



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 08:51 am GMT

PDB ID : 3PMK
Title : Crystal structure of the Vesicular Stomatitis Virus RNA free nucleoprotein/p
hosphoprotein complex
Authors : Leyrat, C.; Yabukarski, F.; Tarbouriech, N.; Ruigrok, R.W.H.; Jamin, M.
Deposited on : 2010-11-17
Resolution : 3.03 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 : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

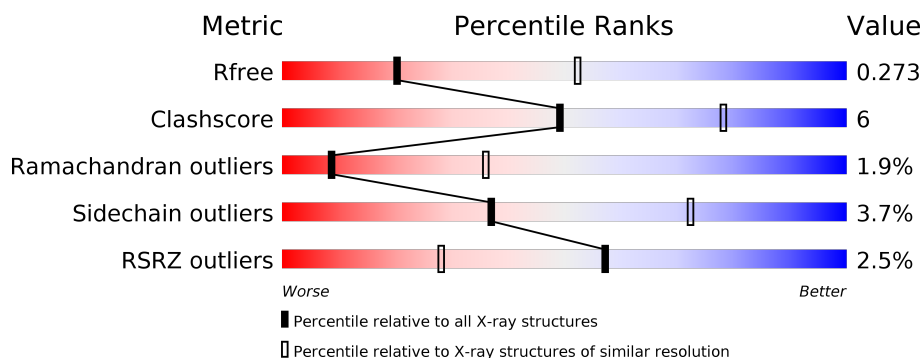
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.03 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}	111664	2391 (3.08-3.00)
Clashscore	122126	2726 (3.08-3.00)
Ramachandran outliers	120053	2639 (3.08-3.00)
Sidechain outliers	120020	2641 (3.08-3.00)
RSRZ outliers	108989	2280 (3.08-3.00)

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. 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	404	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div> </div>
1	B	404	<div> <div>%</div> <div> <div></div> <div>88%</div> <div>10%</div> <div>.</div> </div> </div>
1	C	404	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>.</div> </div> </div>
1	D	404	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div> </div>
1	E	404	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>.</div> </div> </div>
2	N	68	<div> <div></div> <div> <div>38%</div> <div>6%</div> <div>56%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	O	68	<div><div>%</div><div><div></div><div></div><div></div></div><div>31%12%57%</div></div>
2	P	68	<div><div></div><div></div><div></div></div> <div>38%57%</div>
2	Q	68	<div><div>4%</div><div></div><div></div><div></div></div> <div>38%56%</div>
2	R	68	<div><div>%</div><div></div><div></div><div></div></div> <div>37%6%57%</div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17478 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 Nucleocapsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3191	2030	534	608	19			
1	B	404	Total	C	N	O	S	0	0	0
			3191	2030	534	608	19			
1	C	404	Total	C	N	O	S	0	0	0
			3191	2030	534	608	19			
1	D	404	Total	C	N	O	S	0	0	0
			3192	2030	534	609	19			
1	E	404	Total	C	N	O	S	0	0	0
			3191	2030	534	608	19			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	-	EXPRESSION TAG	UNP B7UCZ2
A	20	ALA	-	EXPRESSION TAG	UNP B7UCZ2
A	21	MET	-	EXPRESSION TAG	UNP B7UCZ2
B	19	GLY	-	EXPRESSION TAG	UNP B7UCZ2
B	20	ALA	-	EXPRESSION TAG	UNP B7UCZ2
B	21	MET	-	EXPRESSION TAG	UNP B7UCZ2
C	19	GLY	-	EXPRESSION TAG	UNP B7UCZ2
C	20	ALA	-	EXPRESSION TAG	UNP B7UCZ2
C	21	MET	-	EXPRESSION TAG	UNP B7UCZ2
D	19	GLY	-	EXPRESSION TAG	UNP B7UCZ2
D	20	ALA	-	EXPRESSION TAG	UNP B7UCZ2
D	21	MET	-	EXPRESSION TAG	UNP B7UCZ2
E	19	GLY	-	EXPRESSION TAG	UNP B7UCZ2
E	20	ALA	-	EXPRESSION TAG	UNP B7UCZ2
E	21	MET	-	EXPRESSION TAG	UNP B7UCZ2

