



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:59 PM GMT

PDB ID : 4NFZ
Title : Crystal structure of polymerase subunit PA N-terminal endonuclease domain from bat-derived influenza virus H17N10
Authors : Tefsen, B.; Lu, G.; Zhu, Y.; Haywood, J.; Zhao, L.; Deng, T.; Qi, J.; Gao, G.F.
Deposited on : 2013-11-01
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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

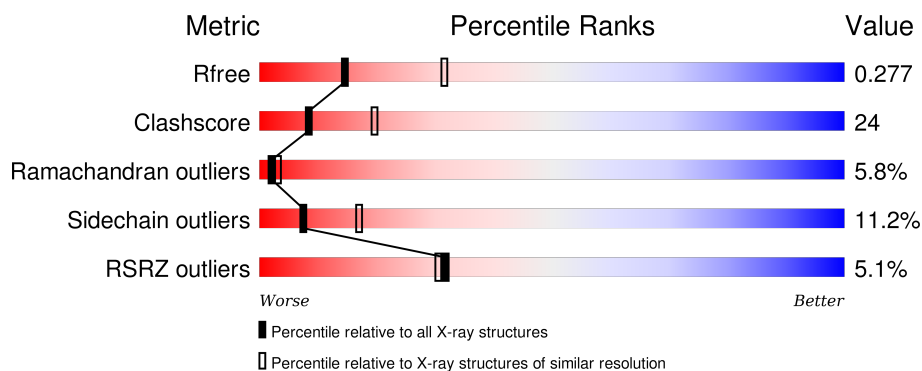
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 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	214	<div> <div>2%</div> <div>54%</div> <div>28%</div> <div>9%</div> <div>8%</div> </div>
1	B	214	<div> <div>5%</div> <div>56%</div> <div>30%</div> <div>8%</div> </div>
1	C	214	<div> <div>7%</div> <div>54%</div> <div>30%</div> <div>7%</div> <div>8%</div> </div>

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
2	MN	B	300	-	-	-	X
2	MN	C	300	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4927 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 Polymerase PA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1634	1031	275	318	10			
1	B	196	Total	C	N	O	S	0	0	0
			1634	1031	275	318	10			
1	C	196	Total	C	N	O	S	0	0	0
			1634	1031	275	318	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	207	LEU	-	EXPRESSION TAG	UNP H6QM92
A	208	GLU	-	EXPRESSION TAG	UNP H6QM92
A	209	HIS	-	EXPRESSION TAG	UNP H6QM92
A	210	HIS	-	EXPRESSION TAG	UNP H6QM92
A	211	HIS	-	EXPRESSION TAG	UNP H6QM92
A	212	HIS	-	EXPRESSION TAG	UNP H6QM92
A	213	HIS	-	EXPRESSION TAG	UNP H6QM92
A	214	HIS	-	EXPRESSION TAG	UNP H6QM92
B	207	LEU	-	EXPRESSION TAG	UNP H6QM92
B	208	GLU	-	EXPRESSION TAG	UNP H6QM92
B	209	HIS	-	EXPRESSION TAG	UNP H6QM92
B	210	HIS	-	EXPRESSION TAG	UNP H6QM92
B	211	HIS	-	EXPRESSION TAG	UNP H6QM92
B	212	HIS	-	EXPRESSION TAG	UNP H6QM92
B	213	HIS	-	EXPRESSION TAG	UNP H6QM92
B	214	HIS	-	EXPRESSION TAG	UNP H6QM92
C	207	LEU	-	EXPRESSION TAG	UNP H6QM92
C	208	GLU	-	EXPRESSION TAG	UNP H6QM92
C	209	HIS	-	EXPRESSION TAG	UNP H6QM92
C	210	HIS	-	EXPRESSION TAG	UNP H6QM92
C	211	HIS	-	EXPRESSION TAG	UNP H6QM92
C	212	HIS	-	EXPRESSION TAG	UNP H6QM92
C	213	HIS	-	EXPRESSION TAG	UNP H6QM92

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Chain	Residue	Modelled	Actual	Comment	Reference
C	214	HIS	-	EXPRESSION TAG	UNP H6QM92

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mn 1 1	0	0
2	A	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	B	10	Total O 10 10	0	0
3	C	7	Total O 7 7	0	0

