Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 04:29 AM EDT

PDB ID	:	7MPL
Title	:	Bartonella henselae NrnC bound to pGG
Authors	:	Lormand, J.D.; Sondermann, H.
Deposited on	:	2021-05-04
Resolution	:	1.80 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.172
Clashscore		1
Ramachandran outliers		0
Sidechain outliers		1.3%
RSRZ outliers		0.4%
RNA backbone		0.42

Worse ... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
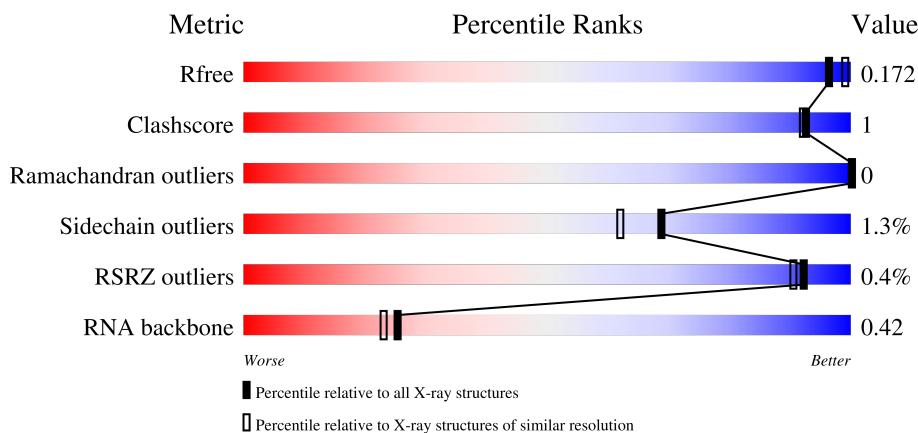
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)
RNA backbone	3102	1060 (2.40-1.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	207	97%
1	C	207	95%
1	E	207	96%
1	G	207	95%
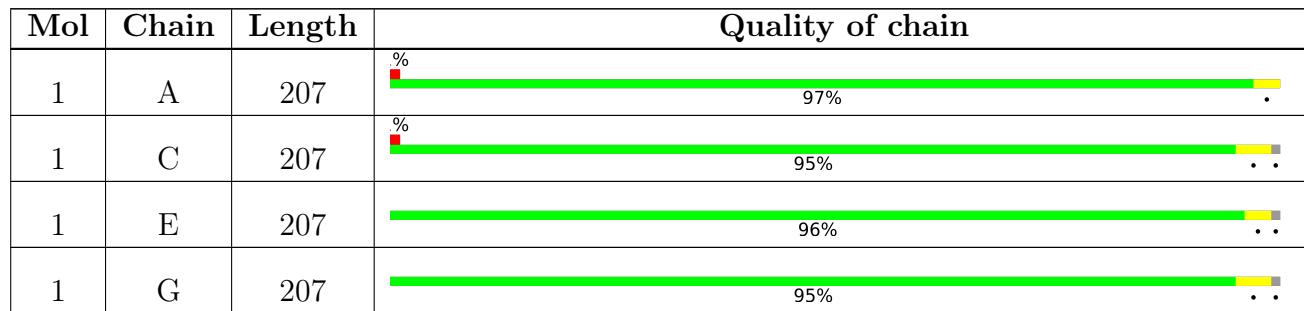
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Mol	Chain	Length	Quality of chain
1	I	207	93% 6%
1	K	207	96%
1	M	207	96%
1	O	207	95%
2	B	2	100%
2	D	2	100%
2	F	2	100%
2	H	2	100%
2	J	2	100%
2	L	2	100%
2	N	2	100%
2	P	2	100%
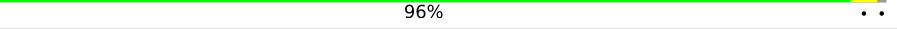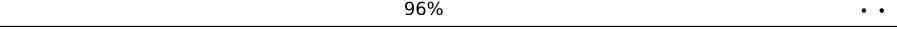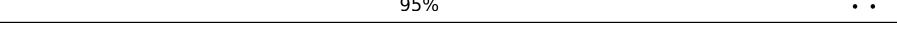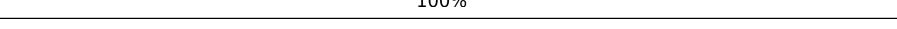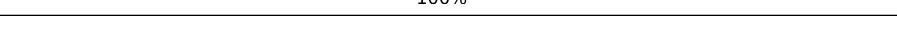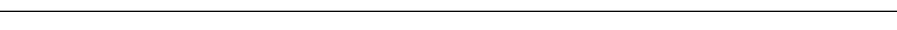
2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 15456 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 NanoRNase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	6	0
			1667	1049	295	316	7			
1	C	205	Total	C	N	O	S	0	5	0
			1660	1045	294	314	7			
1	E	205	Total	C	N	O	S	0	3	0
			1653	1040	296	311	6			
1	G	205	Total	C	N	O	S	0	4	0
			1655	1041	293	315	6			
1	I	205	Total	C	N	O	S	0	3	0
			1650	1038	294	312	6			
1	K	205	Total	C	N	O	S	0	3	0
			1652	1039	297	310	6			
1	M	204	Total	C	N	O	S	0	3	0
			1646	1036	295	309	6			
1	O	204	Total	C	N	O	S	0	1	0
			1631	1026	291	308	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP X5MEI1
C	0	SER	-	expression tag	UNP X5MEI1
E	0	SER	-	expression tag	UNP X5MEI1
G	0	SER	-	expression tag	UNP X5MEI1
I	0	SER	-	expression tag	UNP X5MEI1
K	0	SER	-	expression tag	UNP X5MEI1
M	0	SER	-	expression tag	UNP X5MEI1
O	0	SER	-	expression tag	UNP X5MEI1

