



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:44 PM UTC

PDB ID : 3HHW / pdb_00003hhw
Title : Complex of a vesicular stomatitis virus empty capsid with the nucleocapsid-binding domain of the phosphoprotein
Authors : Green, T.J.; Luo, M.
Deposited on : 2009-05-18
Resolution : 2.70 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

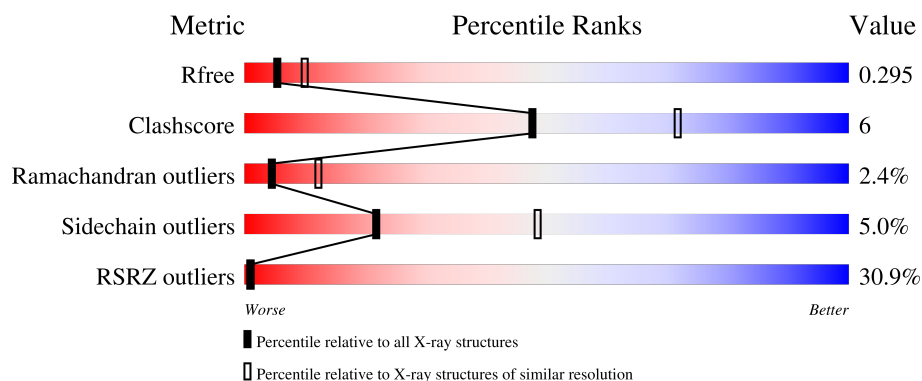
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	87	30% 71% 11% 16%
1	B	87	66% 72% 11% 16%
1	C	87	30% 70% 11% 16%
1	D	87	59% 72% 9% 16%
1	E	87	67% 74% 10% 16%

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Mol	Chain	Length	Quality of chain
2	K	421	
2	L	421	
2	M	421	
2	N	421	
2	O	421	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	TAR	K	423	X	-	-	-
3	TAR	K	424	X	-	-	-
3	TAR	K	425	X	-	-	-
3	TAR	K	426	X	-	-	-
3	TAR	M	1	X	-	-	-
3	TAR	O	423	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19615 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 Phosphoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	73	Total	C	N	O	Se	0	0	0
			576	368	100	106	2			
1	B	73	Total	C	N	O	Se	0	0	0
			576	368	100	106	2			
1	C	73	Total	C	N	O	Se	0	0	0
			576	368	100	106	2			
1	D	73	Total	C	N	O	Se	0	0	0
			576	368	100	106	2			
1	E	73	Total	C	N	O	Se	0	0	0
			576	368	100	106	2			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	179	GLY	-	expression tag	UNP P04880
A	180	SER	-	expression tag	UNP P04880
A	181	HIS	-	expression tag	UNP P04880
A	182	MET	-	expression tag	UNP P04880
B	179	GLY	-	expression tag	UNP P04880
B	180	SER	-	expression tag	UNP P04880
B	181	HIS	-	expression tag	UNP P04880
B	182	MET	-	expression tag	UNP P04880
C	179	GLY	-	expression tag	UNP P04880
C	180	SER	-	expression tag	UNP P04880
C	181	HIS	-	expression tag	UNP P04880
C	182	MET	-	expression tag	UNP P04880
D	179	GLY	-	expression tag	UNP P04880
D	180	SER	-	expression tag	UNP P04880
D	181	HIS	-	expression tag	UNP P04880
D	182	MET	-	expression tag	UNP P04880
E	179	GLY	-	expression tag	UNP P04880
E	180	SER	-	expression tag	UNP P04880
E	181	HIS	-	expression tag	UNP P04880

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Chain	Residue	Modelled	Actual	Comment	Reference
E	182	MET	-	expression tag	UNP P04880

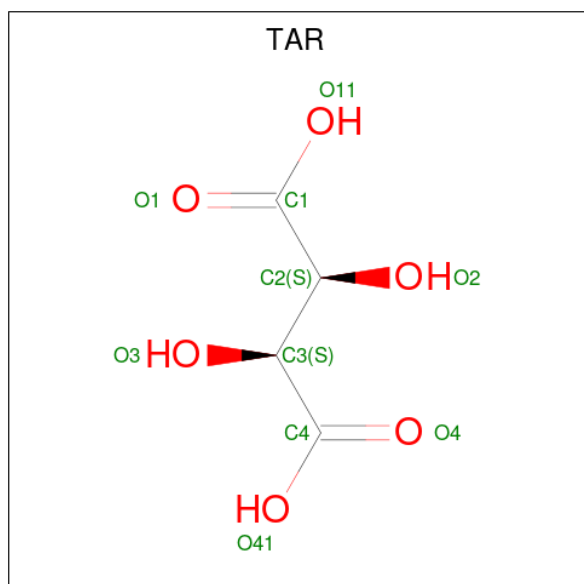
- Molecule 2 is a protein called Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	421	Total	C	N	O	S	0	0	0
			3335	2126	559	632	18			
2	L	421	Total	C	N	O	S	0	0	0
			3335	2126	559	632	18			
2	M	421	Total	C	N	O	S	0	0	0
			3335	2126	559	632	18			
2	N	421	Total	C	N	O	S	0	0	0
			3335	2126	559	632	18			
2	O	421	Total	C	N	O	S	0	0	0
			3335	2126	559	632	18			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	290	TRP	SER	engineered mutation	UNP Q77E03
L	290	TRP	SER	engineered mutation	UNP Q77E03
M	290	TRP	SER	engineered mutation	UNP Q77E03
N	290	TRP	SER	engineered mutation	UNP Q77E03
O	290	TRP	SER	engineered mutation	UNP Q77E03

- Molecule 3 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: C₄H₆O₆).

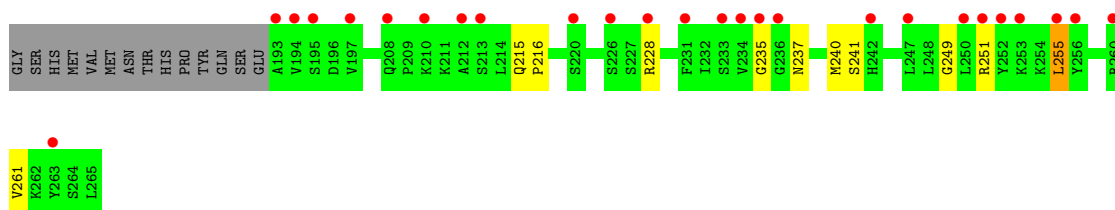


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	K	1	Total	C	O	0	0
			10	4	6		
3	K	1	Total	C	O	0	0
			10	4	6		
3	K	1	Total	C	O	0	0
			10	4	6		
3	K	1	Total	C	O	0	0
			10	4	6		
3	M	1	Total	C	O	0	0
			10	4	6		
3	O	1	Total	C	O	0	0
			10	4	6		

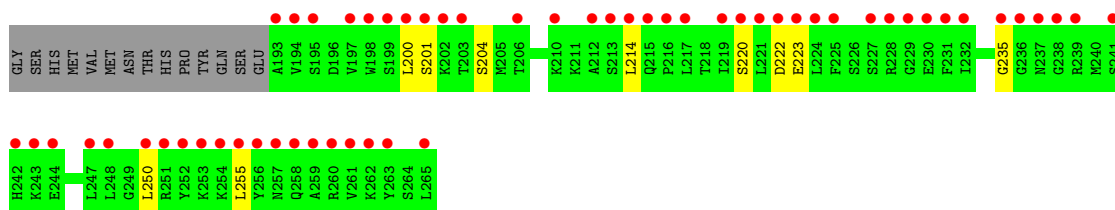
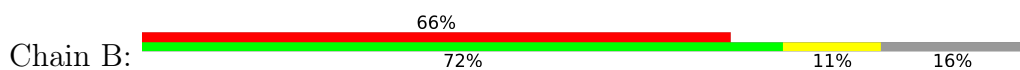
3 Residue-property plots [i](#)

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.

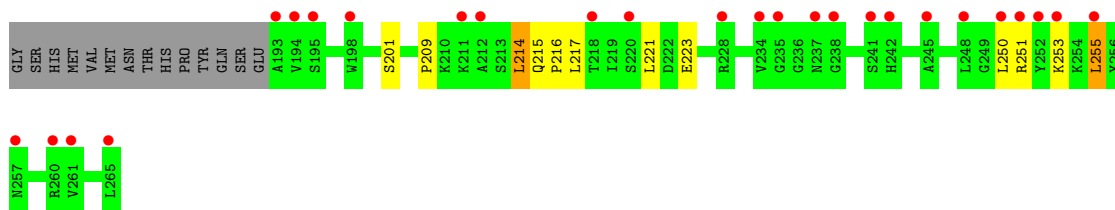
• Molecule 1: Phosphoprotein



• Molecule 1: Phosphoprotein

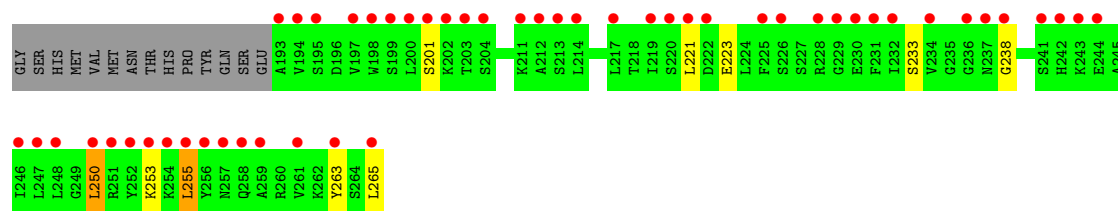


• Molecule 1: Phosphoprotein

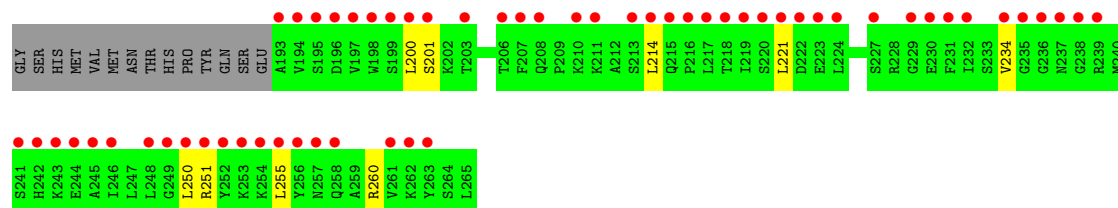
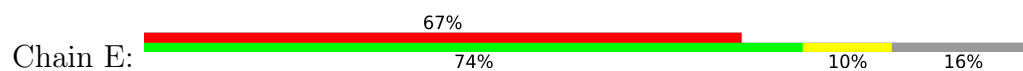