T184	
F191	
R192	
Q193	
S194	
E195	
K196	
GLY	
GLU	
GLU	
THR	
LEU	
GLU	
GLU	
GLU	
PHE	
SER	
LEU	
GLU	
HIS	
HIS	
HIS	
HIS	
HIS	
HIS	

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	74.30 Å 74.30 Å 401.16 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.80 – 2.70 42.80 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (42.80-2.70) 97.6 (42.80-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.70 (at 2.69 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.240 , 0.278 0.236 , 0.277	Depositor DCC
R_{free} test set	962 reflections (5.13%)	DCC
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 19232 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4927	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.67	0/1667	0.78	3/2241 (0.1%)
1	B	0.71	0/1667	0.82	3/2241 (0.1%)
1	C	0.68	0/1667	0.80	3/2241 (0.1%)
All	All	0.69	0/5001	0.80	9/6723 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	108	ASP	CB-CG-OD2	7.50	125.05	118.30
1	B	108	ASP	CB-CG-OD2	6.74	124.37	118.30
1	C	70	ALA	CB-CA-C	-6.59	100.22	110.10
1	A	70	ALA	CB-CA-C	-6.04	101.04	110.10
1	C	108	ASP	CB-CG-OD2	5.61	123.34	118.30
1	C	70	ALA	N-CA-C	5.55	125.98	111.00
1	A	70	ALA	N-CA-C	5.46	125.75	111.00
1	B	67	ASP	CB-CA-C	-5.41	99.57	110.40
1	B	75	ARG	NE-CZ-NH1	-5.08	117.76	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1634	0	1568	81	0
1	B	1634	0	1568	80	2
1	C	1634	0	1568	83	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	5	0	0	10	0
3	B	10	0	0	34	0
3	C	7	0	0	26	0
All	All	4927	0	4704	232	2

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 24.