- Molecule 2 is a RNA chain called 5'-phosphorylated GG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	2	Total 47	C 20	N 10	O 15	P 2	0	0	0
2	D	2	Total 47	C 20	N 10	O 15	P 2	0	0	0
2	F	2	Total 47	C 20	N 10	O 15	P 2	0	0	0
2	H	2	Total 47	C 20	N 10	O 15	P 2	0	0	0
2	J	2	Total 47	C 20	N 10	O 15	P 2	0	0	0
2	L	2	Total 47	C 20	N 10	O 15	P 2	0	0	0
2	N	2	Total 47	C 20	N 10	O 15	P 2	0	0	0
2	P	2	Total 47	C 20	N 10	O 15	P 2	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	263	Total 263	O 263	0	0
3	B	15	Total 15	O 15	0	0
3	C	265	Total 265	O 265	0	0
3	D	11	Total 11	O 11	0	0
3	E	237	Total 237	O 237	0	0
3	F	11	Total 11	O 11	0	0
3	G	249	Total 249	O 249	0	0
3	H	12	Total 12	O 12	0	0
3	I	223	Total 223	O 223	0	0
3	J	10	Total 10	O 10	0	0
3	K	213	Total 213	O 213	0	0
3	L	12	Total 12	O 12	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	M	179	Total 179	O 179	0	0
3	N	10	Total 10	O 10	0	0
3	O	143	Total 143	O 143	0	0
3	P	13	Total 13	O 13	0	0

3 Residue-property plots ⓘ

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: NanoRNase C
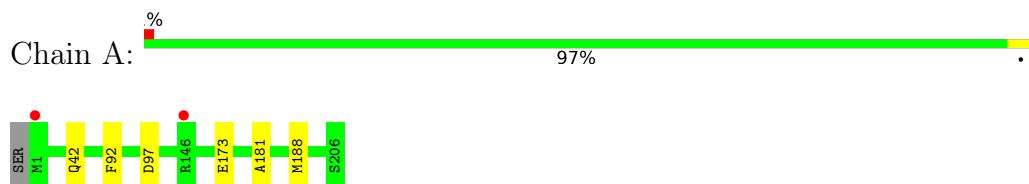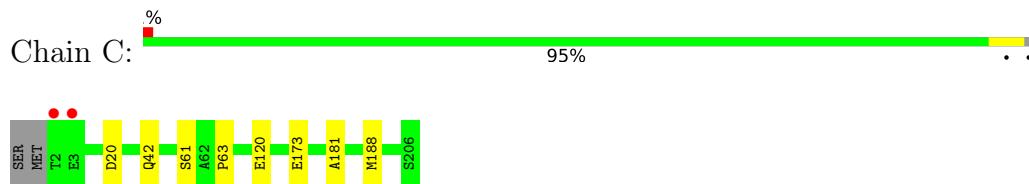
Chain A:

