1:B:218:PRO:O	1:B:222:GLU:HG2	2.18	0.43
1:B:412:SER:CB	1:C:501:PHE:O	2.66	0.43
1:C:328:ASP:HB3	1:C:331:ILE:HD12	2.01	0.43
1:C:385:LYS:HB2	1:C:385:LYS:HE2	1.75	0.43
1:D:177:GLU:HG3	1:D:225:PHE:CE2	2.53	0.43
1:B:125:LEU:CD1	1:B:129:MET:HE3	2.48	0.43
1:B:304:VAL:HG11	1:B:484:VAL:HG13	2.00	0.43
1:D:104:LYS:HB3	1:D:105:PRO:HD3	2.00	0.43
1:B:91:THR:O	1:B:92:ALA:HB3	2.18	0.43
1:C:86:ARG:HG2	1:C:378:PRO:HG2	2.00	0.43
1:A:118:GLU:O	1:A:119:LEU:C	2.61	0.42
1:C:404:PHE:HB3	1:C:436:GLU:OE2	2.19	0.42
1:B:59:ASP:O	1:B:63:GLN:HG2	2.19	0.42
1:C:24:ILE:HG23	1:C:280:LEU:HD13	2.02	0.42
1:A:274:MET:HE1	1:A:313:ALA:CB	2.49	0.42
1:C:414:GLN:HG3	1:D:161:THR:HG21	2.01	0.42
1:D:493:GLN:O	1:D:493:GLN:HG3	2.20	0.42
1:C:53:MET:HE3	1:C:53:MET:HB3	1.98	0.41
1:D:286:ALA:HA	1:D:292:SER:OG	2.19	0.41
1:B:40:ASP:HA	1:B:43:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:LYS:HD2	1:D:101:MET:SD	2.59	0.41
1:B:304:VAL:HB	1:B:395:TRP:CE2	2.56	0.41
1:B:319:PHE:HE1	1:B:321:ILE:HD11	1.86	0.41
1:A:77:ILE:H	1:A:77:ILE:HG12	1.71	0.41
1:A:444:GLU:HG2	1:B:252:LEU:CD2	2.50	0.41
1:D:395:TRP:HH2	1:D:486:LYS:CE	2.34	0.41
1:D:485:THR:O	1:D:486:LYS:HB2	2.20	0.41
1:B:49:SER:HG	1:B:85:CYS:HG	1.65	0.41
1:B:128:ARG:HB2	1:B:129:MET:HE2	2.01	0.41
1:D:134:MET:HA	1:D:168:LEU:HD21	2.02	0.41
1:A:47:SER:HB2	1:A:277:SER:HB3	2.03	0.41
1:B:225:PHE:HA	1:B:228:LYS:HD2	2.02	0.41
1:A:274:MET:HE2	1:A:278:MET:HB3	2.02	0.41
1:C:447:ASP:HA	1:C:451:GLN:OE1	2.21	0.41
1:D:333:GLU:OE2	1:D:374:GLY:HA3	2.21	0.40
1:A:474:THR:HA	1:D:424:GLN:HG3	2.02	0.40
1:B:91:THR:O	1:B:91:THR:HG23	2.20	0.40
1:A:145:GLN:O	1:A:146:ARG:HG2	2.21	0.40
1:A:333:GLU:OE2	1:A:374:GLY:HA3	2.21	0.40
1:B:401:ARG:NH1	1:B:406:SER:O	2.50	0.40
1:A:511:THR:C	1:A:513:ALA:H	2.30	0.40
1:B:333:GLU:OE2	1:B:374:GLY:HA3	2.21	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	456/571 (80%)	449 (98%)	7 (2%)	0	100	100
1	B	444/571 (78%)	437 (98%)	6 (1%)	1 (0%)	43	53
1	C	445/571 (78%)	440 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	448/571 (78%)	442 (99%)	5 (1%)	1 (0%)	43 53
All	All	1793/2284 (78%)	1768 (99%)	23 (1%)	2 (0%)	48 60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	92	ALA
1	B	92	ALA

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	396/476 (83%)	390 (98%)	6 (2%)	57 69
1	B	387/476 (81%)	373 (96%)	14 (4%)	31 42
1	C	387/476 (81%)	379 (98%)	8 (2%)	47 60
1	D	387/476 (81%)	381 (98%)	6 (2%)	55 68
All	All	1557/1904 (82%)	1523 (98%)	34 (2%)	45 59

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LYS
1	A	65	LYS
1	A	76	LYS
1	A	118	GLU
1	A	288	MET
1	A	318	LYS
1	B	43	ILE
1	B	62	TYR
1	B	82	LYS
1	B	128	ARG
1	B	168	LEU
1	B	171	ARG

