Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:25 pm BST

PDB ID	:	5N2U
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 following versions of software and data (see references ⓘ) were used in the production of this report:

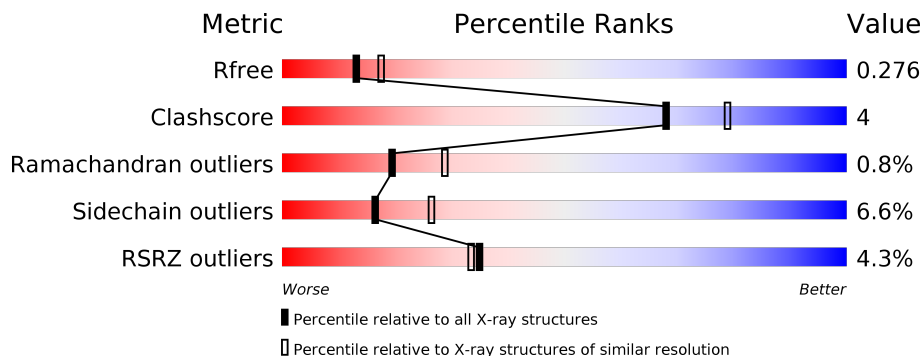|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.40 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	Percentile Ranks	Value
Rfree		0.276
Clashscore		4
Ramachandran outliers		0.8%
Sidechain outliers		6.6%
RSRZ outliers		4.3%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 on 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	552	5% — 68% / 16% / • / 15%
1	B	552	4% — 70% / 12% / • / 17%
1	C	552	3% — 74% / 9% / • / 15%
1	D	552	3% — 75% / 10% / • / 14%

2 Entry composition (i)

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.
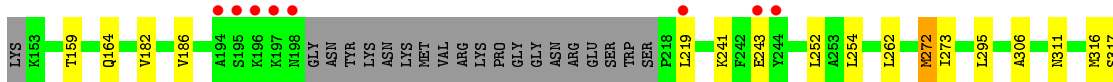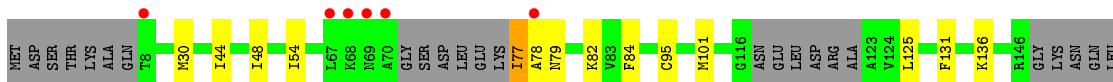
- Molecule 1 is a protein called Nucleoprotein.

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

- Molecule 2 is water.

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

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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:

5% 68% 16% • 15%

- Molecule 1: Nucleoprotein

Chain B:

4% 70% 12% • 17%
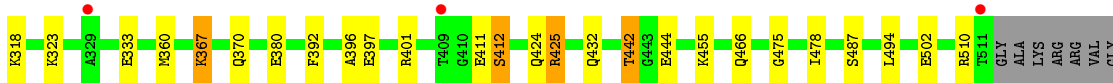
SER SER MET ASP ILE GLU THR VAL GLY GLU ASP

• Molecule 1: Nucleoprotein
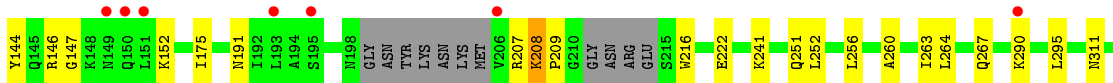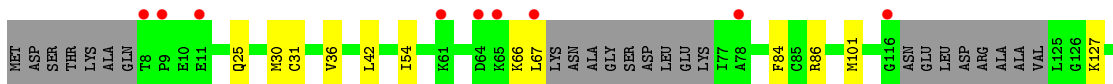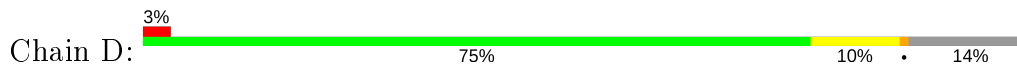
Chain C:

• 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	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
$< I/\sigma(I) >$ [1]	1.44 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.202 , 0.252 0.223 , 0.276	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 , 48.5	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	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.*

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[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 (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	0.47	0/3736	0.70	0/5016
1	B	0.47	0/3649	0.71	1/4898 (0.0%)
1	C	0.46	0/3708	0.67	0/4976
1	D	0.45	0/3793	0.67	0/5088
All	All	0.46	0/14886	0.69	1/19978 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($°$)	Ideal($°$)
1	B	388	SER	C-N-CA	5.10	134.45	121.70

There are no chirality outliers.

There are no planarity outliers.