All (232) 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:29:GLN:HB2	3:A:403:HOH:O	1.34	1.28
1:A:126:LYS:O	1:A:127:VAL:HG22	1.41	1.19
1:C:75:ARG:NH2	1:C:162:ILE:CG2	2.11	1.14
1:C:168:ARG:HG3	3:C:403:HOH:O	1.48	1.13
1:A:85:ASN:ND2	1:A:86:ILE:H	1.45	1.13
1:B:142:ASN:CA	3:B:402:HOH:O	1.97	1.12
1:A:127:VAL:HG21	1:A:153:GLU:HG3	1.26	1.12
1:A:27:ASN:ND2	3:A:403:HOH:O	1.80	1.12
1:C:75:ARG:NH2	1:C:162:ILE:HG23	1.63	1.09
1:C:141:GLU:N	3:C:404:HOH:O	1.84	1.09
1:C:195:GLU:CB	3:C:401:HOH:O	2.01	1.08
1:B:142:ASN:C	3:B:402:HOH:O	1.90	1.07
1:C:132:TYR:HA	3:C:402:HOH:O	1.55	1.07
1:B:188:TRP:CD1	3:B:404:HOH:O	2.06	1.06
1:B:183:ALA:HA	3:B:407:HOH:O	1.55	1.06
1:A:85:ASN:ND2	1:A:86:ILE:N	2.06	1.04
1:B:70:ALA:N	3:B:403:HOH:O	1.91	1.04
1:C:165:GLU:HA	3:C:403:HOH:O	1.56	1.04
1:B:194:SER:N	3:B:409:HOH:O	1.89	1.03
1:C:75:ARG:HH22	1:C:162:ILE:HG23	1.10	1.02
1:B:70:ALA:HA	3:B:403:HOH:O	1.62	0.99
1:B:70:ALA:CA	3:B:403:HOH:O	2.10	0.99
1:C:75:ARG:HH22	1:C:162:ILE:CG2	1.71	0.98
1:C:141:GLU:CA	3:C:404:HOH:O	2.09	0.97
1:A:15:GLU:OE1	1:A:19:LYS:NZ	1.98	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ARG:NH2	1:C:18:GLU:OE2	1.98	0.96
1:B:178:LEU:N	3:B:406:HOH:O	1.96	0.96
1:A:85:ASN:HD22	1:A:86:ILE:N	1.62	0.94
1:B:142:ASN:O	3:B:402:HOH:O	1.82	0.94
1:B:67:ASP:O	1:B:69:ASN:OD1	1.85	0.94
1:C:132:TYR:O	3:C:402:HOH:O	1.85	0.94
1:B:194:SER:CA	3:B:409:HOH:O	2.16	0.94
1:A:167:SER:O	3:A:404:HOH:O	1.85	0.94
1:B:177:VAL:HB	3:B:406:HOH:O	1.66	0.93
1:C:27:ASN:OD1	1:C:28:PRO:O	1.88	0.92
1:C:135:ALA:HB3	3:C:402:HOH:O	1.70	0.91
1:B:27:ASN:OD1	1:B:29:GLN:HB2	1.69	0.91
1:A:160:GLU:N	3:A:402:HOH:O	2.01	0.91
1:A:161:TYR:OH	3:A:401:HOH:O	1.88	0.91
1:A:127:VAL:CG2	1:A:153:GLU:HG3	2.00	0.90
1:B:142:ASN:CG	3:B:402:HOH:O	2.09	0.90
1:B:100:ASN:O	3:B:401:HOH:O	1.89	0.89
1:B:188:TRP:NE1	3:B:404:HOH:O	2.06	0.88
1:A:85:ASN:HD22	1:A:86:ILE:H	0.91	0.87
1:B:3:ASN:ND2	1:C:10:ASN:HB2	1.90	0.85
1:C:164:ASP:O	3:C:403:HOH:O	1.95	0.84
1:C:168:ARG:CG	3:C:403:HOH:O	2.12	0.83
1:B:188:TRP:CE2	3:B:404:HOH:O	2.31	0.83
1:C:141:GLU:C	3:C:404:HOH:O	2.17	0.83
1:A:126:LYS:O	1:A:127:VAL:CG2	2.26	0.83
1:A:29:GLN:OE1	1:A:29:GLN:HA	1.76	0.83
1:B:3:ASN:HD21	1:C:10:ASN:HB2	1.44	0.81
1:A:127:VAL:HG21	1:A:153:GLU:CG	2.08	0.81
1:C:195:GLU:HB3	3:C:401:HOH:O	1.72	0.81
1:B:177:VAL:CB	3:B:406:HOH:O	2.24	0.81
1:B:142:ASN:ND2	3:B:402:HOH:O	2.13	0.79
1:A:29:GLN:OE1	1:A:29:GLN:CA	2.30	0.79
1:A:126:LYS:C	1:A:127:VAL:CG2	2.52	0.78