• Molecule 1: Phosphoprotein

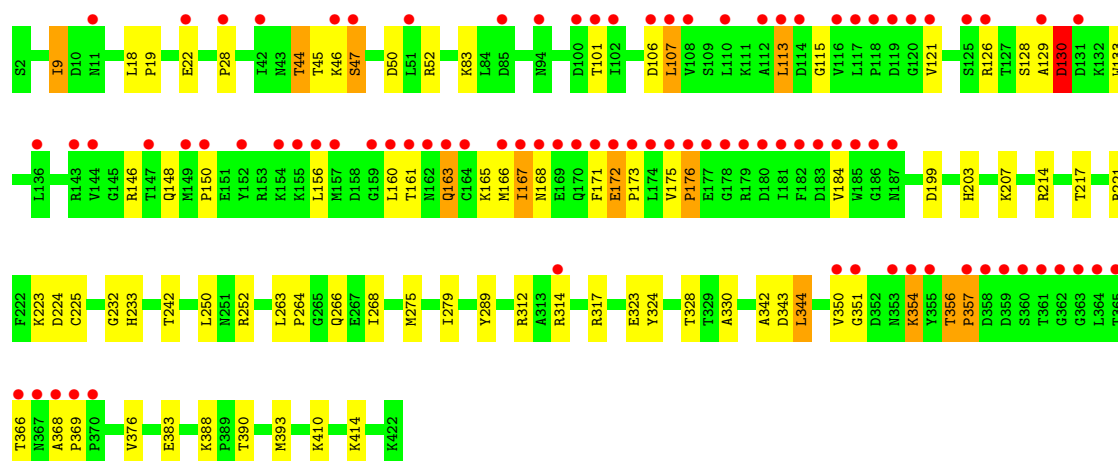
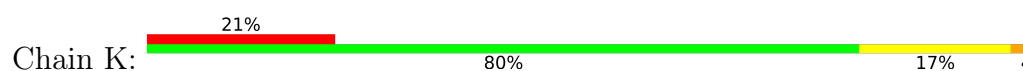




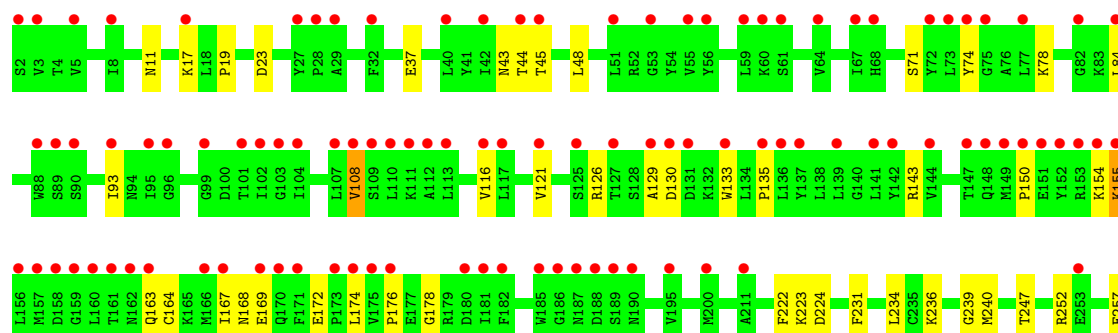
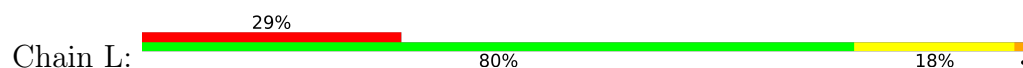
● Molecule 1: Phosphoprotein

