Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2024 – 04:18 PM EDT

PDB ID	:	9BJL
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:

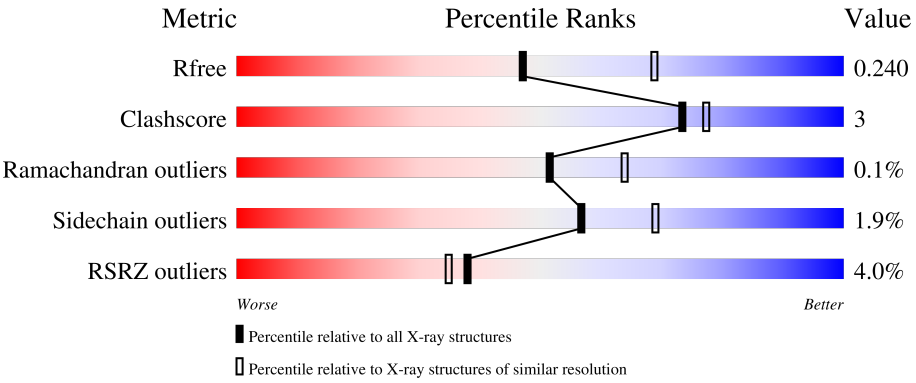
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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}	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (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 <=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	3% 75% 7% 18%
1	B	571	6% 70% 9% 20%
1	C	571	2% 74% 6% 20%
1	D	571	3% 72% 8% 20%

2 Entry composition (i)

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 (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is water.

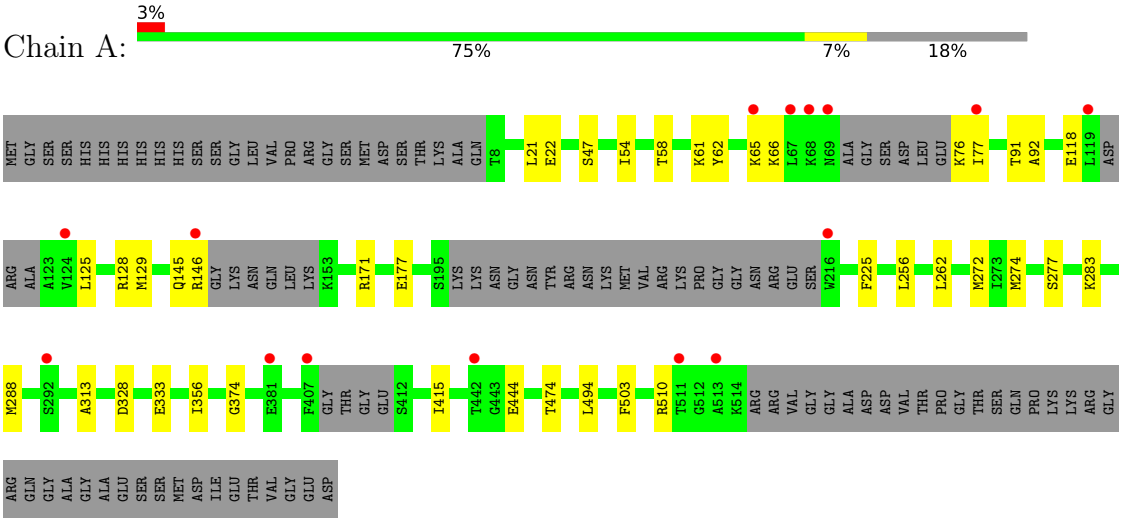
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total O 8 8	0	0
3	B	9	Total O 9 9	0	0
3	C	13	Total O 13 13	0	0
3	D	13	Total O 13 13	0	0

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.