- Molecule 1: NanoRNase C

Chain C:

- Molecule 1: NanoRNase C
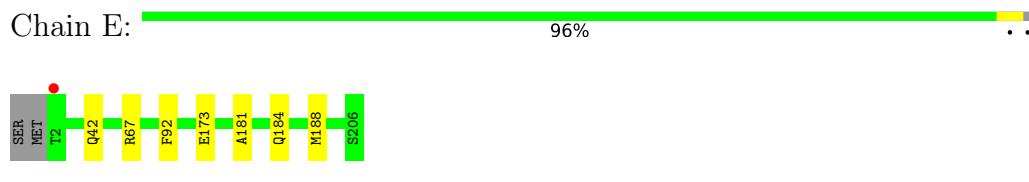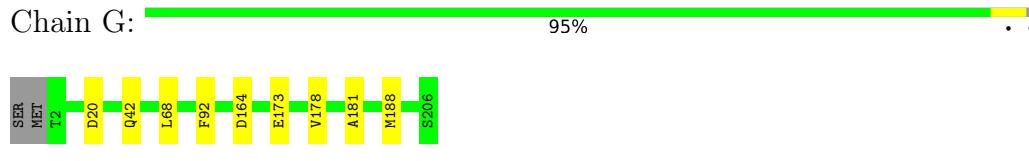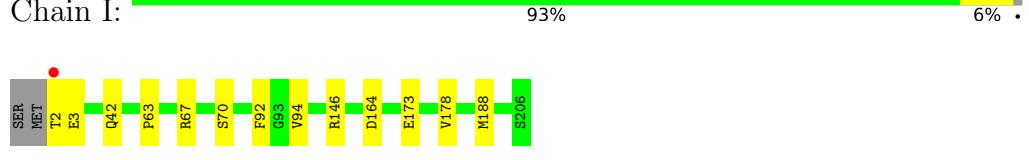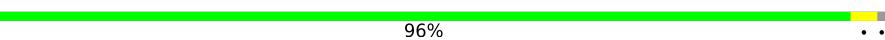
Chain E:

- Molecule 1: NanoRNase C

Chain G:

- Molecule 1: NanoRNase C

Chain I:

- Molecule 1: NanoRNase C

Chain K: 96%

SER MET T2 Q42 E173 V178 A181 M188 S206

• Molecule 1: NanoRNase C

Chain M: 96%

SER MET THR E3 D20 Q42 N127 E173 A181 M188 S206

• Molecule 1: NanoRNase C

Chain O: 95%

SER MET THR E3 Q42 R72 D97 K132 R146 E173 A181 M188 S206
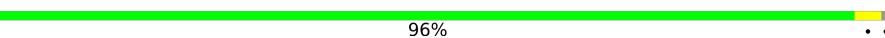
• Molecule 2: 5'-phosphorylated GG