- Molecule 2 is a protein called Phosphoprotein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	N	30	Total	C	N	O	0	0	0
			246	151	44	51			
2	O	29	Total	C	N	O	0	0	0
			238	146	42	50			
2	P	29	Total	C	N	O	0	0	0
			240	148	43	49			
2	Q	30	Total	C	N	O	0	0	0
			247	152	44	51			
2	R	29	Total	C	N	O	0	0	0
			240	148	43	49			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	61	LEU	-	EXPRESSION TAG	UNP B7UCZ3
N	62	GLU	-	EXPRESSION TAG	UNP B7UCZ3
N	63	HIS	-	EXPRESSION TAG	UNP B7UCZ3
N	64	HIS	-	EXPRESSION TAG	UNP B7UCZ3
N	65	HIS	-	EXPRESSION TAG	UNP B7UCZ3
N	66	HIS	-	EXPRESSION TAG	UNP B7UCZ3
N	67	HIS	-	EXPRESSION TAG	UNP B7UCZ3
N	68	HIS	-	EXPRESSION TAG	UNP B7UCZ3
O	61	LEU	-	EXPRESSION TAG	UNP B7UCZ3
O	62	GLU	-	EXPRESSION TAG	UNP B7UCZ3
O	63	HIS	-	EXPRESSION TAG	UNP B7UCZ3
O	64	HIS	-	EXPRESSION TAG	UNP B7UCZ3
O	65	HIS	-	EXPRESSION TAG	UNP B7UCZ3
O	66	HIS	-	EXPRESSION TAG	UNP B7UCZ3
O	67	HIS	-	EXPRESSION TAG	UNP B7UCZ3
O	68	HIS	-	EXPRESSION TAG	UNP B7UCZ3
P	61	LEU	-	EXPRESSION TAG	UNP B7UCZ3
P	62	GLU	-	EXPRESSION TAG	UNP B7UCZ3
P	63	HIS	-	EXPRESSION TAG	UNP B7UCZ3
P	64	HIS	-	EXPRESSION TAG	UNP B7UCZ3
P	65	HIS	-	EXPRESSION TAG	UNP B7UCZ3
P	66	HIS	-	EXPRESSION TAG	UNP B7UCZ3
P	67	HIS	-	EXPRESSION TAG	UNP B7UCZ3
P	68	HIS	-	EXPRESSION TAG	UNP B7UCZ3
Q	61	LEU	-	EXPRESSION TAG	UNP B7UCZ3
Q	62	GLU	-	EXPRESSION TAG	UNP B7UCZ3
Q	63	HIS	-	EXPRESSION TAG	UNP B7UCZ3
Q	64	HIS	-	EXPRESSION TAG	UNP B7UCZ3
Q	65	HIS	-	EXPRESSION TAG	UNP B7UCZ3
Q	66	HIS	-	EXPRESSION TAG	UNP B7UCZ3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
Q	67	HIS	-	EXPRESSION TAG	UNP B7UCZ3
Q	68	HIS	-	EXPRESSION TAG	UNP B7UCZ3
R	61	LEU	-	EXPRESSION TAG	UNP B7UCZ3
R	62	GLU	-	EXPRESSION TAG	UNP B7UCZ3
R	63	HIS	-	EXPRESSION TAG	UNP B7UCZ3
R	64	HIS	-	EXPRESSION TAG	UNP B7UCZ3
R	65	HIS	-	EXPRESSION TAG	UNP B7UCZ3
R	66	HIS	-	EXPRESSION TAG	UNP B7UCZ3
R	67	HIS	-	EXPRESSION TAG	UNP B7UCZ3
R	68	HIS	-	EXPRESSION TAG	UNP B7UCZ3

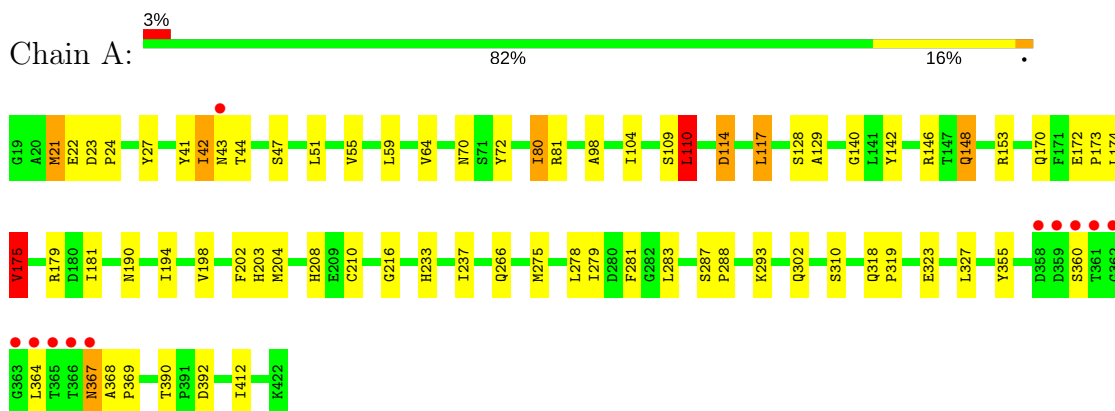
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	51	Total O 51 51	0	0
3	B	71	Total O 71 71	0	0
3	C	62	Total O 62 62	0	0
3	D	51	Total O 51 51	0	0
3	E	47	Total O 47 47	0	0
3	N	7	Total O 7 7	0	0
3	O	7	Total O 7 7	0	0
3	P	7	Total O 7 7	0	0
3	Q	4	Total O 4 4	0	0
3	R	4	Total O 4 4	0	0

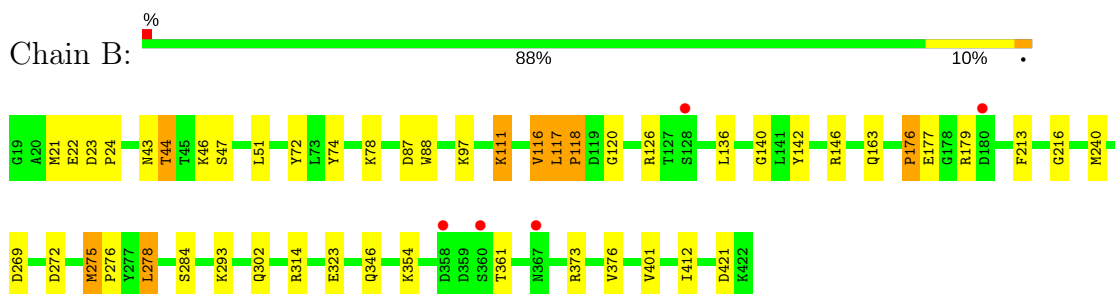
3 Residue-property plots [i](#)

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.