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Mol	Chain	Res	Type
1	B	196	LYS
1	B	197	LYS
1	B	228	LYS
1	B	277	SER
1	B	383	THR
1	B	393	HIS
1	B	394	LYS
1	B	491	ILE
1	C	154	ARG
1	C	221	ARG
1	C	277	SER
1	C	445	THR
1	C	462	THR
1	C	474	THR
1	C	491	ILE
1	C	510	ARG
1	D	145	GLN
1	D	227	ASN
1	D	288	MET
1	D	467	LYS
1	D	478	ILE
1	D	511	THR

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	251	GLN
1	B	179	HIS
1	B	251	GLN
1	B	270	HIS
1	B	289	ASN
1	C	12	GLN
1	C	251	GLN
1	C	270	HIS
1	C	289	ASN
1	D	270	HIS
1	D	289	ASN
1	D	466	GLN

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	468/571 (81%)	0.32	28 (5%)	27 24	35, 50, 88, 115	0
1	B	456/571 (79%)	0.58	28 (6%)	27 23	36, 65, 107, 140	0
1	C	455/571 (79%)	0.15	15 (3%)	49 48	32, 47, 78, 127	0
1	D	458/571 (80%)	0.23	23 (5%)	34 31	32, 49, 88, 144	0
All	All	1837/2284 (80%)	0.32	94 (5%)	33 30	32, 51, 95, 144	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	VAL	6.4
1	A	124	VAL	5.5
1	C	124	VAL	4.3
1	C	123	ALA	4.2
1	A	513	ALA	4.2
1	B	123	ALA	4.1
1	A	67	LEU	3.7
1	A	216	TRP	3.6
1	C	409	THR	3.6
1	A	123	ALA	3.6
1	A	412	SER	3.6
1	C	407	PHE	3.5
1	C	8	THR	3.4
1	C	244	TYR	3.3
1	A	119	LEU	3.2
1	A	407	PHE	3.1
1	D	196	LYS	3.1
1	A	76	LYS	3.1
1	B	116	GLY	3.1
1	D	409	THR	3.0
1	D	124	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	410	GLY	3.0
1	D	81	GLY	3.0
1	A	146	ARG	2.9
1	B	61	LYS	2.9
1	B	153	LYS	2.9
1	B	216	TRP	2.8
1	D	291	GLY	2.8
1	B	474	THR	2.8
1	D	80	ALA	2.8
1	D	123	ALA	2.8
1	B	103	LEU	2.8
1	C	408	GLY	2.7
1	D	93	GLY	2.7
1	C	506	SER	2.7
1	A	511	THR	2.7
1	A	77	ILE	2.7
1	D	411	GLU	2.7
1	A	291	GLY	2.7
1	D	412	SER	2.7
1	A	442	THR	2.7
1	C	410	GLY	2.6
1	A	512	GLY	2.6
1	A	68	LYS	2.6
1	B	285	TYR	2.6
1	D	101	MET	2.6
1	A	243	GLU	2.5
1	A	69	ASN	2.5
1	B	8	THR	2.5
1	A	116	GLY	2.5
1	D	63	GLN	2.5
1	A	443	GLY	2.5
1	B	327	GLY	2.5
1	B	111	LEU	2.5
1	B	115	LEU	2.5
1	C	511	THR	2.5
1	B	369	TYR	2.5
1	B	25	GLN	2.4
1	D	60	LYS	2.4
1	D	118	GLU	2.4
1	B	406	SER	2.4
1	A	92	ALA	2.4
1	B	15	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	511	THR	2.3
1	B	125	LEU	2.3
1	B	62	TYR	2.3
1	D	92	ALA	2.3
1	D	292	SER	2.3
1	B	509	PRO	2.3
1	D	62	TYR	2.3
1	C	60	LYS	2.2
1	A	381	GLU	2.2
1	D	407	PHE	2.2
1	A	292	SER	2.2
1	B	287	GLU	2.2
1	B	109	ALA	2.2
1	B	201	TYR	2.2
1	B	288	MET	2.2
1	D	217	SER	2.2
1	C	153	LYS	2.2
1	A	117	ASN	2.2
1	B	81	GLY	2.1
1	B	91	THR	2.1
1	D	91	THR	2.1
1	C	243	GLU	2.1
1	A	62	TYR	2.1
1	C	493	GLN	2.1
1	C	198	ASN	2.1
1	B	491	ILE	2.1
1	A	66	LYS	2.1
1	B	291	GLY	2.0
1	A	8	THR	2.0
1	A	91	THR	2.0
1	D	153	LYS	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CL	A	601	1/1	0.98	0.10	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.