Chain B: 100%
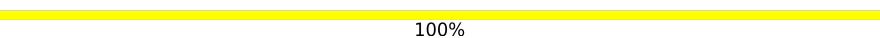
G603 G604

• Molecule 2: 5'-phosphorylated GG

Chain D: 100%
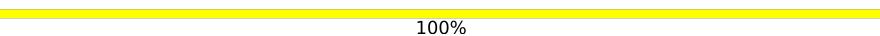
G603 G604

• Molecule 2: 5'-phosphorylated GG

Chain F: 100%
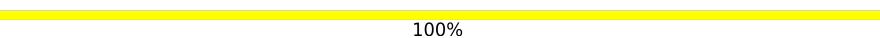
G603 G604

• Molecule 2: 5'-phosphorylated GG

Chain H: 100%
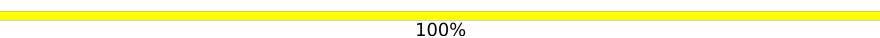
G603 G604

• Molecule 2: 5'-phosphorylated GG

Chain J: 100%
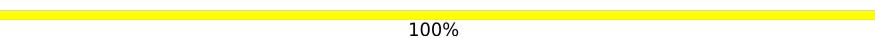
G603
G604

• Molecule 2: 5'-phosphorylated GG

Chain L:

100%
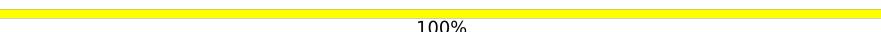
G603
G604

• Molecule 2: 5'-phosphorylated GG

Chain N:

100%
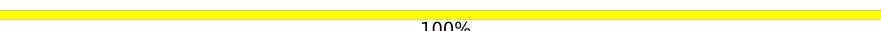
G603
G604

• Molecule 2: 5'-phosphorylated GG

Chain P:
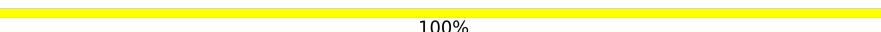
100%

G603
G604

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.16Å 128.26Å 129.28Å 90.00° 94.68° 90.00°	Depositor
Resolution (Å)	64.39 – 1.80 128.85 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (64.39-1.80) 99.3 (128.85-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 1.80Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.151 , 0.171 0.152 , 0.172	Depositor DCC
R_{free} test set	10610 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 53.3	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15456	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0/1713	0.56	0/2314
1	C	0.38	0/1703	0.54	0/2300
1	E	0.36	0/1690	0.52	0/2282
1	G	0.37	0/1695	0.54	0/2290
1	I	0.36	0/1687	0.53	0/2279
1	K	0.34	0/1689	0.51	0/2281
1	M	0.34	0/1683	0.52	0/2272
1	O	0.31	0/1662	0.50	0/2245
2	B	1.50	1/52 (1.9%)	1.25	0/78
2	D	1.59	1/52 (1.9%)	1.29	0/78
2	F	1.57	1/52 (1.9%)	1.32	0/78
2	H	1.55	1/52 (1.9%)	1.02	0/78
2	J	1.55	1/52 (1.9%)	1.22	0/78
2	L	1.62	1/52 (1.9%)	1.25	0/78
2	N	1.55	1/52 (1.9%)	1.33	0/78
2	P	1.49	1/52 (1.9%)	1.01	0/78
All	All	0.45	8/13938 (0.1%)	0.57	0/18887

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	603	G	OP3-P	-10.85	1.48	1.61
2	H	603	G	OP3-P	-10.48	1.48	1.61
2	F	603	G	OP3-P	-10.37	1.48	1.61
2	N	603	G	OP3-P	-10.22	1.48	1.61
2	J	603	G	OP3-P	-10.21	1.49	1.61
2	P	603	G	OP3-P	-10.14	1.49	1.61
2	D	603	G	OP3-P	-9.86	1.49	1.61
2	B	603	G	OP3-P	-9.57	1.49	1.61

There are no bond angle outliers.

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	1667	0	1672	6	0
1	C	1660	0	1664	6	0
1	E	1653	0	1658	5	0
1	G	1655	0	1653	7	0
1	I	1650	0	1651	8	0
1	K	1652	0	1658	4	0
1	M	1646	0	1651	3	0
1	O	1631	0	1628	4	0
2	B	47	0	23	1	0
2	D	47	0	23	1	0
2	F	47	0	23	1	0
2	H	47	0	23	1	0
2	J	47	0	23	1	0
2	L	47	0	23	1	0
2	N	47	0	23	1	0
2	P	47	0	23	1	0
3	A	263	0	0	2	1
3	B	15	0	0	1	0
3	C	265	0	0	2	0
3	D	11	0	0	1	0
3	E	237	0	0	3	1
3	F	11	0	0	1	0
3	G	249	0	0	3	0
3	H	12	0	0	1	0
3	I	223	0	0	3	0
3	J	10	0	0	1	0
3	K	213	0	0	1	0
3	L	12	0	0	1	0
3	M	179	0	0	1	0
3	N	10	0	0	1	0
3	O	143	0	0	0	0
3	P	13	0	0	1	0
All	All	15456	0	13419	40	1

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 1.