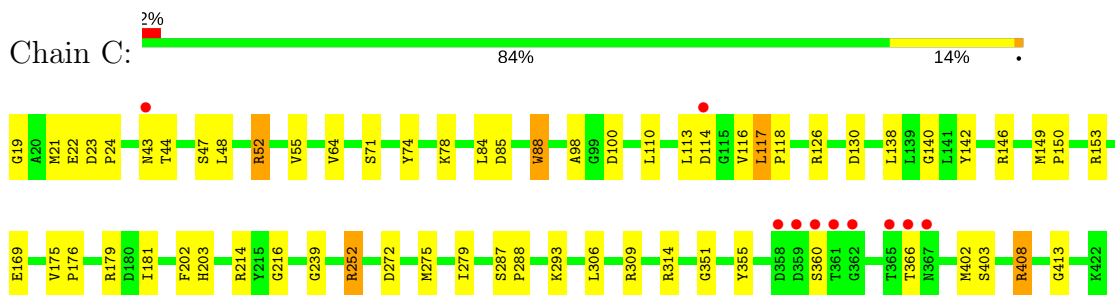
- Molecule 1: Nucleocapsid protein



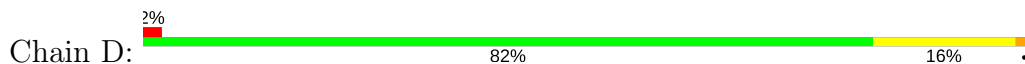
- Molecule 1: Nucleocapsid protein

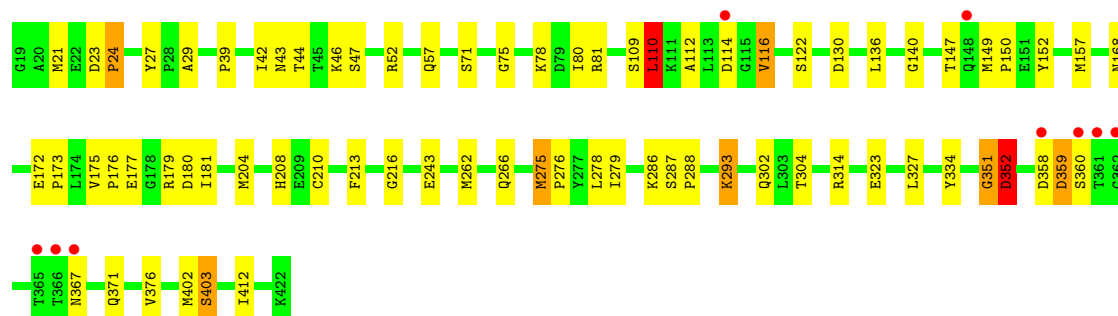


- Molecule 1: Nucleocapsid protein

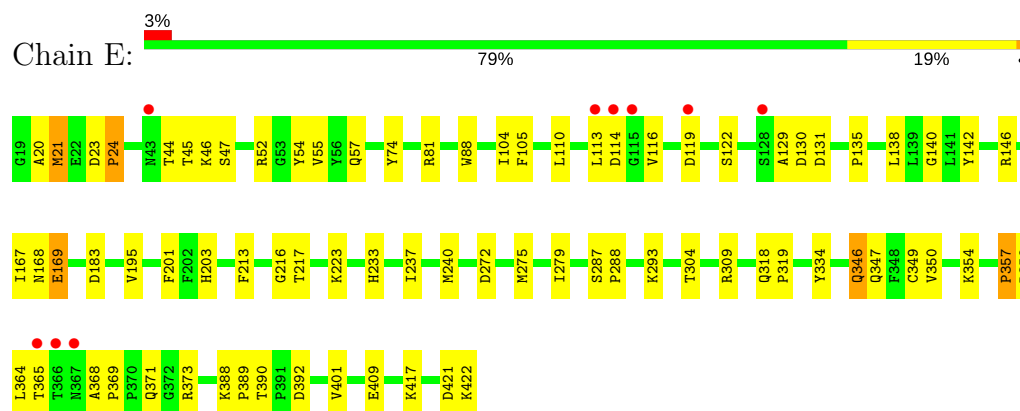


- Molecule 1: Nucleocapsid protein

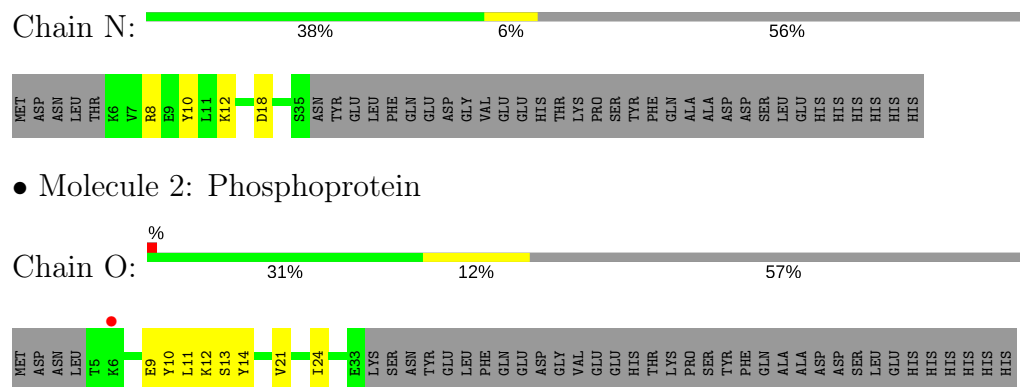




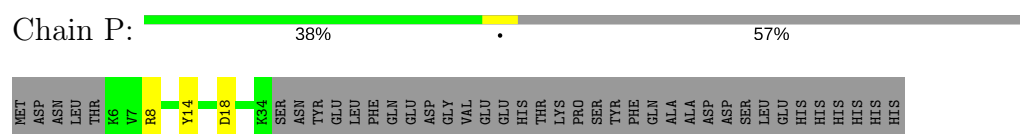
• Molecule 1: Nucleocapsid protein



• Molecule 2: Phosphoprotein

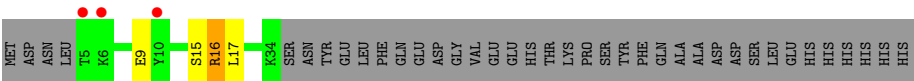


• Molecule 2: Phosphoprotein

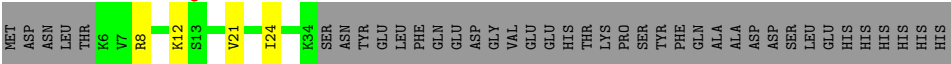
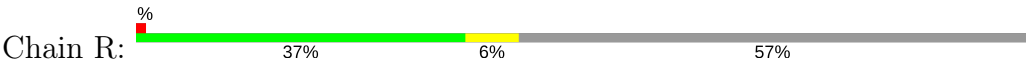