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	3674	0	3715	46	0
1	B	3591	0	3631	34	0
1	C	3649	0	3701	23	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14881	0	14836	113	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 (113) 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:A:274:MET:HE1	1:A:310:PHE:HA	1.70	0.74
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:274:MET:HE1	1:B:310:PHE:HA	1.79	0.63
1:B:452:LEU:O	1:B:456:ILE:HG12	1.98	0.63
1:C:272:MET:HG3	1:C:272:MET:O	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	0.56
1:A:53:MET:HE3	1:A:107:VAL:HG11	1.89	0.55
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: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:C:311:ASN:HD21	1:C:392:PHE:H	1.56	0.52
1:D:311:ASN:HD21	1:D:392:PHE:H	1.58	0.51
1:B:274:MET:HE3	1:B:310:PHE:CD1	2.45	0.51
1:C:442:THR:HG21	1:D:256:LEU:HD13	1.93	0.51
1:A:339:MET:HE1	1:A:387:THR:HG22	1.93	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:PHE:CE1	1:D:101:MET:HG3	2.47	0.49
1:A:272:MET:HE2	1:A:346:CYS:HB3	1.93	0.49
1:A:234:PRO:HB2	1:A:456:ILE:HG13	1.95	0.49
1:D:260:ALA:HB1	1:D:264:LEU:HD12	1.96	0.48
1:B:58:THR:HG21	1:B:125:LEU:HD21	1.95	0.48
1:B:55:ARG:HD3	1:B:132:THR:HG22	1.95	0.48
1:B:53:MET:HE3	1:B:107:VAL:HG11	1.96	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: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:436:GLU:HG3	1:A:463:PHE:HZ	1.80	0.46
1:A:432:GLN:HA	1:A:466:GLN:HE22	1.79	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: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:274:MET:HE2	1:A:278:MET:HB3	1.98	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: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:B:55:ARG:NH1	1:B:132:THR:HG23	2.32	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
1:C:44:ILE:HG12	1:C:318:LYS:O	2.18	0.43
1:B:30:MET:HG3	1:B:54:ILE:HD11	2.00	0.43
1:B:341:ILE:HD11	1:B:371:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ALA:HA	1:B:173:ARG:HG2	2.01	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:B:368:ARG:HA	1:B:371:LEU:HD12	2.01	0.42
1:C:84:PHE:CE1	1:C:101:MET:HG3	2.55	0.42
1:C:44:ILE:O	1:C:48:ILE:HG12	2.20	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:339:MET:HE1	1:B:387:THR:HB	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:275:PRO:HD2	1:A:278:MET:HE2	2.01	0.41
1:A:31:CYS:HB3	1:A:36:VAL:HB	2.01	0.41
1:A:339:MET:HE2	1:A:339:MET:HA	2.01	0.41
1:A:53:MET:CE	1:A:107:VAL:HG11	2.49	0.41
1:A:146:ARG:HH21	1:A:153:LYS:HA	1.84	0.41
1:A:481:ILE:HG13	1:A:481:ILE:H	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
1:C:368:ARG:HD3	1:C:500:PHE:CE2	2.57	0.40
1:B:274:MET:HG2	1:B:278:MET:HE3	2.02	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%)	14	20
1	B	448/552 (81%)	412 (92%)	32 (7%)	4 (1%)	17	25
1	C	457/552 (83%)	440 (96%)	14 (3%)	3 (1%)	22	32
1	D	465/552 (84%)	440 (95%)	22 (5%)	3 (1%)	25	36
All	All	1831/2208 (83%)	1721 (94%)	95 (5%)	15 (1%)	19	29

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
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 (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	395/462 (86%)	368 (93%)	27 (7%)	16	25
1	B	388/462 (84%)	361 (93%)	27 (7%)	15	24
1	C	394/462 (85%)	372 (94%)	22 (6%)	21	34
1	D	403/462 (87%)	375 (93%)	28 (7%)	15	25
All	All	1580/1848 (86%)	1476 (93%)	104 (7%)	16	26

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	38	GLU
1	A	47	SER
1	A	53	MET
1	A	117	ASN
1	A	120	ASP
1	A	125	LEU
1	A	128	ARG
1	A	136	LYS
1	A	148	LYS
1	A	151	LEU
1	A	169	GLU
1	A	191	ASN
1	A	224	SER
1	A	227	ASN
1	A	241	LYS
1	A	264	LEU
1	A	272	MET
1	A	323	LYS
1	A	330	GLU
1	A	375	ASN
1	A	442	THR
1	A	445	THR
1	A	467	LYS
1	A	481	ILE
1	A	494	LEU
1	A	502	GLU
1	B	12	GLN
1	B	13	ARG
1	B	18	LYS
1	B	29	ARG