All (40) 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:I:178:VAL:HG22	1:O:188:MET:HE1	1.65	0.79
1:C:188[B]:MET:HE1	1:K:178:VAL:HG22	1.69	0.74
1:A:188[B]:MET:HE1	1:G:178:VAL:HG22	1.70	0.74
1:I:2:THR:OG1	1:I:3:GLU:N	2.22	0.72
1:G:164:ASP:OD1	3:G:301:HOH:O	2.09	0.69
2:H:604:G:OP1	3:H:701:HOH:O	2.10	0.68
2:N:604:G:OP1	3:N:701:HOH:O	2.11	0.68
2:L:604:G:OP1	3:L:701:HOH:O	2.11	0.68
2:B:604:G:OP1	3:B:701:HOH:O	2.13	0.66
2:J:604:G:OP1	3:J:701:HOH:O	2.14	0.65
1:C:120[B]:GLU:OE1	3:C:301:HOH:O	2.15	0.65
2:D:604:G:OP1	3:D:701:HOH:O	2.14	0.64
2:P:604:G:OP1	3:P:701:HOH:O	2.15	0.64
1:E:184[B]:GLN:NE2	3:E:302:HOH:O	2.27	0.62
1:C:20[B]:ASP:OD1	3:C:302:HOH:O	2.16	0.60
1:G:20[A]:ASP:OD1	3:G:302:HOH:O	2.16	0.59
1:M:20:ASP:OD1	3:M:301:HOH:O	2.17	0.58
2:F:604:G:OP1	3:F:701:HOH:O	2.18	0.55
1:E:181:ALA:CB	1:M:188:MET:HG3	2.40	0.51
1:A:181:ALA:HB3	1:G:188:MET:HG2	1.93	0.50
1:A:188[A]:MET:HG2	1:G:181:ALA:HB3	1.94	0.48
1:E:92:PHE:HB2	3:E:340:HOH:O	2.14	0.48
1:I:188:MET:HG2	1:O:181:ALA:HB3	1.96	0.47
1:C:181:ALA:CB	1:K:188:MET:HG3	2.44	0.47
1:E:188:MET:HG2	1:M:181:ALA:HB3	1.96	0.47
1:A:97:ASP:HB3	3:A:1394:HOH:O	2.15	0.46
1:I:63:PRO:O	1:I:67:ARG:HG3	2.15	0.46
1:A:92:PHE:HB2	3:A:1221:HOH:O	2.14	0.46
1:G:92:PHE:HB2	3:G:330:HOH:O	2.15	0.45
1:I:92:PHE:HB2	3:I:334:HOH:O	2.17	0.45
1:I:146:ARG:NH2	3:I:313:HOH:O	2.50	0.45
1:K:2:THR:N	3:K:305:HOH:O	2.50	0.44
1:I:70:SER:HB3	1:I:94:VAL:HG11	1.99	0.44
1:E:67:ARG:NH2	3:E:306:HOH:O	2.42	0.43
1:I:164:ASP:OD1	3:I:301:HOH:O	2.21	0.43
1:C:188[A]:MET:HG2	1:K:181:ALA:HB3	2.02	0.41
1:O:132:LYS:HE2	1:O:132:LYS:HB3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:72:ARG:HD2	1:O:97:ASP:OD2	2.20	0.41
1:C:61:SER:OG	1:C:63:PRO:HD3	2.21	0.40
1:A:188[B]:MET:HG3	1:G:181:ALA:CB	2.52	0.40

All (1) 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)
3:A:1350:HOH:O	3:E:351:HOH:O[2_655]	2.14	0.06