• Molecule 2: Phosphoprotein





● Molecule 2: Phosphoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	74.56 Å 171.97 Å 239.86 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.97 – 3.03 59.97 – 3.03	Depositor EDS
% Data completeness (in resolution range)	89.0 (59.97-3.03) 89.1 (59.97-3.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.31 (at 3.01 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.244 , 0.278 0.241 , 0.273	Depositor DCC
R_{free} test set	2742 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	17478	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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	0.32	0/3265	0.48	0/4417
1	B	0.32	0/3265	0.48	0/4417
1	C	0.32	0/3265	0.50	0/4417
1	D	0.32	0/3266	0.47	0/4417
1	E	0.32	0/3265	0.48	0/4417
2	N	0.33	0/247	0.46	0/328
2	O	0.33	0/239	0.47	0/319
2	P	0.33	0/241	0.48	0/320
2	Q	0.34	0/248	0.54	0/330
2	R	0.31	0/241	0.46	0/320
All	All	0.32	0/17542	0.48	0/23702

There are no bond length outliers.

There are no bond angle outliers.

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	3191	0	3131	44	0
1	B	3191	0	3131	31	0
1	C	3191	0	3131	46	0
1	D	3192	0	3131	46	0
1	E	3191	0	3131	48	0
2	N	246	0	244	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	238	0	233	5	0
2	P	240	0	239	1	0
2	Q	247	0	246	4	0
2	R	240	0	239	2	0
3	A	51	0	0	0	0
3	B	71	0	0	0	0
3	C	62	0	0	0	0
3	D	51	0	0	0	0
3	E	47	0	0	0	0
3	N	7	0	0	0	0
3	O	7	0	0	0	0
3	P	7	0	0	0	0
3	Q	4	0	0	0	0
3	R	4	0	0	0	0
All	All	17478	0	16856	217	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 6.