1:B:194:SER:HB3	3:B:409:HOH:O	1.83	0.78
1:B:194:SER:CB	3:B:409:HOH:O	2.32	0.77
1:B:174:ARG:O	3:B:406:HOH:O	2.03	0.76
1:B:188:TRP:CG	3:B:404:HOH:O	2.31	0.76
1:B:115:ASN:OD1	3:B:410:HOH:O	2.04	0.75
1:A:126:LYS:C	1:A:127:VAL:HG22	2.04	0.75
1:C:29:GLN:O	1:C:30:ASN:CB	2.32	0.75
1:C:132:TYR:CA	3:C:402:HOH:O	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ASN:HD21	1:C:10:ASN:CB	2.02	0.73
1:A:27:ASN:ND2	1:A:29:GLN:HB2	2.04	0.73
1:C:194:SER:O	3:C:407:HOH:O	2.06	0.71
1:B:190:SER:O	3:B:409:HOH:O	2.07	0.71
1:A:27:ASN:HD21	1:A:29:GLN:HB2	1.55	0.71
1:B:68:ASP:C	1:B:69:ASN:OD1	2.29	0.71
1:C:141:GLU:CG	3:C:404:HOH:O	2.39	0.70
1:B:142:ASN:N	3:B:402:HOH:O	2.12	0.70
1:C:29:GLN:O	1:C:30:ASN:CG	2.30	0.70
1:A:157:THR:O	3:A:402:HOH:O	2.08	0.69
1:B:177:VAL:CG1	3:B:406:HOH:O	2.38	0.69
1:B:188:TRP:CD2	3:B:404:HOH:O	2.46	0.69
1:C:61:ILE:HG12	1:C:62:VAL:H	1.58	0.68
1:C:172:LYS:O	3:C:406:HOH:O	2.10	0.68
1:A:126:LYS:HB2	1:A:129:ASP:OD2	1.94	0.68
1:A:170:ARG:HB3	3:A:404:HOH:O	1.94	0.67
1:A:63:LYS:O	1:A:63:LYS:HG3	1.94	0.67
1:C:61:ILE:HG12	1:C:62:VAL:N	2.10	0.66
1:B:139:LYS:NZ	3:B:408:HOH:O	2.28	0.66
1:B:16:ARG:O	1:B:20:THR:HG23	1.96	0.66
1:C:163:LEU:O	3:C:405:HOH:O	2.14	0.66
1:C:29:GLN:O	1:C:30:ASN:HB2	1.96	0.66
1:A:85:ASN:ND2	1:A:86:ILE:HG12	2.10	0.65
1:B:177:VAL:HG12	3:B:406:HOH:O	1.97	0.65
1:C:16:ARG:O	1:C:20:THR:HG23	1.97	0.65
1:C:195:GLU:HA	3:C:407:HOH:O	1.96	0.65
1:A:113:LYS:O	1:A:113:LYS:HD2	1.98	0.64
1:A:85:ASN:HD21	1:A:86:ILE:HG12	1.63	0.64
1:B:2:GLU:HB3	1:C:12:MET:CE	2.27	0.64
1:C:168:ARG:NE	3:C:403:HOH:O	2.30	0.63
1:B:69:ASN:OD1	1:B:69:ASN:N	2.30	0.63
1:C:195:GLU:N	3:C:401:HOH:O	1.92	0.62
1:B:3:ASN:HD21	1:C:10:ASN:CG	2.03	0.60
1:A:16:ARG:O	1:A:20:THR:HG23	2.02	0.60
1:C:162:ILE:N	1:C:162:ILE:CD1	2.65	0.59
1:A:167:SER:HA	3:A:404:HOH:O	2.03	0.58
1:C:176:PHE:O	1:C:180:GLN:HG3	2.04	0.58
1:C:55:ASP:HB3	1:C:57:GLU:H	1.69	0.58
1:B:183:ALA:O	3:B:407:HOH:O	2.17	0.57
1:B:27:ASN:OD1	1:B:29:GLN:CB	2.47	0.57
1:A:29:GLN:OE1	1:A:29:GLN:C	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:ARG:CB	3:C:403:HOH:O	2.50	0.56
1:C:75:ARG:NH2	1:C:162:ILE:HG22	2.13	0.55
1:A:167:SER:CA	3:A:404:HOH:O	2.53	0.55
1:C:168:ARG:HB2	3:C:403:HOH:O	2.05	0.55
1:A:4:PHE:CZ	1:A:8:ASN:ND2	2.74	0.55
1:A:85:ASN:HD21	1:A:86:ILE:CG1	2.20	0.55
1:A:160:GLU:O	3:A:402:HOH:O	2.17	0.55
1:A:27:ASN:O	1:A:29:GLN:N	2.40	0.54
1:A:85:ASN:HA	1:B:25:GLY:HA2	1.90	0.54
1:A:131:TYR:OH	1:A:157:THR:HA	2.07	0.54