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Mol	Chain	Res	Type
1	B	38	GLU
1	B	53	MET
1	B	60	LYS
1	B	94	LYS
1	B	101	MET
1	B	132	THR
1	B	144	TYR
1	B	152	LYS
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	287	GLU
1	B	317	SER
1	B	330	GLU
1	B	362	SER
1	B	415	ILE
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	182	VAL
1	C	219	LEU
1	C	241	LYS
1	C	243	GLU
1	C	272	MET
1	C	295	LEU
1	C	316	MET
1	C	317	SER
1	C	367	LYS
1	C	451	GLN
1	C	462	THR
1	C	480	ASP
1	C	481	ILE

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Mol	Chain	Res	Type
1	C	490	LYS
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	152	LYS
1	D	175	ILE
1	D	191	ASN
1	D	216	TRP
1	D	222	GLU
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	425	ARG
1	D	442	THR
1	D	444	GLU
1	D	455	LYS
1	D	487	SER
1	D	494	LEU
1	D	502	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	ASN
1	A	340	GLN
1	A	375	ASN
1	A	417	ASN
1	A	424	GLN
1	A	432	GLN
1	B	227	ASN

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Mol	Chain	Res	Type
1	B	255	ASN
1	B	414	GLN
1	B	441	ASN
1	C	69	ASN
1	C	106	ASN
1	C	155	ASN
1	C	311	ASN
1	C	340	GLN
1	C	414	GLN
1	C	424	GLN
1	C	459	GLN
1	C	466	GLN
1	C	497	ASN
1	D	179	HIS
1	D	267	GLN
1	D	311	ASN
1	D	370	GLN
1	D	393	HIS
1	D	424	GLN
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 carbohydrates 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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1
1	D	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 (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	469/552 (84%)	0.29	25 (5%)	26	25	36, 55, 91, 114	0
1	B	460/552 (83%)	0.13	21 (4%)	32	31	35, 51, 81, 108	0
1	C	467/552 (84%)	0.01	15 (3%)	47	46	32, 49, 77, 103	0
1	D	476/552 (86%)	0.10	19 (3%)	38	37	33, 52, 84, 109	0
All	All	1872/2208 (84%)	0.13	80 (4%)	35	33	32, 52, 84, 114	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	ALA	13.0
1	A	124	VAL	9.7
1	A	147	GLY	8.5
1	A	123	ALA	7.9
1	C	67	LEU	5.9
1	A	216	TRP	5.7
1	D	151	LEU	5.1
1	A	150	GLN	5.1
1	A	117	ASN	4.7
1	A	120	ASP	4.5
1	D	149	ASN	4.2
1	A	151	LEU	4.0
1	D	64	ASP	3.6
1	B	78	ALA	3.5
1	A	493	GLN	3.5
1	B	381	GLU	3.4
1	A	61	LYS	3.4
1	A	121	ARG	3.3
1	C	70	ALA	3.2
1	B	77	ILE	3.2
1	A	152	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	290	LYS	3.1
1	C	68	LYS	3.1
1	B	61	LYS	3.1
1	A	487	SER	3.0
1	B	123	ALA	3.0
1	D	8	THR	3.0
1	C	78	ALA	3.0
1	D	409	THR	3.0
1	B	291	GLY	3.0
1	B	409	THR	2.9
1	D	65	LYS	2.9
1	A	10	GLU	2.9
1	D	11	GLU	2.8
1	A	62	TYR	2.7
1	D	193	LEU	2.7
1	A	290	LYS	2.7
1	A	292	SER	2.7
1	B	81	GLY	2.6
1	D	67	LEU	2.6
1	C	197	LYS	2.6
1	B	410	GLY	2.6
1	B	495	GLY	2.6
1	C	488	ASN	2.5
1	C	194	ALA	2.5
1	D	78	ALA	2.5
1	D	206	VAL	2.5
1	D	61	LYS	2.5
1	B	485	THR	2.4
1	D	150	GLN	2.4
1	C	195	SER	2.4
1	D	195	SER	2.4
1	A	92	ALA	2.4
1	C	69	ASN	2.4
1	C	196	LYS	2.4
1	C	198	ASN	2.4
1	A	12	GLN	2.3
1	B	290	LYS	2.2
1	B	327	GLY	2.2
1	A	218	PRO	2.2
1	C	219	LEU	2.2
1	B	324	GLY	2.2
1	C	243	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	124	VAL	2.2
1	B	331	ILE	2.2
1	D	329	ALA	2.2
1	D	9	PRO	2.2
1	A	126	GLY	2.2
1	B	92	ALA	2.1
1	A	192	ILE	2.1
1	C	8	THR	2.1
1	B	80	ALA	2.1
1	D	116	GLY	2.1
1	B	488	ASN	2.1
1	A	513	ALA	2.1
1	A	511	THR	2.1
1	C	244	TYR	2.1
1	D	511	THR	2.0
1	B	494	LEU	2.0
1	B	323	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 carbohydrates 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.