All (217) 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:E:23:ASP:HB3	1:E:293:LYS:HE2	1.38	1.04
1:B:117:LEU:H	1:B:118:PRO:HD3	1.22	1.00
1:C:408:ARG:HG3	1:C:408:ARG:HH11	1.33	0.93
1:A:367:ASN:H	1:A:367:ASN:HD22	1.17	0.87
2:Q:16:ARG:HG3	2:Q:16:ARG:HH11	1.40	0.87
1:C:52:ARG:HB3	1:C:52:ARG:HH11	1.43	0.83
1:C:146:ARG:HG3	1:C:146:ARG:HH11	1.41	0.82
2:O:12:LYS:O	2:O:14:TYR:N	2.12	0.81
1:D:351:GLY:O	1:D:352:ASP:HB2	1.81	0.80
1:C:408:ARG:CG	1:C:408:ARG:HH11	1.94	0.80
1:C:252:ARG:HG3	1:C:252:ARG:HH11	1.48	0.79
1:C:23:ASP:N	1:C:24:PRO:HD2	1.99	0.78
1:D:109:SER:O	1:D:110:LEU:HB2	1.84	0.77
1:B:117:LEU:H	1:B:118:PRO:CD	1.98	0.77
1:B:117:LEU:N	1:B:118:PRO:HD3	2.01	0.76
1:E:146:ARG:HH11	1:E:146:ARG:HG3	1.51	0.75
1:D:23:ASP:N	1:D:24:PRO:HD2	2.05	0.72
1:B:87:ASP:HB3	1:B:97:LYS:HA	1.70	0.71
1:A:55:VAL:O	1:A:59:LEU:HB2	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:TYR:O	1:E:146:ARG:HG2	1.95	0.67
1:D:43:ASN:ND2	1:D:112:ALA:O	2.28	0.67
1:E:349:CYS:O	2:Q:9:GLU:HG3	1.96	0.66
1:A:364:LEU:HB2	1:A:368:ALA:HB2	1.78	0.66
1:A:279:ILE:HD11	1:A:287:SER:HB2	1.76	0.66
1:A:367:ASN:H	1:A:367:ASN:ND2	1.93	0.65
1:E:390:THR:HG22	1:E:392:ASP:H	1.62	0.65
2:Q:16:ARG:HG3	2:Q:16:ARG:NH1	2.12	0.65
1:C:23:ASP:HB3	1:C:293:LYS:HE2	1.81	0.63
1:C:23:ASP:N	1:C:24:PRO:CD	2.61	0.63
1:D:172:GLU:HG2	1:D:173:PRO:HD2	1.79	0.63
1:C:408:ARG:HG3	1:C:408:ARG:NH1	2.08	0.62
1:E:23:ASP:N	1:E:24:PRO:HD2	2.14	0.62
1:B:142:TYR:O	1:B:146:ARG:HG3	2.00	0.61
1:E:130:ASP:O	1:E:131:ASP:HB2	1.99	0.61
1:E:44:THR:H	1:E:113:LEU:HA	1.66	0.61
1:C:142:TYR:O	1:C:146:ARG:HG2	2.01	0.61
1:B:44:THR:HG21	1:B:116:VAL:HG13	1.82	0.60
1:C:88:TRP:CH2	1:C:272:ASP:HB2	2.37	0.60
1:C:52:ARG:NH2	1:C:126:ARG:O	2.34	0.60
1:A:44:THR:HG22	1:A:114:ASP:H	1.67	0.59
1:A:278:LEU:HG	1:A:279:ILE:HD12	1.84	0.59
1:B:21:MET:SD	1:C:203:HIS:HE1	2.25	0.59
1:C:52:ARG:CB	1:C:52:ARG:HH11	2.15	0.58
1:D:57:GLN:HG2	1:D:122:SER:HB2	1.85	0.58
1:D:42:ILE:HD11	1:D:71:SER:HA	1.84	0.58
1:D:358:ASP:O	1:D:360:SER:N	2.36	0.58
1:D:359:ASP:O	1:D:360:SER:HB3	2.02	0.58
1:C:146:ARG:HG3	1:C:146:ARG:NH1	2.17	0.57
1:A:42:ILE:HD11	1:A:194:ILE:HD11	1.85	0.57
1:A:202:PHE:HE1	1:A:208:HIS:CD2	2.22	0.57
1:E:361:THR:HG22	1:E:371:GLN:HE22	1.70	0.57
1:A:367:ASN:N	1:A:367:ASN:HD22	1.96	0.57
1:C:140:GLY:HA2	1:C:216:GLY:HA3	1.87	0.57
1:B:21:MET:C	1:B:23:ASP:H	2.09	0.56
1:C:74:TYR:O	1:C:78:LYS:HG3	2.06	0.55
1:D:208:HIS:HD2	1:D:210:CYS:H	1.54	0.55
1:A:81:ARG:HD2	1:A:208:HIS:CE1	2.40	0.55
1:D:29:ALA:H	1:D:266:GLN:HE22	1.54	0.55
1:D:402:MET:O	1:D:403:SER:HB2	2.06	0.54
1:B:88:TRP:HE3	1:B:272:ASP:HB3	1.71	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:ASP:HB3	1:D:293:LYS:NZ	2.22	0.54
1:C:252:ARG:CG	1:C:252:ARG:HH11	2.18	0.54
1:C:43:ASN:HB2	1:C:71:SER:OG	2.09	0.53
1:E:146:ARG:NH1	1:E:146:ARG:HG3	2.22	0.53
1:D:302:GLN:HB2	1:D:412:ILE:HD13	1.91	0.53
1:B:140:GLY:HA2	1:B:216:GLY:HA3	1.92	0.52
2:O:10:TYR:CD2	2:O:12:LYS:HG3	2.44	0.52
1:E:240:MET:HE2	1:E:373:ARG:HD3	1.91	0.52
1:E:23:ASP:N	1:E:24:PRO:CD	2.72	0.52
1:D:351:GLY:O	1:D:352:ASP:CB	2.56	0.52
1:B:240:MET:CE	1:B:373:ARG:HD3	2.39	0.52
1:E:364:LEU:H	1:E:368:ALA:HB2	1.75	0.52
1:E:57:GLN:HG2	1:E:122:SER:HB2	1.90	0.52
1:A:390:THR:HG22	1:A:392:ASP:H	1.75	0.51
1:A:293:LYS:HA	1:A:293:LYS:HE2	1.93	0.51
1:C:55:VAL:HG11	1:C:138:LEU:HD11	1.93	0.51
1:A:64:VAL:HG12	1:A:181:ILE:HD11	1.92	0.51
1:E:104:ILE:HG22	1:E:201:PHE:CD2	2.46	0.51
1:C:402:MET:O	1:C:403:SER:HB2	2.12	0.50
1:A:23:ASP:N	1:A:24:PRO:HD2	2.26	0.50
1:A:43:ASN:HD21	1:A:70:ASN:HB2	1.75	0.50
1:E:240:MET:CE	1:E:373:ARG:HD3	2.41	0.50
1:D:136:LEU:HD13	1:D:213:PHE:HA	1.93	0.50
1:B:117:LEU:N	1:B:118:PRO:CD	2.68	0.50
1:B:275:MET:HG3	1:B:276:PRO:HD3	1.93	0.49
2:R:12:LYS:HD2	2:R:12:LYS:H	1.77	0.49
1:B:23:ASP:N	1:B:24:PRO:HD2	2.26	0.49
1:D:147:THR:HG21	1:D:152:TYR:HD2	1.77	0.49
1:E:279:ILE:HD11	1:E:287:SER:HB2	1.93	0.49
1:A:153:ARG:HE	1:A:179:ARG:HD2	1.77	0.49
2:Q:15:SER:C	2:Q:17:LEU:H	2.16	0.49
1:D:179:ARG:O	1:D:181:ILE:N	2.39	0.49
1:A:140:GLY:HA2	1:A:216:GLY:HA3	1.95	0.49
1:A:194:ILE:O	1:A:198:VAL:HG23	2.13	0.49
1:A:355:TYR:HB2	1:D:376:VAL:HG13	1.95	0.49
1:D:140:GLY:HA2	1:D:216:GLY:HA3	1.95	0.49
1:D:402:MET:O	1:D:403:SER:CB	2.60	0.49
1:A:23:ASP:N	1:A:24:PRO:CD	2.76	0.49
1:B:23:ASP:N	1:B:24:PRO:CD	2.76	0.49
1:D:179:ARG:C	1:D:181:ILE:H	2.15	0.49
1:A:80:ILE:O	1:A:80:ILE:HG22	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ARG:HD2	1:A:208:HIS:HE1	1.77	0.48
1:E:388:LYS:HD2	1:E:389:PRO:HD2	1.95	0.48
1:A:59:LEU:HD23	1:A:174:LEU:HD22	1.96	0.48
1:B:346:GLN:HE22	1:B:354:LYS:HA	1.78	0.48
1:A:302:GLN:HB2	1:A:412:ILE:HD13	1.95	0.48
1:E:21:MET:O	1:E:23:ASP:N	2.38	0.48
1:C:52:ARG:HH12	1:C:130:ASP:HB2	1.79	0.47
1:A:281:PHE:HB3	1:A:283:LEU:HD13	1.96	0.47
1:D:23:ASP:N	1:D:24:PRO:CD	2.77	0.47
1:E:346:GLN:HE22	1:E:354:LYS:HA	1.78	0.47
1:A:172:GLU:HG2	1:A:173:PRO:HD2	1.95	0.47
1:D:149:MET:HA	1:D:150:PRO:HD3	1.76	0.47
1:A:174:LEU:O	1:A:175:VAL:HG12	2.15	0.46