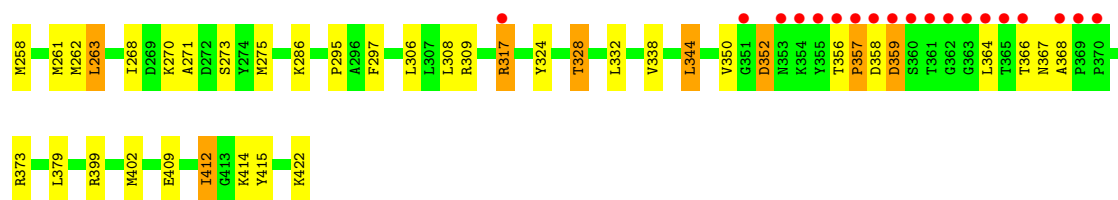


● Molecule 2: Nucleoprotein

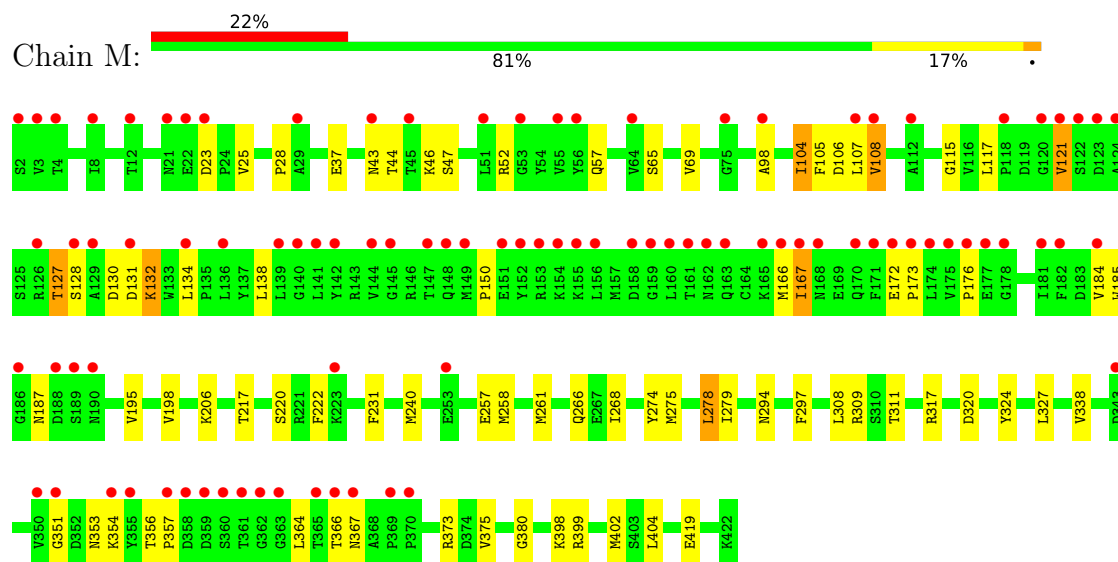


● Molecule 2: Nucleoprotein

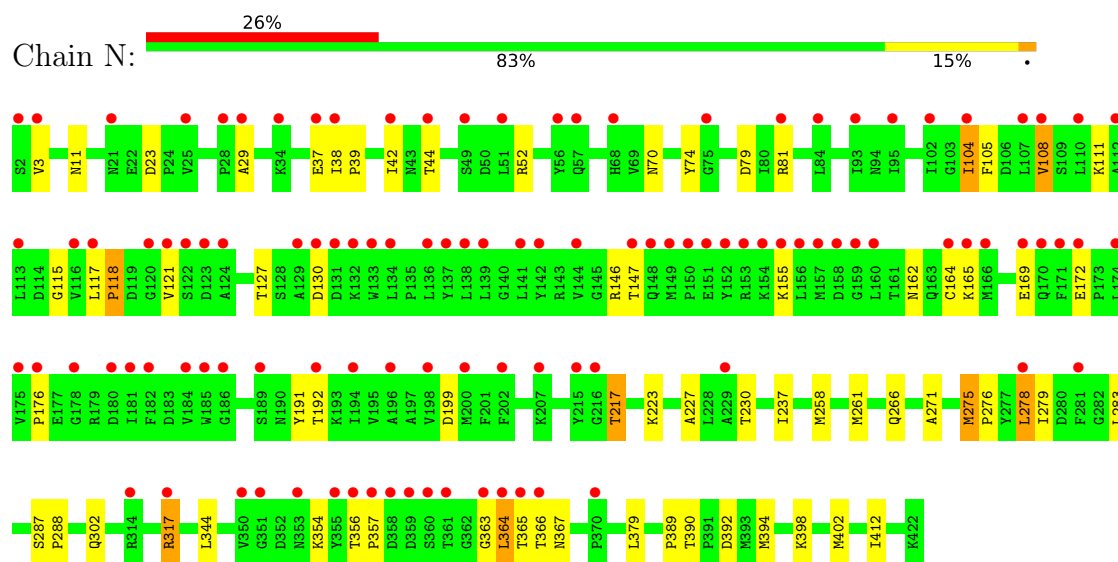




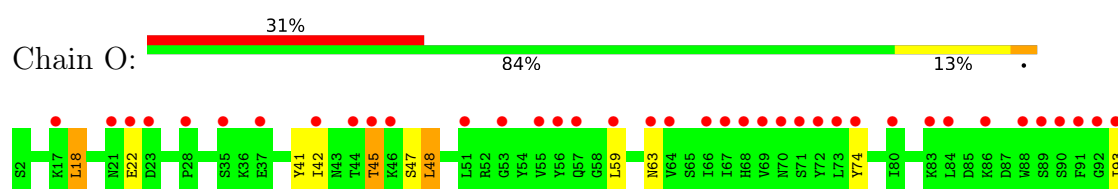
• Molecule 2: Nucleoprotein

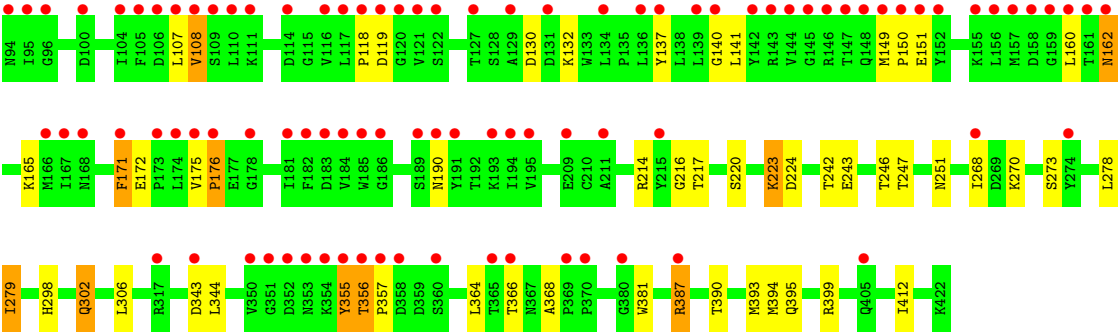


• Molecule 2: Nucleoprotein



• Molecule 2: Nucleoprotein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	170.60Å 234.52Å 95.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	73.7 (30.00-2.70) 73.6 (30.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.263 , 0.296 0.262 , 0.295	Depositor DCC
R_{free} test set	3839 reflections (3.64%)	wwPDB-VP
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	19615	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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](#)

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

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	0.43	0/584	0.80	0/778
1	B	0.46	0/584	0.75	0/778
1	C	0.44	0/584	0.84	0/778
1	D	0.45	0/584	0.77	0/778
1	E	0.43	0/584	0.73	0/778
2	K	0.48	0/3413	0.83	2/4622 (0.0%)
2	L	0.45	0/3413	0.79	2/4622 (0.0%)
2	M	0.46	0/3413	0.80	1/4622 (0.0%)
2	N	0.44	0/3413	0.80	0/4622
2	O	0.47	0/3413	0.79	0/4622
All	All	0.46	0/19985	0.80	5/27000 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	356	THR	CA-C-N	6.72	128.24	119.84
2	K	356	THR	C-N-CA	6.72	128.24	119.84
2	L	263	LEU	CA-C-N	5.71	125.83	119.32
2	L	263	LEU	C-N-CA	5.71	125.83	119.32
2	M	43	ASN	CB-CA-C	-5.19	110.57	116.54