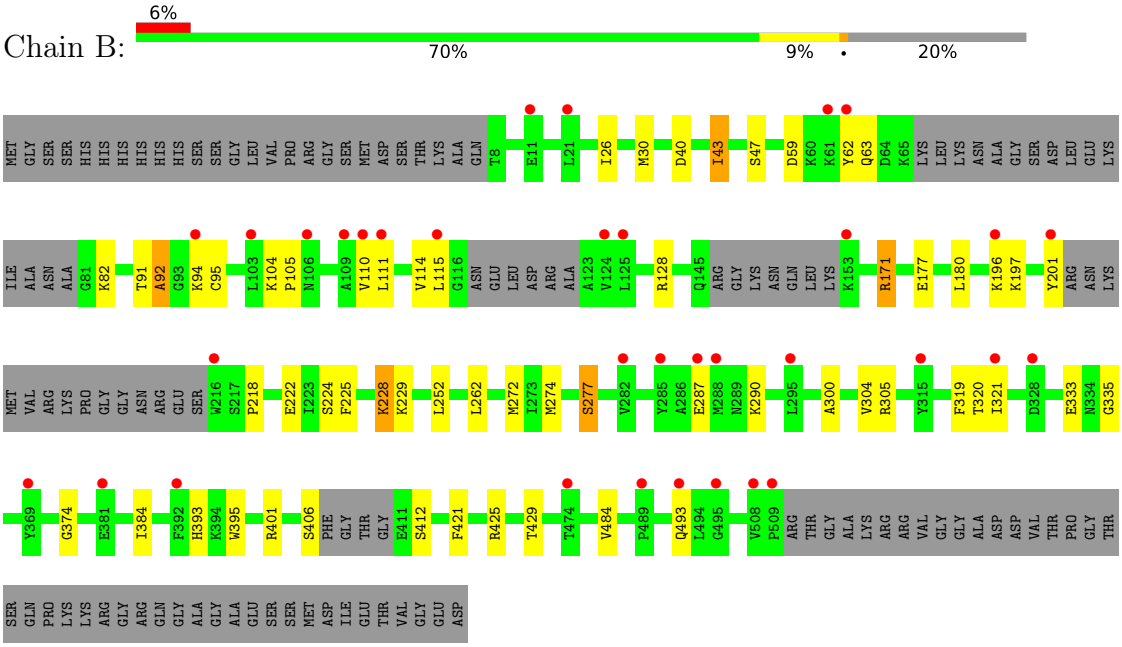
- Molecule 1: Nucleoprotein

Chain A:



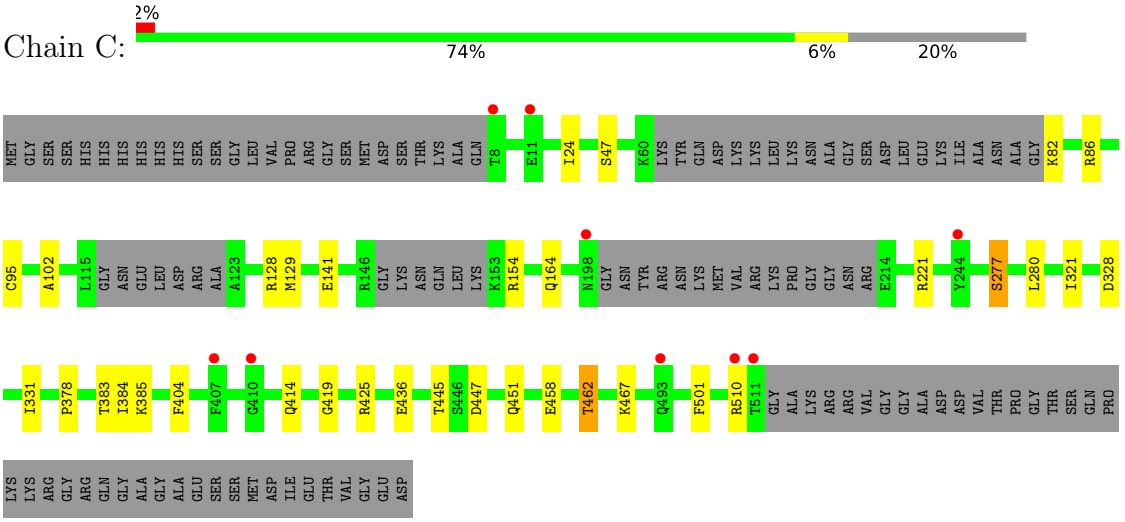
- Molecule 1: Nucleoprotein

Chain B:



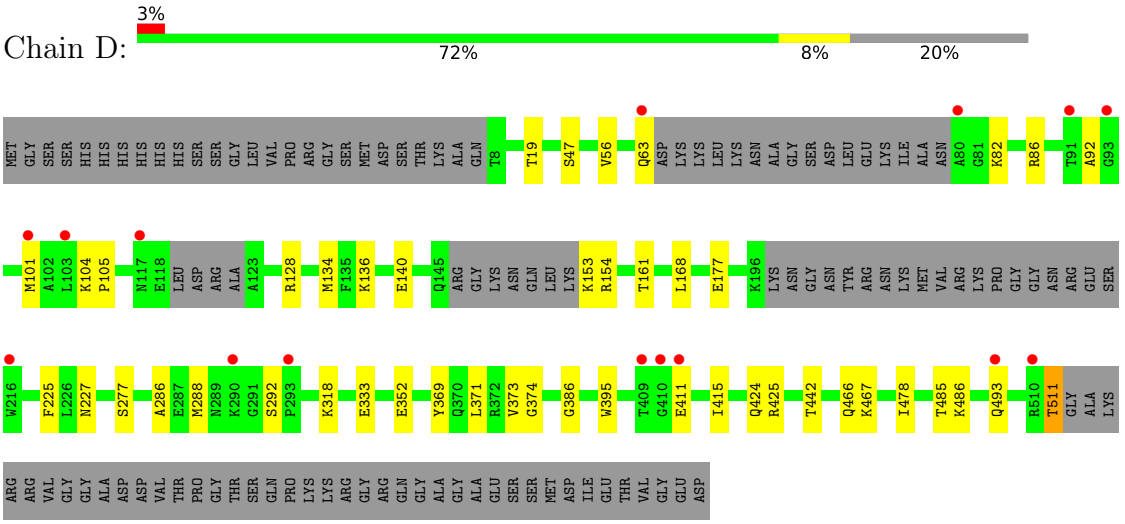
- Molecule 1: Nucleoprotein

Chain C:



• Molecule 1: Nucleoprotein

Chain D:



4 Data and refinement statistics (i)

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 85.57 – 2.43	Depositor EDS
% Data completeness (in resolution range)	91.8 (85.57-2.43) 91.9 (85.57-2.43)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, R_{free}	0.203 , 0.241 0.204 , 0.240	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)	0.38 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.35	0/3733	0.54	0/5011
1	B	0.33	0/3640	0.54	0/4888
1	C	0.34	0/3631	0.55	0/4878
1	D	0.33	0/3649	0.55	0/4903
All	All	0.34	0/14653	0.54	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 (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	3673	0	3721	24	0
1	B	3580	0	3608	36	0
1	C	3571	0	3604	17	0
1	D	3588	0	3614	29	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	96	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 3.

All (96) 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: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: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:B:287:GLU:HG2	1:B:290:LYS:HZ1	1.70	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:125:LEU:HD12	1:A:129:MET:HE2	1.92	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:62:TYR:CE2	1:A:66:LYS:HD2	2.48	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:A:274:MET:HE1	1:A:313:ALA:CB	2.45	0.46
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: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: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: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:B:30:MET:CE	1:B:111:LEU:HG	2.46	0.44
1:B:94:LYS:HG2	1:B:95:CYS:H	1.82	0.44
1:B:180:LEU:O	1:B:229:LYS:NZ	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:THR:HG22	1:B:384:ILE:HD13	1.99	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: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: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: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: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
1:D:82:LYS:HD2	1:D:101:MET:SD	2.59	0.41
1:C:128:ARG:HG3	1:C:129:MET:CE	2.50	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: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:D:466:GLN:O	1:D:467:LYS:C	2.60	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: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%)	47	57
1	C	445/571 (78%)	440 (99%)	5 (1%)	0	100	100
1	D	448/571 (78%)	442 (99%)	5 (1%)	1 (0%)	47	57
All	All	1793/2284 (78%)	1768 (99%)	23 (1%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