1:B:68:ASP:C	1:B:69:ASN:CG	2.66	0.54
1:B:29:GLN:HG3	1:C:16:ARG:HH21	1.73	0.54
1:C:151:ASP:HB2	1:C:153:GLU:OE2	2.07	0.54
1:B:166:GLU:O	1:B:169:ALA:HB3	2.08	0.53
1:A:22:LYS:HG2	1:A:22:LYS:O	2.08	0.53
1:B:149:SER:OG	1:B:153:GLU:HG2	2.07	0.53
1:B:131:TYR:OH	1:B:157:THR:HA	2.09	0.53
1:A:127:VAL:CG2	1:A:153:GLU:OE1	2.56	0.53
1:B:2:GLU:HB3	1:C:12:MET:HE1	1.92	0.52
1:A:151:ASP:HB2	1:A:153:GLU:OE2	2.10	0.52
1:B:151:ASP:HB2	1:B:153:GLU:OE2	2.11	0.51
1:B:167:SER:O	3:B:405:HOH:O	2.19	0.51
1:C:117:PHE:HB2	1:C:143:VAL:HG22	1.93	0.51
1:A:27:ASN:HD21	1:A:29:GLN:CB	2.22	0.51
1:A:63:LYS:HD2	1:A:66:ASP:H	1.75	0.51
1:C:55:ASP:HB3	1:C:57:GLU:N	2.26	0.51
1:B:68:ASP:HB2	1:B:74:HIS:NE2	2.25	0.51
1:A:97:MET:HG3	1:C:97:MET:HG3	1.93	0.50
1:B:67:ASP:C	1:B:69:ASN:OD1	2.50	0.50
1:B:170:ARG:HB3	3:B:405:HOH:O	2.11	0.50
1:C:142:ASN:ND2	1:C:142:ASN:O	2.45	0.50
1:B:165:GLU:HG3	1:B:168:ARG:NH2	2.26	0.50
1:A:29:GLN:OE1	1:A:29:GLN:O	2.30	0.50
1:C:131:TYR:OH	1:C:157:THR:HA	2.11	0.50
1:C:28:PRO:O	1:C:29:GLN:O	2.30	0.49
1:A:127:VAL:CG2	1:A:153:GLU:CG	2.79	0.49
1:A:75:ARG:HG2	1:A:76:PHE:CE2	2.48	0.49
1:A:63:LYS:NZ	1:A:72:LEU:HD12	2.28	0.49
1:B:142:ASN:O	1:B:142:ASN:ND2	2.46	0.49
1:B:134:LYS:O	1:B:138:LEU:HB2	2.12	0.49
1:B:178:LEU:HG	3:B:406:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ASP:O	1:A:69:ASN:HB2	2.12	0.49
1:B:68:ASP:O	1:B:69:ASN:CB	2.61	0.49
1:A:68:ASP:O	1:A:69:ASN:CB	2.61	0.49
1:C:162:ILE:N	1:C:162:ILE:HD12	2.28	0.48
1:C:78:ILE:HA	1:C:109:LEU:HD23	1.95	0.48
1:A:109:LEU:HB2	1:A:118:ILE:HB	1.96	0.48
1:B:140:GLY:O	1:B:142:ASN:N	2.46	0.48
1:A:22:LYS:O	1:A:22:LYS:CG	2.59	0.48
1:A:56:LEU:HD11	1:A:71:MET:HE2	1.96	0.48
1:C:27:ASN:C	1:C:28:PRO:O	2.51	0.48
1:C:134:LYS:O	1:C:138:LEU:HB2	2.14	0.47
1:A:21:MET:CE	1:A:31:GLU:HB2	2.44	0.47
1:B:3:ASN:ND2	1:C:10:ASN:CB	2.67	0.47
1:C:132:TYR:C	3:C:402:HOH:O	2.26	0.47
1:B:2:GLU:HB3	1:C:12:MET:HE2	1.94	0.47
1:B:124:ARG:HD3	1:B:191:PHE:CE2	2.50	0.47
1:B:55:ASP:HB3	1:B:57:GLU:H	1.80	0.47
1:A:55:ASP:HB3	1:A:57:GLU:N	2.30	0.46
1:C:12:MET:HG3	1:C:13:ILE:N	2.29	0.46
1:A:55:ASP:HB3	1:A:57:GLU:H	1.81	0.46
1:B:139:LYS:HZ1	1:B:140:GLY:H	1.64	0.46
1:B:93:SER:O	1:B:97:MET:HG2	2.15	0.46
1:B:78:ILE:HA	1:B:109:LEU:HD23	1.96	0.46
1:B:77:GLU:HG2	1:B:90:ILE:HG21	1.98	0.46
1:B:4:PHE:CZ	1:B:8:ASN:ND2	2.84	0.46
1:B:139:LYS:CE	1:B:140:GLY:H	2.30	0.45
1:A:149:SER:OG	1:A:153:GLU:HG2	2.17	0.45
1:C:195:GLU:HB2	3:C:401:HOH:O	1.90	0.45
1:A:141:GLU:O	1:A:143:VAL:N	2.50	0.45