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	576	0	597	13	0
1	B	576	0	597	3	0
1	C	576	0	597	7	0
1	D	576	0	597	4	0
1	E	576	0	597	3	0
2	K	3335	0	3292	54	0
2	L	3335	0	3292	46	0
2	M	3335	0	3292	48	0
2	N	3335	0	3292	33	0
2	O	3335	0	3292	36	0
3	K	40	0	16	0	0
3	M	10	0	4	0	0
3	O	10	0	4	0	0
All	All	19615	0	19469	219	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 (219) 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)
2:K:390:THR:H	2:K:393:MET:HE3	1.27	0.96
1:A:255:LEU:CD2	2:K:366:THR:HG23	2.00	0.90
2:M:356:THR:H	2:M:357:PRO:HD2	1.41	0.83
2:M:240:MET:HE2	2:M:373:ARG:HD3	1.60	0.83
2:M:356:THR:N	2:M:357:PRO:HD2	1.95	0.82
2:K:214:ARG:HA	2:K:217:THR:HG22	1.63	0.79
2:O:390:THR:H	2:O:393:MET:HE3	1.48	0.78
2:O:220:SER:O	2:O:223:LYS:HG3	1.82	0.77
2:N:389:PRO:HB2	2:N:394:MET:HE1	1.69	0.74
2:N:302:GLN:HB2	2:N:412:ILE:HD13	1.68	0.74
2:K:324:TYR:O	2:K:328:THR:HG23	1.87	0.74
2:L:399:ARG:HA	2:L:402:MET:HE2	1.71	0.73
2:L:324:TYR:O	2:L:328:THR:HG23	1.89	0.71
2:O:302:GLN:HB3	2:O:412:ILE:HD13	1.70	0.71
1:A:255:LEU:HD22	2:K:366:THR:CG2	2.22	0.70
1:A:261:VAL:HG21	2:K:376:VAL:HG12	1.72	0.70
2:L:317:ARG:H	2:L:317:ARG:NE	1.89	0.70
1:A:255:LEU:HD22	2:K:366:THR:HG23	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:356:THR:N	2:O:357:PRO:HD3	2.09	0.67
2:O:381:TRP:CH2	2:O:393:MET:HE2	2.30	0.66
2:M:366:THR:HG23	2:M:367:ASN:H	1.61	0.66
2:M:130:ASP:C	2:M:132:LYS:H	2.04	0.65
2:M:356:THR:H	2:M:357:PRO:CD	2.09	0.65
2:M:320:ASP:HA	2:M:324:TYR:OH	1.96	0.65
1:A:251:ARG:HG2	1:A:251:ARG:HH21	1.61	0.64
2:M:356:THR:N	2:M:357:PRO:CD	2.61	0.63
1:A:255:LEU:CD2	2:K:366:THR:CG2	2.74	0.62
2:L:366:THR:C	2:L:368:ALA:H	2.07	0.62
2:K:160:LEU:HD13	2:K:171:PHE:HD2	1.65	0.62
2:N:29:ALA:H	2:N:266:GLN:HE22	1.47	0.62
2:K:172:GLU:H	2:K:173:PRO:HD3	1.65	0.62
2:L:222:PHE:HE1	2:L:275:MET:HE1	1.65	0.62
2:L:17:LYS:HB2	2:M:268:ILE:HD11	1.81	0.61
2:K:9:ILE:HD13	2:L:252:ARG:HH22	1.64	0.61
2:K:172:GLU:N	2:K:173:PRO:CD	2.63	0.61
2:N:146:ARG:HE	2:N:223:LYS:HE2	1.65	0.61
2:L:422:LYS:HE2	2:M:399:ARG:HB3	1.82	0.61
2:K:172:GLU:H	2:K:173:PRO:CD	2.13	0.60
2:K:47:SER:HB2	2:K:50:ASP:HB2	1.85	0.59
2:N:390:THR:HG22	2:N:392:ASP:H	1.68	0.59
1:D:250:LEU:HD12	1:D:255:LEU:HD13	1.85	0.58
2:O:364:LEU:C	2:O:366:THR:H	2.12	0.58
2:K:342:ALA:HB1	2:K:344:LEU:HD23	1.84	0.58
2:L:317:ARG:H	2:L:317:ARG:HE	1.50	0.58
2:O:387:ARG:CG	2:O:387:ARG:HH11	2.17	0.57
2:N:70:ASN:HD21	2:N:191:TYR:HB2	1.68	0.57
2:M:37:GLU:HB2	2:M:108:VAL:HG21	1.87	0.57
2:M:268:ILE:HG22	2:M:275:MET:HE3	1.84	0.57
2:L:240:MET:HE2	2:L:373:ARG:HD3	1.88	0.56
2:L:268:ILE:HA	2:L:275:MET:HE2	1.88	0.56
2:M:28:PRO:HG3	2:M:278:LEU:HD23	1.86	0.56
2:O:395:GLN:O	2:O:399:ARG:HG2	2.06	0.56
2:N:278:LEU:HA	2:N:283:LEU:HD12	1.88	0.56
2:K:160:LEU:HD23	2:K:163:GLN:HE21	1.71	0.55
2:K:354:LYS:HE3	2:K:356:THR:HA	1.88	0.55
2:M:106:ASP:C	2:M:107:LEU:HD12	2.31	0.55
2:M:65:SER:HB2	2:M:117:LEU:HD22	1.87	0.55
2:O:107:LEU:O	2:O:108:VAL:HB	2.06	0.55
1:A:251:ARG:HG2	1:A:251:ARG:NH2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:106:ASP:OD1	2:K:107:LEU:N	2.39	0.55
1:A:255:LEU:HD23	2:K:366:THR:HG23	1.87	0.55
2:L:379:LEU:HB3	2:M:354:LYS:HD2	1.89	0.54
2:O:270:LYS:HD2	2:O:273:SER:HB2	1.89	0.54
2:L:240:MET:CE	2:L:338:VAL:HG22	2.37	0.54
2:K:224:ASP:OD1	2:K:279:ILE:HG21	2.08	0.54
2:K:184:VAL:HG11	2:L:164:CYS:HB2	1.89	0.54
2:K:390:THR:N	2:K:393:MET:HE3	2.09	0.54
2:K:350:VAL:HG23	2:O:247:THR:HG21	1.90	0.54
2:N:398:LYS:O	2:N:402:MET:HB2	2.07	0.54
2:K:366:THR:HG23	2:K:366:THR:O	2.07	0.53
2:K:52:ARG:HD3	2:K:130:ASP:HB3	1.88	0.53
2:O:381:TRP:HH2	2:O:393:MET:HE2	1.71	0.53
2:N:258:MET:HA	2:N:261:MET:HE3	1.89	0.53
2:N:44:THR:H	2:N:111:LYS:HE3	1.74	0.52
2:K:113:LEU:H	2:K:113:LEU:HD13	1.74	0.52
1:B:201:SER:HB2	1:B:222:ASP:HB2	1.91	0.51
2:M:57:GLN:HB3	2:M:121:VAL:HB	1.93	0.51
2:O:45:THR:HG21	2:O:48:LEU:HD12	1.90	0.51
2:O:140:GLY:HA2	2:O:216:GLY:HA3	1.92	0.51
2:L:223:LYS:O	2:L:224:ASP:HB2	2.10	0.51
2:O:387:ARG:HH11	2:O:387:ARG:HG2	1.76	0.51
1:A:255:LEU:HD22	2:K:366:THR:HG21	1.93	0.51
1:E:234:VAL:HG12	1:E:251:ARG:HH21	1.75	0.51
2:M:130:ASP:O	2:M:132:LYS:N	2.44	0.51
2:K:223:LYS:O	2:K:224:ASP:HB2	2.11	0.50
2:M:172:GLU:HB2	2:M:173:PRO:HD3	1.91	0.50
2:M:130:ASP:C	2:M:132:LYS:N	2.67	0.50
2:O:242:THR:O	2:O:246:THR:HG23	2.11	0.50
1:C:201:SER:HA	1:C:221:LEU:HB2	1.93	0.50
1:D:253:LYS:HD2	2:N:367:ASN:HB2	1.94	0.50
2:M:184:VAL:HG13	2:N:165:LYS:HG2	1.94	0.50
2:N:389:PRO:HB2	2:N:394:MET:CE	2.41	0.49
2:K:167:ILE:HG12	2:K:168:ASN:H	1.77	0.49
2:O:41:TYR:HB2	2:O:190:ASN:HD21	1.75	0.49
2:O:366:THR:C	2:O:368:ALA:H	2.21	0.49
2:N:364:LEU:C	2:N:366:THR:H	2.20	0.49
2:L:357:PRO:C	2:L:359:ASP:H	2.21	0.49
2:M:132:LYS:HG3	2:M:166:MET:HB2	1.94	0.49
2:L:174:LEU:HB2	2:L:178:GLY:HA3	1.94	0.48
2:L:133:TRP:HE3	2:L:163:GLN:HE22	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:83:LYS:HB2	2:K:101:THR:HG22	1.95	0.48
2:L:257:GLU:OE2	2:L:295:PRO:HD2	2.14	0.48
2:M:132:LYS:HG2	2:M:167:ILE:HG12	1.96	0.48
1:E:260:ARG:HG2	2:K:357:PRO:HB3	1.95	0.48
2:K:376:VAL:HG21	2:L:352:ASP:HB3	1.95	0.48
2:O:387:ARG:HG2	2:O:387:ARG:NH1	2.29	0.47
2:L:328:THR:HG21	2:L:415:TYR:OH	2.15	0.47
2:K:203:HIS:HD2	2:K:214:ARG:HH22	1.62	0.47
2:L:366:THR:C	2:L:368:ALA:N	2.73	0.47
2:K:232:GLY:HA2	2:O:18:LEU:HD21	1.97	0.47
2:M:44:THR:HG23	2:M:46:LYS:HE2	1.97	0.47
2:N:147:THR:HG21	2:N:155:LYS:HG3	1.97	0.47
2:O:42:ILE:HD13	2:O:74:TYR:HB2	1.96	0.47
1:D:201:SER:HA	1:D:221:LEU:HB2	1.97	0.47
2:N:164:CYS:HB3	2:N:169:GLU:HG2	1.97	0.47
2:O:162:ASN:HA	2:O:165:LYS:HE3	1.96	0.47
2:K:203:HIS:CG	2:K:221:ARG:HH21	2.33	0.46
2:K:225:CYS:HA	2:K:289:TYR:HB2	1.96	0.46
2:O:214:ARG:HA	2:O:217:THR:OG1	2.15	0.46
2:O:149:MET:C	2:O:151:GLU:H	2.23	0.46
1:C:223:GLU:HB3	2:M:364:LEU:HD21	1.97	0.46
2:M:278:LEU:HD13	2:M:279:ILE:HG12	1.96	0.46
2:K:242:THR:HG22	2:O:18:LEU:HD22	1.97	0.46
2:K:45:THR:HG22	2:K:46:LYS:H	1.81	0.45
2:K:224:ASP:CG	2:K:279:ILE:HG21	2.41	0.45
2:M:132:LYS:HG3	2:M:166:MET:CB	2.46	0.45
2:M:231:PHE:CE2	2:M:258:MET:HE1	2.52	0.45
2:M:217:THR:O	2:M:220:SER:HB3	2.16	0.45
2:N:275:MET:HG3	2:N:276:PRO:HD3	1.98	0.45
1:C:209:PRO:HB3	1:C:214:LEU:HB3	1.98	0.45
2:K:368:ALA:HB1	2:K:369:PRO:HD2	1.98	0.45
2:L:270:LYS:HD3	2:L:273:SER:HB2	1.99	0.45
2:M:380:GLY:HA2	2:N:354:LYS:HE2	1.99	0.45
1:A:249:GLY:C	1:A:251:ARG:H	2.25	0.45
1:C:253:LYS:HB2	1:C:255:LEU:HG	1.99	0.44
2:K:133:TRP:HB2	2:K:163:GLN:HG3	2.00	0.44
2:L:37:GLU:HB2	2:L:108:VAL:HG21	1.99	0.44
2:L:306:LEU:HD22	2:L:412:ILE:HD12	2.00	0.44
2:K:161:THR:HG22	2:K:165:LYS:HE3	1.99	0.44
2:K:323:GLU:CD	2:L:239:GLY:HA3	2.42	0.44
2:L:350:VAL:O	2:L:350:VAL:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:69:VAL:HG13	2:M:138:LEU:HD13	2.00	0.44
2:L:143:ARG:HH21	2:L:155:LYS:HE2	1.82	0.44
2:M:364:LEU:O	2:M:366:THR:HG22	2.18	0.44
2:N:104:ILE:HG22	2:N:105:PHE:H	1.83	0.44
2:N:162:ASN:HA	2:N:165:LYS:HE3	2.00	0.44
2:L:261:MET:HE1	2:L:297:PHE:CD2	2.53	0.44
2:M:185:TRP:C	2:M:187:ASN:H	2.26	0.44
2:L:422:LYS:HB3	2:M:402:MET:SD	2.58	0.44
2:N:37:GLU:HB2	2:N:108:VAL:HG21	2.00	0.44
2:L:167:ILE:HG22	2:L:168:ASN:N	2.32	0.43
2:O:160:LEU:HD22	2:O:171:PHE:HD2	1.83	0.43
2:K:28:PRO:HD2	2:K:266:GLN:OE1	2.19	0.43
2:K:268:ILE:HA	2:K:275:MET:HE2	2.00	0.43
2:L:130:ASP:O	2:L:135:PRO:HD3	2.17	0.43
2:O:298:HIS:O	2:O:302:GLN:HB2	2.19	0.43
2:O:387:ARG:CG	2:O:387:ARG:NH1	2.81	0.43
1:A:235:GLY:HA3	2:L:364:LEU:HD13	2.00	0.43
2:K:175:VAL:HB	2:K:176:PRO:HD3	2.01	0.43
2:L:126:ARG:HH21	2:L:129:ALA:HB2	1.83	0.43
2:N:79:ASP:HB2	2:N:81:ARG:HG3	2.00	0.43
1:D:263:TYR:C	1:D:265:LEU:H	2.26	0.43
2:M:105:PHE:C	2:M:107:LEU:H	2.26	0.43
1:A:215:GLN:HA	1:A:216:PRO:HD3	1.95	0.43
2:L:409:GLU:HA	2:L:414:LYS:HD2	2.01	0.43
2:M:308:LEU:C	2:M:309:ARG:HG2	2.44	0.43
1:A:237:ASN:HB2	1:A:240:MSE:HG3	2.01	0.42
2:K:126:ARG:NH2	2:K:129:ALA:HB3	2.34	0.42
2:M:240:MET:CE	2:M:373:ARG:HD3	2.40	0.42
2:N:363:GLY:C	2:N:365:THR:H	2.27	0.42
2:O:278:LEU:HG	2:O:279:ILE:HD12	2.00	0.42
2:M:195:VAL:HG13	2:M:217:THR:HG22	2.00	0.42
2:M:366:THR:HG23	2:M:367:ASN:N	2.31	0.42
2:O:137:TYR:O	2:O:141:LEU:HG	2.19	0.42
2:L:74:TYR:O	2:L:78:LYS:HB2	2.19	0.42
2:M:52:ARG:HD3	2:M:130:ASP:OD2	2.20	0.42
2:N:317:ARG:H	2:N:317:ARG:HG2	1.56	0.42
2:L:164:CYS:SG	2:L:169:GLU:HG2	2.60	0.42
2:M:104:ILE:HD13	2:M:198:VAL:HG22	2.02	0.42
2:N:117:LEU:N	2:N:118:PRO:CD	2.83	0.42
1:B:220:SER:HB3	1:B:223:GLU:HG2	2.01	0.42
2:K:44:THR:O	2:K:45:THR:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:23:ASP:HB3	2:L:286:LYS:HE3	2.02	0.42
2:K:19:PRO:HB3	2:L:222:PHE:CZ	2.55	0.42
2:L:275:MET:HE3	2:L:275:MET:HB3	1.93	0.42
2:M:257:GLU:HB3	2:M:294:ASN:HD22	1.85	0.42
2:O:130:ASP:C	2:O:132:LYS:H	2.28	0.42
2:O:387:ARG:HH11	2:O:387:ARG:CB	2.32	0.42
1:C:215:GLN:HA	1:C:216:PRO:HD3	1.95	0.41
2:K:314:ARG:H	2:K:314:ARG:HG2	1.60	0.41
2:N:278:LEU:HD13	2:N:279:ILE:HG12	2.02	0.41
2:O:223:LYS:HE3	2:O:224:ASP:CG	2.45	0.41
2:O:387:ARG:HH11	2:O:387:ARG:HB3	1.86	0.41
1:C:253:LYS:HD2	2:M:367:ASN:HB2	2.02	0.41
1:E:201:SER:HA	1:E:221:LEU:HB2	2.02	0.41
2:M:261:MET:HE1	2:M:297:PHE:CD2	2.55	0.41
2:N:38:ILE:HA	2:N:39:PRO:HD3	1.86	0.41
2:N:287:SER:HA	2:N:288:PRO:HD3	1.86	0.41
2:K:330:ALA:HB2	2:L:344:LEU:HD21	2.03	0.41
2:L:19:PRO:HB3	2:M:222:PHE:CZ	2.56	0.41
2:L:222:PHE:CE1	2:L:275:MET:HE1	2.52	0.41
2:M:127:THR:OG1	2:M:128:SER:N	2.52	0.41
2:K:199:ASP:OD1	2:K:217:THR:HG23	2.21	0.41
2:M:28:PRO:HD2	2:M:266:GLN:OE1	2.21	0.41
2:M:107:LEU:HD23	2:M:274:TYR:HE2	1.86	0.41
2:N:199:ASP:HB2	2:N:217:THR:HG22	2.01	0.41
2:N:227:ALA:HA	2:N:230:THR:HG22	2.03	0.41
2:O:175:VAL:HB	2:O:176:PRO:HD3	2.03	0.41
2:L:231:PHE:CE2	2:L:258:MET:HE1	2.57	0.40
2:N:52:ARG:NH2	2:N:127:THR:HA	2.36	0.40
2:K:263:LEU:HA	2:K:264:PRO:HD3	1.93	0.40
2:N:42:ILE:HD13	2:N:74:TYR:HB2	2.04	0.40
2:N:356:THR:N	2:N:357:PRO:HD3	2.36	0.40
2:K:233:HIS:CE1	2:K:312:ARG:HD2	2.57	0.40
2:L:43:ASN:HA	2:L:44:THR:HA	1.74	0.40
2:L:258:MET:HE3	2:L:262:MET:HG3	2.02	0.40
1:B:204:SER:HB3	1:B:220:SER:HB2	2.03	0.40
1:C:214:LEU:HD23	1:C:215:GLN:H	1.86	0.40
2:O:355:TYR:HB2	2:O:357:PRO:HD3	2.04	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	71/87 (82%)	62 (87%)	8 (11%)	1 (1%)	9	23
1	B	71/87 (82%)	59 (83%)	11 (16%)	1 (1%)	9	23
1	C	71/87 (82%)	60 (84%)	10 (14%)	1 (1%)	9	23
1	D	71/87 (82%)	58 (82%)	11 (16%)	2 (3%)	4	9
1	E	71/87 (82%)	64 (90%)	7 (10%)	0	100	100
2	K	419/421 (100%)	377 (90%)	29 (7%)	13 (3%)	3	8
2	L	419/421 (100%)	373 (89%)	35 (8%)	11 (3%)	4	11
2	M	419/421 (100%)	372 (89%)	37 (9%)	10 (2%)	4	12
2	N	419/421 (100%)	376 (90%)	36 (9%)	7 (2%)	7	19
2	O	419/421 (100%)	369 (88%)	37 (9%)	13 (3%)	3	8
All	All	2450/2540 (96%)	2170 (89%)	221 (9%)	59 (2%)	4	12