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%)	65	76
1	B	387/476 (81%)	376 (97%)	11 (3%)	43	56
1	C	387/476 (81%)	380 (98%)	7 (2%)	59	71
1	D	387/476 (81%)	382 (99%)	5 (1%)	69	80
All	All	1557/1904 (82%)	1528 (98%)	29 (2%)	57	69

All (29) 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	171	ARG
1	A	288	MET
1	B	43	ILE
1	B	62	TYR
1	B	82	LYS
1	B	128	ARG
1	B	171	ARG
1	B	196	LYS
1	B	197	LYS
1	B	201	TYR
1	B	228	LYS
1	B	277	SER
1	B	393	HIS
1	C	154	ARG
1	C	221	ARG
1	C	277	SER
1	C	425	ARG
1	C	445	THR
1	C	462	THR
1	C	510	ARG
1	D	227	ASN
1	D	288	MET
1	D	425	ARG
1	D	478	ILE
1	D	511	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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, 95^{th} 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%)	0.27	15 (3%)	47	44	35, 50, 88, 115	0
1	B	456/571 (79%)	0.53	34 (7%)	14	11	36, 65, 107, 140	0
1	C	455/571 (79%)	0.17	9 (1%)	65	61	32, 47, 78, 127	0
1	D	458/571 (80%)	0.22	15 (3%)	46	43	32, 49, 88, 144	0
All	All	1837/2284 (80%)	0.30	73 (3%)	38	35	32, 51, 95, 144	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	62	TYR	5.9
1	B	61	LYS	5.0
1	D	409	THR	4.6
1	A	67	LEU	4.5
1	B	315	TYR	4.5
1	D	63	GLN	4.4
1	D	80	ALA	4.2
1	A	292	SER	4.2
1	A	216	TRP	3.9
1	A	511	THR	3.8
1	B	111	LEU	3.7
1	D	411	GLU	3.6
1	B	282	VAL	3.5
1	B	285	TYR	3.4
1	A	68	LYS	3.4
1	C	8	THR	3.3
1	B	109	ALA	3.3
1	C	407	PHE	3.3
1	D	493	GLN	3.2
1	B	106	ASN	3.2
1	B	125	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	288	MET	3.0
1	B	287	GLU	3.0
1	A	513	ALA	3.0
1	A	407	PHE	3.0
1	B	103	LEU	3.0
1	A	119	LEU	3.0
1	B	11	GLU	2.9
1	B	94	LYS	2.9
1	C	198	ASN	2.9
1	B	153	LYS	2.8
1	B	321	ILE	2.8
1	D	93	GLY	2.8
1	B	369	TYR	2.7
1	B	115	LEU	2.7
1	B	509	PRO	2.6
1	B	110	VAL	2.6
1	C	410	GLY	2.6
1	B	201	TYR	2.6
1	A	442	THR	2.6
1	B	216	TRP	2.5
1	C	244	TYR	2.4
1	B	392	PHE	2.4
1	B	381	GLU	2.4
1	B	493	GLN	2.4
1	C	11	GLU	2.4
1	D	103	LEU	2.4
1	D	91	THR	2.4
1	B	124	VAL	2.4
1	B	495	GLY	2.4
1	B	508	VAL	2.4
1	B	295	LEU	2.3
1	D	510	ARG	2.3
1	A	69	ASN	2.3
1	B	474	THR	2.3
1	C	493	GLN	2.3
1	B	328	ASP	2.3
1	D	117	ASN	2.2
1	C	511	THR	2.2
1	D	216	TRP	2.2
1	D	293	PRO	2.2
1	D	410	GLY	2.2
1	A	77	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	65	LYS	2.1
1	C	510	ARG	2.1
1	B	21	LEU	2.1
1	A	146	ARG	2.1
1	B	489	PRO	2.1
1	A	124	VAL	2.1
1	D	101	MET	2.1
1	B	196	LYS	2.1
1	D	290	LYS	2.1
1	A	381	GLU	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 monosaccharides 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, 95^{th} 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	0.96	0.12	69,69,69,69	0

6.5 Other polymers (i)

There are no such residues in this entry.