1:A:202:PHE:HE1	1:A:208:HIS:HD2	1.62	0.46
1:E:421:ASP:O	1:E:422:LYS:HB2	2.16	0.46
1:D:81:ARG:HB3	1:D:208:HIS:HE1	1.80	0.46
1:E:168:ASN:CG	1:E:169:GLU:H	2.19	0.46
1:A:203:HIS:HE1	1:D:21:MET:SD	2.38	0.46
1:E:129:ALA:HB1	1:E:169:GLU:OE1	2.16	0.46
1:E:304:THR:HG21	1:E:334:TYR:CD2	2.51	0.46
1:D:359:ASP:O	1:D:360:SER:CB	2.64	0.46
1:E:360:SER:C	1:E:362:GLY:H	2.19	0.45
1:A:41:TYR:H	1:A:190:ASN:ND2	2.13	0.45
1:C:408:ARG:CG	1:C:408:ARG:NH1	2.64	0.45
1:B:136:LEU:HD13	1:B:213:PHE:HA	1.98	0.45
1:C:146:ARG:CG	1:C:146:ARG:HH11	2.20	0.45
1:D:46:LYS:O	1:D:47:SER:HB3	2.16	0.45
1:A:142:TYR:O	1:A:146:ARG:HG2	2.17	0.45
1:B:269:ASP:HB3	2:P:14:TYR:HB3	1.99	0.45
1:B:240:MET:HE2	1:B:373:ARG:HD3	1.98	0.45
1:D:75:GLY:HA2	1:D:78:LYS:HE2	1.98	0.45
1:E:55:VAL:HG11	1:E:138:LEU:HD11	1.99	0.45
1:D:262:MET:HB3	2:O:12:LYS:HD2	1.98	0.45
1:A:109:SER:O	1:A:110:LEU:HB2	2.17	0.44
1:E:149:MET:HA	1:E:150:PRO:HD3	1.82	0.44
1:A:148:GLN:HB3	1:A:148:GLN:HE21	1.59	0.44
1:C:22:GLU:C	1:C:24:PRO:HD2	2.37	0.44
1:B:136:LEU:HD21	1:B:163:GLN:HB3	1.98	0.44
1:D:52:ARG:HD3	1:D:130:ASP:HB2	1.99	0.44
1:E:146:ARG:HH22	1:E:223:LYS:HE3	1.82	0.44
1:D:109:SER:O	1:D:110:LEU:CB	2.58	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:VAL:HG12	1:C:181:ILE:HD11	2.00	0.44
1:B:401:VAL:HG23	1:B:421:ASP:HB2	2.00	0.44
1:D:46:LYS:HD2	1:D:116:VAL:HG21	1.99	0.44
1:D:275:MET:HG3	1:D:276:PRO:HD3	2.00	0.44
1:B:88:TRP:CE3	1:B:272:ASP:HB3	2.52	0.44
1:B:51:LEU:HB3	1:B:72:TYR:HB2	1.99	0.44
1:C:279:ILE:HD11	1:C:287:SER:HB2	1.99	0.44
1:A:42:ILE:HD12	1:A:42:ILE:HA	1.74	0.43
1:E:401:VAL:HB	1:E:417:LYS:HA	2.00	0.43
1:C:202:PHE:HB2	1:C:214:ARG:HD2	2.01	0.43
1:B:323:GLU:CD	1:C:239:GLY:HA3	2.39	0.43
1:A:117:LEU:H	1:A:117:LEU:HD13	1.83	0.43
1:C:146:ARG:CG	1:C:146:ARG:NH1	2.81	0.43
2:R:21:VAL:HA	2:R:24:ILE:HD12	2.01	0.43
1:B:278:LEU:HD12	1:B:284:SER:HB3	2.00	0.43
1:B:46:LYS:HG2	1:B:46:LYS:O	2.19	0.43
1:C:175:VAL:HA	1:C:176:PRO:HD3	1.91	0.43
1:C:48:LEU:O	1:C:52:ARG:HG3	2.19	0.42
1:C:84:LEU:HD21	1:C:88:TRP:CD1	2.54	0.42
1:C:19:GLY:N	1:C:293:LYS:HZ1	2.18	0.42
1:C:287:SER:HA	1:C:288:PRO:HD3	1.86	0.42
1:C:402:MET:O	1:C:403:SER:CB	2.67	0.42
1:D:278:LEU:H	1:D:278:LEU:HD23	1.84	0.42
1:E:368:ALA:HA	1:E:369:PRO:HD3	1.86	0.42
1:A:27:TYR:HB3	1:A:266:GLN:OE1	2.19	0.42
1:B:74:TYR:O	1:B:78:LYS:HG3	2.18	0.42
1:E:140:GLY:HA2	1:E:216:GLY:HA3	2.02	0.42
1:B:302:GLN:HB2	1:B:412:ILE:HD13	2.02	0.42
1:C:252:ARG:HD3	1:E:347:GLN:HE22	1.85	0.42
1:E:135:PRO:HB2	1:E:213:PHE:HE2	1.85	0.42
1:E:233:HIS:O	1:E:237:ILE:HG12	2.19	0.42
1:D:287:SER:HA	1:D:288:PRO:HD3	1.92	0.42
1:D:175:VAL:HA	1:D:176:PRO:HD3	1.88	0.42
1:E:146:ARG:HH11	1:E:146:ARG:CG	2.28	0.42
1:B:176:PRO:HB2	1:B:177:GLU:H	1.61	0.42
1:A:233:HIS:O	1:A:237:ILE:HG12	2.19	0.42
1:C:117:LEU:HA	1:C:118:PRO:HD3	1.90	0.42
1:E:21:MET:C	1:E:23:ASP:H	2.18	0.42
1:E:46:LYS:HG3	1:E:46:LYS:O	2.20	0.41
1:A:323:GLU:HB2	1:A:327:LEU:HD13	2.03	0.41
1:A:51:LEU:HB3	1:A:72:TYR:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:HIS:CD2	1:A:210:CYS:H	2.39	0.41
2:O:21:VAL:HA	2:O:24:ILE:HD12	2.02	0.41
1:C:114:ASP:OD2	1:C:114:ASP:N	2.54	0.41
1:D:23:ASP:HB3	1:D:293:LYS:HZ1	1.85	0.41
1:D:304:THR:HG21	1:D:334:TYR:CD2	2.55	0.41
1:E:81:ARG:O	1:E:201:PHE:HZ	2.03	0.41
1:E:287:SER:HA	1:E:288:PRO:HD3	1.94	0.41
1:C:21:MET:SD	1:E:203:HIS:HE1	2.43	0.41
1:C:52:ARG:HH11	1:C:52:ARG:CG	2.33	0.41
1:D:39:PRO:HA	1:D:109:SER:O	2.21	0.41
1:D:27:TYR:HB3	1:D:266:GLN:NE2	2.36	0.41
1:D:23:ASP:HA	1:D:286:LYS:HE3	2.01	0.41
1:E:164:CYS:HA	1:E:167:ILE:HD12	2.01	0.41
1:E:54:TYR:CD1	1:E:119:ASP:HB3	2.55	0.41
1:D:279:ILE:HD11	1:D:287:SER:HB2	2.03	0.41
1:A:287:SER:HA	1:A:288:PRO:HD3	1.91	0.41
1:C:44:THR:HA	1:C:113:LEU:HG	2.02	0.41
1:D:323:GLU:O	1:D:327:LEU:HG	2.21	0.41
1:E:52:ARG:HD2	1:E:130:ASP:HB2	2.02	0.41
1:E:318:GLN:HA	1:E:319:PRO:HD3	1.91	0.41
1:E:357:PRO:HB2	1:E:358:ASP:H	1.63	0.41
1:A:318:GLN:HA	1:A:319:PRO:HD3	1.94	0.41
1:B:23:ASP:O	1:B:24:PRO:C	2.58	0.40
1:E:57:GLN:CG	1:E:122:SER:HB2	2.51	0.40
2:N:10:TYR:HB3	2:N:12:LYS:HE3	2.03	0.40
1:B:376:VAL:HG13	1:C:355:TYR:HB2	2.03	0.40
1:E:195:VAL:HG13	1:E:217:THR:HG22	2.02	0.40
1:A:368:ALA:HA	1:A:369:PRO:HD3	1.97	0.40
1:E:74:TYR:HA	1:E:105:PHE:CZ	2.57	0.40
1:D:243:GLU:HG3	2:O:9:GLU:HG2	2.03	0.40
1:C:149:MET:HA	1:C:150:PRO:HD3	1.87	0.40
1:C:153:ARG:HH21	1:C:179:ARG:HG3	1.87	0.40
1:C:306:LEU:HD21	1:C:413:GLY:HA2	2.03	0.40
1:D:57:GLN:CG	1:D:122:SER:HB2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	402/404 (100%)	378 (94%)	15 (4%)	9 (2%)	7	31
1	B	402/404 (100%)	364 (90%)	29 (7%)	9 (2%)	7	31
1	C	402/404 (100%)	373 (93%)	25 (6%)	4 (1%)	17	53
1	D	402/404 (100%)	369 (92%)	23 (6%)	10 (2%)	6	28
1	E	402/404 (100%)	363 (90%)	32 (8%)	7 (2%)	10	39
2	N	28/68 (41%)	27 (96%)	1 (4%)	0	100	100
2	O	27/68 (40%)	24 (89%)	1 (4%)	2 (7%)	1	5
2	P	27/68 (40%)	26 (96%)	1 (4%)	0	100	100
2	Q	28/68 (41%)	26 (93%)	2 (7%)	0	100	100
2	R	27/68 (40%)	24 (89%)	3 (11%)	0	100	100
All	All	2147/2360 (91%)	1974 (92%)	132 (6%)	41 (2%)	9	36