1:A:121:GLY:HA3	1:A:130:TYR:HE2	1.81	0.45
1:C:164:ASP:C	3:C:403:HOH:O	2.48	0.45
1:C:124:ARG:HD3	1:C:191:PHE:CE2	2.51	0.45
1:A:125:ARG:HB3	1:A:126:LYS:H	1.66	0.45
1:A:141:GLU:HG2	1:A:141:GLU:H	1.54	0.45
1:C:140:GLY:O	1:C:142:ASN:N	2.49	0.44
1:B:55:ASP:HB3	1:B:57:GLU:N	2.32	0.44
1:B:17:ALA:O	1:B:21:MET:HG3	2.17	0.44
1:A:96:ASN:HD22	1:A:96:ASN:HA	1.60	0.44
1:A:166:GLU:O	1:A:169:ALA:HB3	2.18	0.44
1:B:12:MET:HG2	1:B:16:ARG:NH1	2.32	0.44
1:C:125:ARG:NH2	1:C:195:GLU:OE1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:GLY:O	1:A:142:ASN:N	2.51	0.44
1:B:75:ARG:HG2	1:B:76:PHE:CE2	2.52	0.44
1:A:27:ASN:ND2	1:A:29:GLN:CB	2.80	0.43
1:C:71:MET:O	1:C:72:LEU:HD23	2.18	0.43
1:A:124:ARG:HD3	1:A:191:PHE:CE2	2.53	0.43
1:B:173:THR:O	1:B:176:PHE:N	2.51	0.43
1:C:111:ASP:OD2	1:C:162:ILE:HG21	2.18	0.43
1:C:149:SER:OG	1:C:153:GLU:HG2	2.18	0.43
1:A:53:PHE:CE1	1:A:63:LYS:HG2	2.53	0.43
1:C:166:GLU:O	1:C:169:ALA:HB3	2.19	0.43
1:C:4:PHE:CZ	1:C:8:ASN:ND2	2.87	0.43
1:A:1:MET:HE3	1:A:3:ASN:HB2	2.01	0.43
1:B:139:LYS:HE3	1:B:140:GLY:H	1.84	0.43
1:A:63:LYS:HD2	1:A:65:ASN:H	1.83	0.43
1:C:109:LEU:HB2	1:C:118:ILE:HB	2.00	0.43
1:A:144:TYR:CE1	1:A:162:ILE:HD13	2.53	0.43
1:C:139:LYS:CE	1:C:140:GLY:H	2.32	0.42
1:C:121:GLY:HA3	1:C:130:TYR:HE2	1.83	0.42
1:B:56:LEU:HD23	1:B:56:LEU:HA	1.91	0.42
1:C:75:ARG:HG2	1:C:76:PHE:CE2	2.54	0.42
1:C:154:GLU:OE2	1:C:168:ARG:HD2	2.19	0.42
1:B:64:GLU:HG2	1:B:64:GLU:H	1.54	0.42
1:A:1:MET:HG3	1:A:2:GLU:N	2.35	0.42
1:B:117:PHE:HB2	1:B:143:VAL:HG22	2.02	0.42
1:A:93:SER:O	1:A:96:ASN:HB2	2.19	0.42
1:A:27:ASN:C	1:A:29:GLN:N	2.73	0.42
1:B:68:ASP:O	1:B:69:ASN:CG	2.58	0.42
1:A:89:THR:HG21	1:C:86:ILE:HG23	2.02	0.42
1:C:93:SER:O	1:C:97:MET:HG2	2.20	0.42
1:A:124:ARG:HD3	1:A:191:PHE:CD2	2.55	0.41
1:C:141:GLU:HG2	3:C:404:HOH:O	2.12	0.41
1:A:63:LYS:HZ1	1:A:72:LEU:HD12	1.85	0.41
1:C:139:LYS:HE3	1:C:140:GLY:H	1.84	0.41
1:A:142:ASN:O	1:A:142:ASN:ND2	2.53	0.41
1:A:154:GLU:OE2	1:A:168:ARG:HD2	2.21	0.41
1:B:99:GLU:C	3:B:401:HOH:O	2.58	0.41
1:A:173:THR:O	1:A:176:PHE:HB3	2.21	0.41
1:A:67:ASP:N	1:A:67:ASP:OD1	2.53	0.41
1:C:85:ASN:HB3	1:C:86:ILE:H	1.75	0.41
1:C:125:ARG:HB3	1:C:126:LYS:H	1.55	0.41
1:C:68:ASP:O	1:C:69:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ASN:C	1:A:10:ASN:OD1	2.59	0.40
1:C:68:ASP:O	1:C:69:ASN:CB	2.69	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LYS:NZ	1:C:180:GLN:OE1[7_655]	1.15	1.05
1:B:173:THR:OG1	1:C:173:THR:OG1[7_655]	1.86	0.34