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	K	44	THR
2	K	357	PRO
2	L	357	PRO
2	M	176	PRO
2	K	115	GLY
2	K	176	PRO
2	M	98	ALA
2	M	131	ASP
2	N	118	PRO
2	N	130	ASP
2	N	176	PRO
2	O	22	GLU
2	O	108	VAL
1	D	238	GLY

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Mol	Chain	Res	Type
2	K	146	ARG
2	K	351	GLY
2	L	150	PRO
2	L	176	PRO
2	L	271	ALA
2	M	115	GLY
2	M	127	THR
2	N	271	ALA
2	O	47	SER
2	O	119	ASP
2	O	343	ASP
1	A	228	ARG
1	C	251	ARG
2	L	45	THR
2	L	121	VAL
2	L	358	ASP
2	L	359	ASP
2	O	63	ASN
2	O	344	LEU
1	D	233	SER
2	K	130	ASP
2	K	150	PRO
2	K	172	GLU
2	K	343	ASP
2	K	344	LEU
2	L	172	GLU
2	L	367	ASN
2	M	47	SER
2	M	108	VAL
2	O	45	THR
2	O	118	PRO
2	K	121	VAL
2	K	167	ILE
2	L	108	VAL
2	M	351	GLY
1	B	235	GLY
2	N	115	GLY
2	O	356	THR
2	M	150	PRO
2	M	167	ILE
2	N	121	VAL
2	O	172	GLU

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Mol	Chain	Res	Type
2	N	172	GLU
2	O	150	PRO
2	O	176	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	64/75 (85%)	62 (97%)	2 (3%)	35	65
1	B	64/75 (85%)	60 (94%)	4 (6%)	16	39
1	C	64/75 (85%)	60 (94%)	4 (6%)	16	39
1	D	64/75 (85%)	61 (95%)	3 (5%)	23	51
1	E	64/75 (85%)	60 (94%)	4 (6%)	16	39
2	K	362/362 (100%)	341 (94%)	21 (6%)	18	42
2	L	362/362 (100%)	341 (94%)	21 (6%)	18	42
2	M	362/362 (100%)	345 (95%)	17 (5%)	23	51
2	N	362/362 (100%)	348 (96%)	14 (4%)	28	57
2	O	362/362 (100%)	346 (96%)	16 (4%)	25	53
All	All	2130/2185 (98%)	2024 (95%)	106 (5%)	22	48

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	SER
1	A	255	LEU
1	B	200	LEU
1	B	214	LEU
1	B	250	LEU
1	B	255	LEU
1	C	214	LEU
1	C	217	LEU
1	C	250	LEU
1	C	255	LEU

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Mol	Chain	Res	Type
1	D	223	GLU
1	D	250	LEU
1	D	255	LEU
1	E	200	LEU
1	E	214	LEU
1	E	250	LEU
1	E	255	LEU
2	K	9	ILE
2	K	18	LEU
2	K	22	GLU
2	K	47	SER
2	K	107	LEU
2	K	113	LEU
2	K	128	SER
2	K	130	ASP
2	K	148	GLN
2	K	156	LEU
2	K	163	GLN
2	K	166	MET
2	K	207	LYS
2	K	250	LEU
2	K	252	ARG
2	K	317	ARG
2	K	354	LYS
2	K	383	GLU
2	K	388	LYS
2	K	410	LYS
2	K	414	LYS
2	L	11	ASN
2	L	48	LEU
2	L	71	SER
2	L	84	LEU
2	L	93	ILE
2	L	116	VAL
2	L	154	LYS
2	L	155	LYS
2	L	234	LEU
2	L	236	LYS
2	L	247	THR
2	L	263	LEU
2	L	308	LEU
2	L	309	ARG

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Mol	Chain	Res	Type
2	L	317	ARG
2	L	328	THR
2	L	332	LEU
2	L	344	LEU
2	L	352	ASP
2	L	356	THR
2	L	412	ILE
2	M	23	ASP
2	M	25	VAL
2	M	104	ILE
2	M	121	VAL
2	M	132	LYS
2	M	134	LEU
2	M	206	LYS
2	M	278	LEU
2	M	311	THR
2	M	317	ARG
2	M	327	LEU
2	M	338	VAL
2	M	353	ASN
2	M	375	VAL
2	M	398	LYS
2	M	404	LEU
2	M	419	GLU
2	N	3	VAL
2	N	11	ASN
2	N	23	ASP
2	N	104	ILE
2	N	108	VAL
2	N	192	THR
2	N	217	THR
2	N	237	ILE
2	N	275	MET
2	N	278	LEU
2	N	317	ARG
2	N	344	LEU
2	N	364	LEU
2	N	379	LEU
2	O	18	LEU
2	O	48	LEU
2	O	59	LEU
2	O	93	ILE

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Mol	Chain	Res	Type
2	O	162	ASN
2	O	171	PHE
2	O	223	LYS
2	O	243	GLU
2	O	251	ASN
2	O	268	ILE
2	O	279	ILE
2	O	302	GLN
2	O	306	LEU
2	O	355	TYR
2	O	387	ARG
2	O	394	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	257	ASN
1	B	215	GLN
1	B	237	ASN
1	B	258	GLN
1	C	237	ASN
1	D	237	ASN
1	D	242	HIS
1	E	242	HIS
2	K	148	GLN
2	K	163	GLN
2	K	203	HIS
2	K	260	GLN
2	K	294	ASN
2	K	395	GLN
2	L	162	ASN
2	L	163	GLN
2	L	170	GLN
2	L	298	HIS
2	L	346	GLN
2	L	386	ASN
2	L	395	GLN
2	M	203	HIS
2	M	251	ASN
2	M	260	GLN
2	M	294	ASN
2	M	347	GLN

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Mol	Chain	Res	Type
2	M	371	GLN
2	N	11	ASN
2	N	57	GLN
2	N	70	ASN
2	N	251	ASN
2	N	260	GLN
2	N	266	GLN
2	N	294	ASN
2	N	302	GLN
2	N	371	GLN
2	N	385	GLN
2	O	43	ASN
2	O	57	GLN
2	O	70	ASN
2	O	163	GLN
2	O	203	HIS
2	O	251	ASN
2	O	298	HIS
2	O	302	GLN
2	O	347	GLN
2	O	353	ASN
2	O	395	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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TAR	K	426	-	9,9,9	1.13	0	12,12,12	0.96	0
3	TAR	M	1	-	9,9,9	1.23	0	12,12,12	0.85	0
3	TAR	K	425	-	9,9,9	1.20	0	12,12,12	0.95	1 (8%)
3	TAR	K	424	-	9,9,9	1.16	0	12,12,12	0.95	0
3	TAR	O	423	-	9,9,9	1.18	0	12,12,12	0.94	0
3	TAR	K	423	-	9,9,9	1.12	0	12,12,12	1.03	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TAR	K	426	-	1/1/4/4	5/12/12/12	-
3	TAR	M	1	-	1/1/4/4	5/12/12/12	-
3	TAR	K	425	-	1/1/4/4	7/12/12/12	-
3	TAR	K	424	-	1/1/4/4	7/12/12/12	-
3	TAR	O	423	-	1/1/4/4	5/12/12/12	-
3	TAR	K	423	-	1/1/4/4	10/12/12/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	425	TAR	O41-C4-C3	2.07	119.06	113.31