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	LEU
1	B	47	SER
1	B	117	LEU
1	B	176	PRO
1	D	110	LEU
1	D	352	ASP
1	D	359	ASP
2	O	13	SER
1	A	129	ALA
1	C	47	SER
1	D	168	ASN
1	E	20	ALA
1	E	350	VAL
1	E	361	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	O	11	LEU
1	A	21	MET
1	A	360	SER
1	B	22	GLU
1	B	111	LYS
1	B	179	ARG
1	C	98	ALA
1	D	351	GLY
1	E	47	SER
1	E	110	LEU
1	E	357	PRO
1	A	128	SER
1	C	360	SER
1	A	98	ALA
1	A	175	VAL
1	B	44	THR
1	B	118	PRO
1	D	44	THR
1	D	403	SER
1	E	24	PRO
1	A	47	SER
1	D	180	ASP
1	D	80	ILE
1	C	351	GLY
1	A	80	ILE
1	B	120	GLY
1	D	24	PRO

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	344/344 (100%)	330 (96%)	14 (4%)	33	70
1	B	344/344 (100%)	335 (97%)	9 (3%)	49	80
1	C	344/344 (100%)	330 (96%)	14 (4%)	33	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	344/344 (100%)	332 (96%)	12 (4%)	39	74
1	E	344/344 (100%)	331 (96%)	13 (4%)	36	71
2	N	26/61 (43%)	24 (92%)	2 (8%)	14	44
2	O	25/61 (41%)	25 (100%)	0	100	100
2	P	25/61 (41%)	23 (92%)	2 (8%)	13	42
2	Q	26/61 (43%)	25 (96%)	1 (4%)	36	71
2	R	25/61 (41%)	24 (96%)	1 (4%)	34	70
All	All	1847/2025 (91%)	1779 (96%)	68 (4%)	37	72