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	194/214 (91%)	170 (88%)	12 (6%)	12 (6%)	2	2
1	B	194/214 (91%)	172 (89%)	13 (7%)	9 (5%)	3	6
1	C	194/214 (91%)	169 (87%)	12 (6%)	13 (7%)	1	2
All	All	582/642 (91%)	511 (88%)	37 (6%)	34 (6%)	2	3

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	LYS
1	A	127	VAL
1	A	137	LYS
1	A	142	ASN
1	B	29	GLN
1	B	137	LYS
1	B	142	ASN
1	C	137	LYS
1	C	142	ASN

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Mol	Chain	Res	Type
1	A	66	ASP
1	A	67	ASP
1	A	69	ASN
1	A	70	ALA
1	A	141	GLU
1	B	55	ASP
1	B	66	ASP
1	B	67	ASP
1	B	69	ASN
1	B	70	ALA
1	B	125	ARG
1	C	29	GLN
1	C	30	ASN
1	C	66	ASP
1	C	67	ASP
1	C	69	ASN
1	C	70	ALA
1	C	85	ASN
1	A	68	ASP
1	C	55	ASP
1	C	125	ARG
1	A	125	ARG
1	A	28	PRO
1	C	28	PRO
1	C	25	GLY

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	178/195 (91%)	153 (86%)	25 (14%)	4	10
1	B	178/195 (91%)	158 (89%)	20 (11%)	7	17
1	C	178/195 (91%)	163 (92%)	15 (8%)	14	30
All	All	534/585 (91%)	474 (89%)	60 (11%)	7	17

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	12	MET
1	A	15	GLU
1	A	19	LYS
1	A	20	THR
1	A	21	MET
1	A	22	LYS
1	A	24	TYR
1	A	26	GLU
1	A	29	GLN
1	A	55	ASP
1	A	61	ILE
1	A	63	LYS
1	A	64	GLU
1	A	67	ASP
1	A	73	LYS
1	A	75	ARG
1	A	84	ARG
1	A	85	ASN
1	A	126	LYS
1	A	127	VAL
1	A	138	LEU
1	A	162	ILE
1	A	163	LEU
1	A	184	THR
1	B	1	MET
1	B	3	ASN
1	B	12	MET
1	B	20	THR
1	B	22	LYS
1	B	26	GLU
1	B	27	ASN
1	B	29	GLN
1	B	30	ASN
1	B	31	GLU
1	B	55	ASP
1	B	63	LYS
1	B	67	ASP
1	B	69	ASN
1	B	73	LYS
1	B	84	ARG
1	B	138	LEU

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Mol	Chain	Res	Type
1	B	154	GLU
1	B	163	LEU
1	B	184	THR
1	C	1	MET
1	C	20	THR
1	C	22	LYS
1	C	26	GLU
1	C	31	GLU
1	C	55	ASP
1	C	63	LYS
1	C	67	ASP
1	C	73	LYS
1	C	84	ARG
1	C	138	LEU
1	C	162	ILE
1	C	163	LEU
1	C	165	GLU
1	C	184	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	85	ASN
1	A	96	ASN
1	B	3	ASN
1	C	3	ASN
1	C	10	ASN
1	C	180	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	196/214 (91%)	0.18	5 (2%) 59 59	28, 52, 93, 148	0
1	B	196/214 (91%)	0.32	10 (5%) 32 30	32, 56, 110, 163	0
1	C	196/214 (91%)	0.47	15 (7%) 16 14	33, 62, 123, 156	0
All	All	588/642 (91%)	0.33	30 (5%) 32 30	28, 57, 110, 163	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	MET	7.4
1	C	193	GLN	5.8
1	A	136	SER	3.8
1	C	196	LYS	3.6
1	C	136	SER	3.4
1	A	71	MET	3.3
1	C	176	PHE	3.2
1	C	104	ARG	3.2
1	C	126	LYS	3.0
1	A	132	TYR	3.0
1	B	132	TYR	2.9
1	B	104	ARG	2.7
1	B	24	TYR	2.7
1	B	176	PHE	2.7
1	A	126	LYS	2.6
1	B	151	ASP	2.5
1	B	67	ASP	2.5
1	B	125	ARG	2.3
1	C	139	LYS	2.3
1	B	28	PRO	2.2
1	C	105	PHE	2.2
1	C	65	ASN	2.2
1	B	136	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	24	TYR	2.1
1	C	84	ARG	2.1
1	C	99	GLU	2.1
1	C	143	VAL	2.1
1	C	162	ILE	2.0
1	C	165	GLU	2.0
1	A	15	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	MN	B	300	1/1	0.93	0.38	4.92	45,45,45,45	0
2	MN	C	300	1/1	0.91	0.28	4.65	51,51,51,51	0
2	MN	A	300	1/1	0.87	0.25	1.78	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.