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	K	423	TAR	C2
3	K	424	TAR	C2
3	K	425	TAR	C2
3	K	426	TAR	C2
3	M	1	TAR	C2

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Mol	Chain	Res	Type	Atom
3	O	423	TAR	C2

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	K	423	TAR	O1-C1-C2-O2
3	K	423	TAR	O11-C1-C2-O2
3	K	426	TAR	O1-C1-C2-O2
3	K	426	TAR	O11-C1-C2-O2
3	K	426	TAR	O3-C3-C4-O4
3	K	426	TAR	O3-C3-C4-O41
3	K	423	TAR	O2-C2-C3-O3
3	K	423	TAR	O3-C3-C4-O4
3	K	423	TAR	O3-C3-C4-O41
3	K	424	TAR	O3-C3-C4-O4
3	K	424	TAR	O3-C3-C4-O41
3	K	425	TAR	O3-C3-C4-O4
3	K	425	TAR	O3-C3-C4-O41
3	O	423	TAR	O3-C3-C4-O4
3	O	423	TAR	O3-C3-C4-O41
3	K	423	TAR	C2-C3-C4-O4
3	K	423	TAR	C2-C3-C4-O41
3	K	423	TAR	C1-C2-C3-O3
3	K	424	TAR	O2-C2-C3-O3
3	K	425	TAR	O11-C1-C2-O2
3	M	1	TAR	O1-C1-C2-O2
3	M	1	TAR	O11-C1-C2-O2
3	M	1	TAR	O3-C3-C4-O4
3	O	423	TAR	O1-C1-C2-O2
3	O	423	TAR	O11-C1-C2-O2
3	K	425	TAR	O1-C1-C2-O2
3	M	1	TAR	O3-C3-C4-O41
3	K	423	TAR	O2-C2-C3-C4
3	K	424	TAR	C1-C2-C3-O3
3	K	426	TAR	O2-C2-C3-O3
3	K	424	TAR	O2-C2-C3-C4
3	K	423	TAR	C1-C2-C3-C4
3	K	425	TAR	C2-C3-C4-O4
3	K	424	TAR	C1-C2-C3-C4
3	K	425	TAR	C2-C3-C4-O41
3	K	425	TAR	O2-C2-C3-O3
3	M	1	TAR	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	O	423	TAR	O2-C2-C3-O3
3	K	424	TAR	C2-C3-C4-O41

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	71/87 (81%)	1.87	26 (36%) 1 0	59, 84, 88, 89	0
1	B	71/87 (81%)	3.17	57 (80%) 0 0	137, 145, 147, 147	0
1	C	71/87 (81%)	1.97	26 (36%) 1 0	71, 87, 92, 92	0
1	D	71/87 (81%)	2.80	51 (71%) 0 0	107, 126, 127, 127	0
1	E	71/87 (81%)	3.01	58 (81%) 0 0	119, 133, 135, 135	0
2	K	421/421 (100%)	0.87	88 (20%) 2 2	31, 49, 111, 120	0
2	L	421/421 (100%)	1.34	122 (28%) 1 1	33, 62, 132, 139	0
2	M	421/421 (100%)	1.11	93 (22%) 2 2	31, 53, 116, 126	0
2	N	421/421 (100%)	1.26	109 (25%) 1 1	36, 66, 139, 145	0
2	O	421/421 (100%)	1.39	130 (30%) 1 1	34, 62, 135, 139	0
All	All	2460/2540 (96%)	1.39	760 (30%) 1 1	31, 64, 137, 147	0

All (760) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	107	LEU	8.4
1	B	194	VAL	8.2
2	M	178	GLY	8.1
2	M	131	ASP	7.6
2	O	186	GLY	7.6
2	M	2	SER	7.5
2	M	156	LEU	7.4
2	O	156	LEU	7.2
2	L	358	ASP	7.1
2	N	2	SER	7.0
2	K	364	LEU	6.6
2	O	365	THR	6.5
2	L	107	LEU	6.5