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	MET
1	A	22	GLU
1	A	42	ILE
1	A	104	ILE
1	A	110	LEU
1	A	114	ASP
1	A	117	LEU
1	A	148	GLN
1	A	170	GLN
1	A	175	VAL
1	A	204	MET
1	A	275	MET
1	A	310	SER
1	A	367	ASN
1	B	43	ASN
1	B	111	LYS
1	B	116	VAL
1	B	126	ARG
1	B	275	MET
1	B	278	LEU
1	B	293	LYS
1	B	314	ARG
1	B	361	THR
1	C	52	ARG
1	C	85	ASP
1	C	88	TRP
1	C	100	ASP
1	C	110	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	116	VAL
1	C	117	LEU
1	C	169	GLU
1	C	252	ARG
1	C	275	MET
1	C	309	ARG
1	C	314	ARG
1	C	366	THR
1	C	408	ARG
1	D	110	LEU
1	D	114	ASP
1	D	116	VAL
1	D	157	MET
1	D	177	GLU
1	D	204	MET
1	D	275	MET
1	D	293	LYS
1	D	314	ARG
1	D	352	ASP
1	D	367	ASN
1	D	371	GLN
1	E	21	MET
1	E	45	THR
1	E	88	TRP
1	E	114	ASP
1	E	116	VAL
1	E	169	GLU
1	E	183	ASP
1	E	272	ASP
1	E	275	MET
1	E	309	ARG
1	E	346	GLN
1	E	365	THR
1	E	409	GLU
2	N	8	ARG
2	N	18	ASP
2	P	8	ARG
2	P	18	ASP
2	Q	16	ARG
2	R	8	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	148	GLN
1	A	170	GLN
1	A	190	ASN
1	A	203	HIS
1	A	208	HIS
1	A	251	ASN
1	A	298	HIS
1	A	302	GLN
1	A	318	GLN
1	A	367	ASN
1	B	187	ASN
1	B	190	ASN
1	B	251	ASN
1	B	294	ASN
1	B	346	GLN
1	B	385	GLN
1	B	395	GLN
1	C	70	ASN
1	C	190	ASN
1	C	203	HIS
1	C	251	ASN
1	C	302	GLN
1	C	371	GLN
1	C	385	GLN
1	D	43	ASN
1	D	208	HIS
1	D	251	ASN
1	D	266	GLN
1	D	367	ASN
1	D	371	GLN
1	D	385	GLN
1	D	386	ASN
1	E	190	ASN
1	E	203	HIS
1	E	233	HIS
1	E	251	ASN
1	E	346	GLN
1	E	347	GLN
1	E	371	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](#)

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	404/404 (100%)	-0.25	11 (2%) 54 25	13, 23, 44, 51	0
1	B	404/404 (100%)	-0.23	5 (1%) 79 53	15, 25, 47, 57	0
1	C	404/404 (100%)	-0.31	10 (2%) 57 28	12, 21, 44, 49	0
1	D	404/404 (100%)	-0.22	9 (2%) 62 33	13, 26, 50, 58	0
1	E	404/404 (100%)	-0.18	14 (3%) 44 19	14, 29, 53, 59	0
2	N	30/68 (44%)	-0.19	0 100 100	23, 35, 57, 72	0
2	O	29/68 (42%)	0.08	1 (3%) 45 19	22, 38, 72, 87	0
2	P	29/68 (42%)	-0.11	0 100 100	22, 34, 57, 61	0
2	Q	30/68 (44%)	0.17	3 (10%) 7 2	22, 37, 86, 98	0
2	R	29/68 (42%)	-0.15	1 (3%) 45 19	21, 35, 65, 78	0
All	All	2167/2360 (91%)	-0.22	54 (2%) 57 28	12, 25, 50, 98	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	360	SER	4.9
1	A	360	SER	4.7
1	E	362	GLY	4.3
1	E	365	THR	4.2
1	C	365	THR	4.0
1	C	360	SER	3.9
1	D	362	GLY	3.9
1	A	363	GLY	3.8
1	D	360	SER	3.7
1	A	358	ASP	3.4
1	A	366	THR	3.4
1	A	365	THR	3.4
1	C	366	THR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	128	SER	3.3
1	A	361	THR	3.2
1	C	362	GLY	3.2
1	E	367	ASN	3.2
1	E	114	ASP	3.2
1	C	367	ASN	3.1
1	C	358	ASP	3.1
1	E	43	ASN	3.1
1	A	362	GLY	3.0
1	C	114	ASP	3.0
1	C	361	THR	2.9
1	D	361	THR	2.8
1	B	358	ASP	2.7
1	E	361	THR	2.7
1	E	366	THR	2.7
1	E	115	GLY	2.5
1	D	365	THR	2.5
1	A	367	ASN	2.5
1	D	367	ASN	2.5
1	E	363	GLY	2.5
1	A	359	ASP	2.4
1	B	128	SER	2.4
2	Q	10	TYR	2.4
2	R	13	SER	2.3
2	O	6	LYS	2.3
1	D	358	ASP	2.2
1	E	113	LEU	2.2
1	E	119	ASP	2.2
1	C	43	ASN	2.2
2	Q	6	LYS	2.2
1	D	366	THR	2.2
2	Q	5	THR	2.2
1	A	364	LEU	2.2
1	C	359	ASP	2.2
1	D	148	GLN	2.2
1	B	180	ASP	2.1
1	B	360	SER	2.1
1	D	114	ASP	2.1
1	B	367	ASN	2.1
1	E	359	ASP	2.1
1	A	43	ASN	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.