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	210/207 (101%)	209 (100%)	1 (0%)	0	100	100
1	C	208/207 (100%)	207 (100%)	1 (0%)	0	100	100
1	E	206/207 (100%)	205 (100%)	1 (0%)	0	100	100
1	G	207/207 (100%)	206 (100%)	1 (0%)	0	100	100
1	I	206/207 (100%)	205 (100%)	1 (0%)	0	100	100
1	K	206/207 (100%)	205 (100%)	1 (0%)	0	100	100
1	M	205/207 (99%)	204 (100%)	1 (0%)	0	100	100
1	O	203/207 (98%)	202 (100%)	1 (0%)	0	100	100
All	All	1651/1656 (100%)	1643 (100%)	8 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	184/180 (102%)	182 (99%)	2 (1%)	73	68
1	C	183/180 (102%)	181 (99%)	2 (1%)	73	68
1	E	181/180 (101%)	179 (99%)	2 (1%)	73	68
1	G	182/180 (101%)	179 (98%)	3 (2%)	62	54
1	I	181/180 (101%)	179 (99%)	2 (1%)	73	68
1	K	181/180 (101%)	179 (99%)	2 (1%)	73	68
1	M	180/180 (100%)	177 (98%)	3 (2%)	60	51
1	O	178/180 (99%)	176 (99%)	2 (1%)	73	68
All	All	1450/1440 (101%)	1432 (99%)	18 (1%)	69	65

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	173	GLU
1	C	42	GLN
1	C	173	GLU
1	E	42	GLN
1	E	173	GLU
1	G	42	GLN
1	G	68	LEU
1	G	173	GLU
1	I	42	GLN
1	I	173	GLU
1	K	42	GLN
1	K	173	GLU
1	M	42	GLN
1	M	127	ASN
1	M	173	GLU
1	O	42	GLN
1	O	173	GLU

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	1/2 (50%)	0	0
2	D	1/2 (50%)	0	0
2	F	1/2 (50%)	0	0
2	H	1/2 (50%)	0	0
2	J	1/2 (50%)	0	0
2	L	1/2 (50%)	0	0
2	N	1/2 (50%)	0	0
2	P	1/2 (50%)	0	0
All	All	8/16 (50%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	206/207 (99%)	-0.30	2 (0%)	82	80	20, 28, 45, 77	0
1	C	205/207 (99%)	-0.30	2 (0%)	82	80	23, 29, 45, 74	0
1	E	205/207 (99%)	-0.37	1 (0%)	91	89	24, 32, 47, 60	0
1	G	205/207 (99%)	-0.36	0	100	100	22, 32, 47, 59	0
1	I	205/207 (99%)	-0.34	1 (0%)	91	89	26, 34, 48, 88	0
1	K	205/207 (99%)	-0.39	0	100	100	26, 38, 54, 71	0
1	M	204/207 (98%)	-0.30	0	100	100	26, 40, 60, 74	0
1	O	204/207 (98%)	-0.17	1 (0%)	91	89	28, 45, 66, 81	0
2	B	2/2 (100%)	-0.68	0	100	100	26, 26, 26, 27	0
2	D	2/2 (100%)	-0.76	0	100	100	28, 28, 28, 28	0
2	F	2/2 (100%)	-0.65	0	100	100	31, 31, 31, 31	0
2	H	2/2 (100%)	-0.76	0	100	100	29, 29, 29, 30	0
2	J	2/2 (100%)	-0.70	0	100	100	32, 32, 32, 32	0
2	L	2/2 (100%)	-0.78	0	100	100	34, 34, 34, 36	0
2	N	2/2 (100%)	-0.72	0	100	100	31, 31, 31, 32	0
2	P	2/2 (100%)	-0.70	0	100	100	38, 38, 38, 38	0
All	All	1655/1672 (98%)	-0.32	7 (0%)	92	90	20, 34, 54, 88	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	2	THR	6.5
1	C	2	THR	5.5
1	A	146	ARG	2.9
1	A	1	MET	2.7
1	C	3	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	O	146	ARG	2.4
1	E	2	THR	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.