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Mol	Chain	Res	Type	RSRZ
2	M	121	VAL	6.5
1	B	222	ASP	6.5
2	O	93	ILE	6.5
1	C	194	VAL	6.5
2	M	162	ASN	6.2
2	O	354	LYS	6.1
2	K	131	ASP	6.0
1	D	253	LYS	6.0
2	M	163	GLN	5.9
2	L	160	LEU	5.9
2	O	162	ASN	5.9
2	K	175	VAL	5.8
2	M	160	LEU	5.8
2	L	186	GLY	5.8
2	O	144	VAL	5.8
1	E	255	LEU	5.8
2	M	172	GLU	5.7
1	B	261	VAL	5.7
2	K	350	VAL	5.7
2	L	159	GLY	5.6
1	B	195	SER	5.5
1	B	254	LYS	5.5
2	O	161	THR	5.5
2	K	167	ILE	5.5
2	O	358	ASP	5.4
2	M	370	PRO	5.4
2	N	142	TYR	5.4
2	O	357	PRO	5.4
2	K	144	VAL	5.4
2	L	181	ILE	5.4
1	C	251	ARG	5.4
1	E	198	TRP	5.3
2	L	354	LYS	5.3
1	D	242	HIS	5.3
1	C	250	LEU	5.2
2	M	161	THR	5.2
2	K	159	GLY	5.1
1	E	253	LYS	5.1
2	M	145	GLY	5.1
2	O	88	TRP	5.0
1	B	258	GLN	5.0
1	A	194	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
2	L	162	ASN	5.0
2	O	175	VAL	5.0
1	D	226	SER	5.0
2	N	81	ARG	4.9
1	E	195	SER	4.9
1	B	201	SER	4.9
2	K	182	PHE	4.9
1	A	226	SER	4.8
2	M	129	ALA	4.8
1	B	239	ARG	4.8
1	D	250	LEU	4.8
2	M	361	THR	4.8
2	O	353	ASN	4.8
2	O	370	PRO	4.8
2	N	108	VAL	4.8
2	O	95	ILE	4.7
2	K	149	MET	4.7
2	N	152	TYR	4.7
2	L	182	PHE	4.7
1	D	194	VAL	4.7
2	O	182	PHE	4.7
2	N	357	PRO	4.7
1	E	213	SER	4.7
1	B	200	LEU	4.7
1	E	197	VAL	4.7
2	K	178	GLY	4.7
1	D	247	LEU	4.7
2	M	167	ILE	4.6
1	B	255	LEU	4.6
2	O	68	HIS	4.6
2	K	156	LEU	4.6
2	L	131	ASP	4.6
1	E	220	SER	4.6
2	N	112	ALA	4.6
1	E	221	LEU	4.6
1	B	220	SER	4.6
2	L	189	SER	4.6
1	D	214	LEU	4.5
2	L	110	LEU	4.5
2	L	351	GLY	4.5
2	L	8	ILE	4.5
1	A	252	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
2	M	107	LEU	4.5
2	M	159	GLY	4.5
2	M	176	PRO	4.5
2	K	143	ARG	4.5
1	B	263	TYR	4.5
1	C	212	ALA	4.5
2	K	160	LEU	4.5
2	O	110	LEU	4.5
2	K	172	GLU	4.5
2	L	356	THR	4.4
2	N	192	THR	4.4
2	K	155	LYS	4.4
2	L	359	ASP	4.4
1	D	197	VAL	4.4
1	E	234	VAL	4.4
2	L	96	GLY	4.4
1	E	211	LYS	4.4
2	N	356	THR	4.4
1	D	237	ASN	4.3
1	E	224	LEU	4.3
2	L	174	LEU	4.3
2	M	98	ALA	4.3
2	N	186	GLY	4.3
2	L	142	TYR	4.3
2	L	357	PRO	4.3
1	A	234	VAL	4.3
2	L	144	VAL	4.3
1	B	237	ASN	4.3
2	O	167	ILE	4.3
2	O	74	TYR	4.3
1	C	198	TRP	4.2
2	K	365	THR	4.2
1	C	193	ALA	4.2
2	O	159	GLY	4.2
2	K	176	PRO	4.2
2	L	149	MET	4.2
2	N	121	VAL	4.2
1	B	248	LEU	4.2
2	O	59	LEU	4.2
2	O	142	TYR	4.2
2	O	215	TYR	4.2
2	L	129	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
2	L	51	LEU	4.2
1	D	234	VAL	4.1
2	L	156	LEU	4.1
2	M	175	VAL	4.1
2	M	166	MET	4.1
1	E	194	VAL	4.1
2	N	154	LYS	4.1
2	K	129	ALA	4.1
2	K	351	GLY	4.1
1	B	219	ILE	4.1
1	B	257	ASN	4.1
2	L	364	LEU	4.1
2	O	171	PHE	4.1
2	K	370	PRO	4.1
2	K	163	GLN	4.1
2	M	120	GLY	4.1
2	O	53	GLY	4.1
2	N	181	ILE	4.1
2	N	156	LEU	4.0
1	D	203	THR	4.0
2	N	365	THR	4.0
1	E	210	LYS	4.0
2	O	42	ILE	4.0
2	O	147	THR	4.0
1	E	235	GLY	4.0
2	N	351	GLY	4.0
2	O	129	ALA	4.0
2	N	117	LEU	4.0
1	B	227	SER	3.9
2	M	357	PRO	3.9
1	B	232	ILE	3.9
1	B	221	LEU	3.9
2	N	113	LEU	3.9
2	M	358	ASP	3.9
2	M	158	ASP	3.9
2	M	43	ASN	3.9
2	K	118	PRO	3.9
2	M	122	SER	3.9
2	L	361	THR	3.9
1	D	254	LYS	3.9
1	D	255	LEU	3.9
1	E	252	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
2	O	94	ASN	3.8
2	K	117	LEU	3.8
2	L	113	LEU	3.8
2	O	149	MET	3.8
2	O	184	VAL	3.8
2	L	176	PRO	3.8
1	D	258	GLN	3.8
2	K	170	GLN	3.8
2	L	365	THR	3.8
2	L	55	VAL	3.8
1	D	202	LYS	3.8
2	M	182	PHE	3.8
1	B	197	VAL	3.8
2	K	164	CYS	3.8
2	O	148	GLN	3.8
2	N	136	LEU	3.8
2	L	121	VAL	3.8
2	L	187	ASN	3.7
2	N	137	TYR	3.7
2	N	159	GLY	3.7
2	K	354	LYS	3.7
1	D	225	PHE	3.7
2	O	157	MET	3.7
2	K	187	ASN	3.7
1	E	219	ILE	3.7
1	E	217	LEU	3.7
2	M	350	VAL	3.7
2	N	175	VAL	3.7
2	N	198	VAL	3.7
2	O	173	PRO	3.7
2	N	160	LEU	3.7
2	K	177	GLU	3.7
2	L	353	ASN	3.6
1	B	238	GLY	3.6
2	M	141	LEU	3.6
2	O	136	LEU	3.6
2	O	139	LEU	3.6
1	B	203	THR	3.6
1	E	222	ASP	3.6
2	L	74	TYR	3.6
2	L	355	TYR	3.6
2	M	355	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
2	N	171	PHE	3.6
2	O	105	PHE	3.6
1	C	261	VAL	3.6
1	E	199	SER	3.6
2	M	3	VAL	3.6
2	O	160	LEU	3.6
1	E	239	ARG	3.6
2	K	161	THR	3.6
2	K	152	TYR	3.6
1	B	241	SER	3.6
1	D	220	SER	3.6
2	O	46	LYS	3.6
2	O	166	MET	3.5
1	E	238	GLY	3.5
2	M	253	GLU	3.5
1	B	253	LYS	3.5
2	L	154	LYS	3.5
2	O	83	LYS	3.5
1	E	250	LEU	3.5
2	L	59	LEU	3.5
1	D	213	SER	3.5
2	L	104	ILE	3.5
2	O	104	ILE	3.5
1	B	206	THR	3.5
2	M	190	ASN	3.5
2	M	186	GLY	3.5
2	L	88	TRP	3.5
2	L	369	PRO	3.5
1	E	214	LEU	3.5
1	B	193	ALA	3.5
1	C	265	LEU	3.5
1	C	241	SER	3.5
2	O	152	TYR	3.4
1	A	212	ALA	3.4
2	N	21	ASN	3.4
2	O	91	PHE	3.4
2	M	75	GLY	3.4
2	N	150	PRO	3.4
2	O	352	ASP	3.4
1	B	224	LEU	3.4
2	K	174	LEU	3.4
2	L	139	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	L	171	PHE	3.4
2	N	149	MET	3.4
2	O	90	SER	3.4
2	O	355	TYR	3.4
1	E	200	LEU	3.4
1	E	257	ASN	3.4
2	L	130	ASP	3.4
1	E	207	PHE	3.4
2	L	90	SER	3.4
2	O	72	TYR	3.4
2	O	366	THR	3.4
2	L	82	GLY	3.4
2	K	183	ASP	3.4
2	M	23	ASP	3.4
2	M	108	VAL	3.4
1	E	232	ILE	3.3
1	A	253	LYS	3.3
1	E	263	TYR	3.3
1	C	228	ARG	3.3
1	D	244	GLU	3.3
2	N	37	GLU	3.3
2	L	362	GLY	3.3
2	M	351	GLY	3.3
1	E	262	LYS	3.3
1	D	198	TRP	3.3
1	E	248	LEU	3.3
1	E	229	GLY	3.3
1	D	230	GLU	3.3
1	E	256	TYR	3.3
2	L	147	THR	3.3
2	M	153	ARG	3.3
2	N	153	ARG	3.3
2	K	110	LEU	3.3
2	N	68	HIS	3.3
1	D	229	GLY	3.3
2	L	111	LYS	3.3
1	E	261	VAL	3.3
2	L	93	ILE	3.3
2	K	179	ARG	3.3
1	E	206	THR	3.3
2	L	2	SER	3.3
1	D	231	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
2	L	64	VAL	3.3
2	O	343	ASP	3.3
1	B	198	TRP	3.2
2	N	110	LEU	3.2
1	C	242	HIS	3.2
2	L	109	SER	3.2
2	M	152	TYR	3.2
1	A	193	ALA	3.2
1	A	255	LEU	3.2
2	O	174	LEU	3.2
2	N	363	GLY	3.2
1	D	246	ILE	3.2
2	K	171	PHE	3.2
2	M	181	ILE	3.2
2	K	106	ASP	3.2
2	K	166	MET	3.2
1	B	214	LEU	3.2
2	N	185	TRP	3.2
1	B	213	SER	3.2
2	O	178	GLY	3.2
2	K	181	ILE	3.2
2	M	144	VAL	3.2
2	O	116	VAL	3.2
2	L	151	GLU	3.2
2	M	51	LEU	3.2
2	O	134	LEU	3.2
2	N	176	PRO	3.2
2	O	150	PRO	3.2
2	L	170	GLN	3.2
1	B	259	ALA	3.2
2	L	29	ALA	3.2
2	K	102	ILE	3.2
2	N	180	ASP	3.1
1	B	250	LEU	3.1
2	M	151	GLU	3.1
2	O	57	GLN	3.1
2	L	366	THR	3.1
2	O	181	ILE	3.1
1	B	243	LYS	3.1
2	K	168	ASN	3.1
2	O	28	PRO	3.1
1	D	241	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	261	VAL	3.1
1	B	262	LYS	3.1
2	N	155	LYS	3.1
2	O	193	LYS	3.1
1	A	220	SER	3.1
2	N	200	MET	3.1
2	L	56	TYR	3.1
2	K	100	ASP	3.1
2	M	188	ASP	3.1
2	O	96	GLY	3.1
2	O	120	GLY	3.1
2	L	42	ILE	3.1
2	K	185	TRP	3.1
2	N	281	PHE	3.1
1	D	195	SER	3.1
1	D	252	TYR	3.0
2	N	56	TYR	3.0
2	O	107	LEU	3.0
2	L	53	GLY	3.0
2	N	361	THR	3.0
2	N	95	ILE	3.0
1	B	260	ARG	3.0
2	L	108	VAL	3.0
1	D	265	LEU	3.0
2	K	357	PRO	3.0
1	C	253	LYS	3.0
2	K	366	THR	3.0
2	O	356	THR	3.0
2	M	21	ASN	3.0
2	M	165	LYS	3.0
2	M	343	ASP	3.0
1	B	228	ARG	3.0
1	C	238	GLY	3.0
2	K	186	GLY	3.0
2	M	124	ALA	3.0
1	A	231	PHE	3.0
2	N	144	VAL	3.0
2	L	169	GLU	3.0
2	K	353	ASN	3.0
2	N	42	ILE	3.0
2	N	124	ALA	3.0
1	B	223	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	195	SER	2.9
2	L	28	PRO	2.9
2	N	207	LYS	2.9
2	L	167	ILE	2.9
2	O	194	ILE	2.9
1	B	231	PHE	2.9
2	M	171	PHE	2.9
2	N	202	PHE	2.9
2	N	139	LEU	2.9
1	B	242	HIS	2.9
2	O	118	PRO	2.9
2	K	359	ASP	2.9
1	D	236	GLY	2.9
1	E	249	GLY	2.9
1	B	247	LEU	2.9
2	L	370	PRO	2.9
1	C	220	SER	2.9
2	L	188	ASP	2.9
2	O	351	GLY	2.9
2	L	40	LEU	2.9
2	M	174	LEU	2.9
2	N	151	GLU	2.9
1	B	199	SER	2.9
2	L	61	SER	2.9
2	O	66	ILE	2.9
2	M	365	THR	2.9
2	L	141	LEU	2.9
2	O	155	LYS	2.9
1	E	231	PHE	2.9
2	O	69	VAL	2.9
2	L	157	MET	2.8
1	E	258	GLN	2.8
2	K	47	SER	2.8
2	M	189	SER	2.8
2	O	71	SER	2.8
2	N	165	LYS	2.8
2	O	92	GLY	2.8
1	E	203	THR	2.8
2	K	147	THR	2.8
2	M	366	THR	2.8
2	N	44	THR	2.8
2	M	170	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
2	N	131	ASP	2.8
2	O	140	GLY	2.8
2	L	84	LEU	2.8
2	O	51	LEU	2.8
2	K	108	VAL	2.8
2	M	55	VAL	2.8
2	M	177	GLU	2.8
2	M	149	MET	2.8
2	L	360	SER	2.8
1	B	236	GLY	2.8
1	D	238	GLY	2.8
2	L	77	LEU	2.8
2	L	44	THR	2.8
2	N	350	VAL	2.8
2	K	157	MET	2.8
2	N	166	MET	2.8
2	O	209	GLU	2.8
2	O	317	ARG	2.8
2	O	89	SER	2.8
2	O	168	ASN	2.8
1	D	221	LEU	2.8
2	L	136	LEU	2.8
1	B	244	GLU	2.8
1	E	218	THR	2.8
2	K	361	THR	2.8
2	M	22	GLU	2.8
1	B	256	TYR	2.8
2	L	72	TYR	2.8
2	L	152	TYR	2.8
2	O	387	ARG	2.8
2	M	173	PRO	2.7
1	E	243	LYS	2.7
2	L	155	LYS	2.7
1	D	204	SER	2.7
2	O	117	LEU	2.7
2	O	189	SER	2.7
2	M	168	ASN	2.7
2	N	353	ASN	2.7
2	L	175	VAL	2.7
2	M	184	VAL	2.7
2	O	67	ILE	2.7
1	A	213	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	M	140	GLY	2.7
2	N	189	SER	2.7
2	N	216	GLY	2.7
2	L	3	VAL	2.7
2	L	153	ARG	2.7
2	M	64	VAL	2.7
1	D	243	LYS	2.7
2	L	137	TYR	2.7
2	N	194	ILE	2.7
2	O	84	LEU	2.7
2	L	116	VAL	2.7
2	N	366	THR	2.7
2	O	131	ASP	2.7
2	O	111	LYS	2.7
2	K	363	GLY	2.7
2	M	126	ARG	2.7
1	E	244	GLU	2.7
1	B	212	ALA	2.7
1	C	245	ALA	2.7
2	M	29	ALA	2.7
2	N	29	ALA	2.7
2	N	132	LYS	2.7
2	O	121	VAL	2.7
2	L	45	THR	2.7
2	N	170	GLN	2.6
2	M	142	TYR	2.6
1	D	232	ILE	2.6
2	L	95	ILE	2.6
1	C	248	LEU	2.6
2	N	134	LEU	2.6
1	A	251	ARG	2.6
1	E	251	ARG	2.6
2	M	112	ALA	2.6
2	O	108	VAL	2.6
2	L	135	PRO	2.6
2	N	370	PRO	2.6
2	O	45	THR	2.6
1	D	222	ASP	2.6
1	B	252	TYR	2.6
2	N	174	LEU	2.6
2	L	68	HIS	2.6
1	A	236	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	229	GLY	2.6
1	E	254	LYS	2.6
2	K	46	LYS	2.6
2	O	195	VAL	2.6
2	O	350	VAL	2.6
2	L	150	PRO	2.6
2	L	161	THR	2.6
2	K	114	ASP	2.6
2	N	130	ASP	2.6
2	O	106	ASP	2.6
1	D	219	ILE	2.6
2	M	8	ILE	2.6
2	M	155	LYS	2.6
1	D	193	ALA	2.6
2	K	116	VAL	2.6
2	L	173	PRO	2.6
2	O	55	VAL	2.6
1	E	227	SER	2.6
2	L	125	SER	2.6
2	N	57	GLN	2.6
2	O	122	SER	2.6
2	L	158	ASP	2.6
2	N	358	ASP	2.6
1	C	235	GLY	2.6
1	D	257	ASN	2.6
2	K	11	ASN	2.6
2	N	129	ALA	2.6
2	M	148	GLN	2.6
2	M	360	SER	2.5
2	L	166	MET	2.5
2	N	157	MET	2.5
2	O	100	ASP	2.5
2	L	102	ILE	2.5
1	B	210	LYS	2.5
1	E	230	GLU	2.5
2	K	369	PRO	2.5
1	E	245	ALA	2.5
1	E	196	ASP	2.5
1	D	251	ARG	2.5
2	O	137	TYR	2.5
2	M	362	GLY	2.5
2	K	121	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	M	45	THR	2.5
2	O	109	SER	2.5
2	K	154	LYS	2.5
2	L	317	ARG	2.5
2	L	363	GLY	2.5
2	K	367	ASN	2.5
2	O	44	THR	2.5
1	E	241	SER	2.5
2	L	117	LEU	2.5
1	B	230	GLU	2.5
2	N	215	TYR	2.5
2	O	191	TYR	2.5
1	B	215	GLN	2.5
2	L	148	GLN	2.5
2	L	127	THR	2.4
2	K	94	ASN	2.4
2	O	143	ARG	2.4
1	B	265	LEU	2.4
1	E	246	ILE	2.4
2	N	93	ILE	2.4
1	E	201	SER	2.4
2	N	158	ASP	2.4
2	K	120	GLY	2.4
1	B	202	LYS	2.4
2	L	368	ALA	2.4
1	C	260	ARG	2.4
1	D	200	LEU	2.4
2	L	190	ASN	2.4
1	D	199	SER	2.4
2	O	185	TRP	2.4
2	O	37	GLU	2.4
1	A	235	GLY	2.4
2	L	17	LYS	2.4
2	M	56	TYR	2.4
1	B	225	PHE	2.4
1	C	237	ASN	2.4
2	K	162	ASN	2.4
2	L	185	TRP	2.4
1	E	236	GLY	2.4
2	N	28	PRO	2.4
1	E	208	GLN	2.4
1	A	197	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	251	ARG	2.4
1	C	252	TYR	2.4
1	D	259	ALA	2.4
2	K	112	ALA	2.4
2	K	126	ARG	2.4
2	K	355	TYR	2.4
2	N	317	ARG	2.4
2	K	51	LEU	2.4
2	K	107	LEU	2.4
2	N	104	ILE	2.4
1	E	237	ASN	2.4
2	O	63	ASN	2.4
2	N	360	SER	2.4
2	M	123	ASP	2.4
2	M	354	LYS	2.4
2	N	34	LYS	2.4
2	O	369	PRO	2.4
2	L	103	GLY	2.4
1	E	215	GLN	2.4
1	C	234	VAL	2.4
2	L	253	GLU	2.3
2	N	172	GLU	2.3
2	O	17	LYS	2.3
2	O	176	PRO	2.3
1	A	260	ARG	2.3
2	O	405	GLN	2.3
2	N	116	VAL	2.3
2	O	64	VAL	2.3
1	B	217	LEU	2.3
2	N	141	LEU	2.3
2	O	70	ASN	2.3
1	C	195	SER	2.3
2	L	89	SER	2.3
2	K	150	PRO	2.3
2	K	184	VAL	2.3
1	A	247	LEU	2.3
1	E	242	HIS	2.3
1	C	218	THR	2.3
1	A	210	LYS	2.3
1	E	223	GLU	2.3
2	O	35	SER	2.3
2	K	173	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	M	369	PRO	2.3
2	L	67	ILE	2.3
2	N	38	ILE	2.3
2	N	229	ALA	2.3
1	C	211	LYS	2.3
2	L	60	LYS	2.3
1	A	263	TYR	2.3
2	L	27	TYR	2.3
2	O	21	ASN	2.3
1	D	201	SER	2.3
2	K	360	SER	2.3
2	L	99	GLY	2.3
2	L	133	TRP	2.3
2	M	139	LEU	2.3
2	N	3	VAL	2.3
2	N	25	VAL	2.3
2	L	32	PHE	2.3
1	E	193	ALA	2.2
2	K	42	ILE	2.2
2	N	164	CYS	2.2
2	O	268	ILE	2.2
1	A	242	HIS	2.2
1	D	211	LYS	2.2
2	K	101	THR	2.2
2	M	147	THR	2.2
2	K	169	GLU	2.2
1	D	256	TYR	2.2
2	N	355	TYR	2.2
2	M	367	ASN	2.2
2	K	28	PRO	2.2
1	B	235	GLY	2.2
1	C	255	LEU	2.2
1	D	248	LEU	2.2
2	N	133	TRP	2.2
2	N	147	THR	2.2
1	A	256	TYR	2.2
1	D	228	ARG	2.2
2	O	190	ASN	2.2
2	M	359	ASP	2.2
2	N	123	ASP	2.2
2	O	114	ASP	2.2
2	O	145	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	M	136	LEU	2.2
2	O	73	LEU	2.2
2	N	182	PHE	2.2
2	K	368	ALA	2.2
2	N	169	GLU	2.2
2	K	314	ARG	2.2
2	N	314	ARG	2.2
2	M	118	PRO	2.2
2	K	180	ASP	2.2
2	M	154	LYS	2.2
2	N	359	ASP	2.2
2	O	23	ASP	2.2
2	N	184	VAL	2.2
2	O	80	ILE	2.2
2	L	211	ALA	2.2
2	M	4	THR	2.2
2	O	127	THR	2.2
1	E	216	PRO	2.2
2	O	274	TYR	2.2
2	K	362	GLY	2.2
2	L	73	LEU	2.2
2	K	119	ASP	2.2
2	L	180	ASP	2.2
2	O	360	SER	2.2
2	O	211	ALA	2.1
2	O	151	GLU	2.1
1	A	208	GLN	2.1
1	D	263	TYR	2.1
1	D	217	LEU	2.1
2	M	53	GLY	2.1
2	N	178	GLY	2.1
2	L	5	VAL	2.1
2	O	183	ASP	2.1
2	M	128	SER	2.1
1	D	212	ALA	2.1
2	L	112	ALA	2.1
2	K	22	GLU	2.1
2	O	146	ARG	2.1
2	M	12	THR	2.1
1	B	216	PRO	2.1
1	C	257	ASN	2.1
2	L	200	MET	2.1

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Mol	Chain	Res	Type	RSRZ
2	N	84	LEU	2.1
2	N	364	LEU	2.1
2	L	195	VAL	2.1
2	N	102	ILE	2.1
2	K	125	SER	2.1
2	N	196	ALA	2.1
2	N	148	GLN	2.1
2	O	22	GLU	2.1
2	O	86	LYS	2.1
2	L	163	GLN	2.1
2	M	134	LEU	2.1
2	L	75	GLY	2.1
2	O	380	GLY	2.1
2	O	56	TYR	2.1
2	K	85	ASP	2.0
2	O	119	ASP	2.0
2	M	223	LYS	2.0
2	K	113	LEU	2.0
2	N	51	LEU	2.0
2	N	138	LEU	2.0
2	M	363	GLY	2.0
1	A	228	ARG	2.0
2	K	358	ASP	2.0
2	O	158	ASP	2.0
1	A	233	SER	2.0
2	N	49	SER	2.0
2	N	122	SER	2.0
2	L	101	THR	2.0
1	A	250	LEU	2.0
2	K	136	LEU	2.0
2	N	278	LEU	2.0
2	N	75	GLY	2.0
2	N	120	GLY	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($\text{\AA}^2$)	Q<0.9
3	TAR	K	424	10/10	0.41	0.18	92,93,93,93	0
3	TAR	K	423	10/10	0.56	0.18	120,120,120,120	0
3	TAR	M	1	10/10	0.60	0.24	117,118,118,118	0
3	TAR	O	423	10/10	0.64	0.18	108,108,108,108	0
3	TAR	K	426	10/10	0.69	0.19	87,88,88,88	0
3	TAR	K	425	10/10	0.70	0.20	67,69,70,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.