



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2026 – 08:05 PM UTC

PDB ID : 3P1Z / pdb_00003p1z
Title : Crystal structure of the Aperopyrum pernix RNA splicing endonuclease
Authors : Hirata, A.
Deposited on : 2010-10-01
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
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

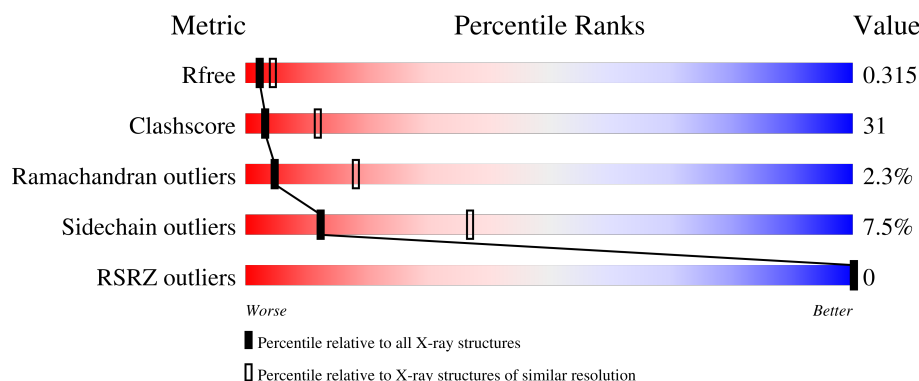
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	170	
1	C	170	
1	E	170	
1	G	170	
1	I	170	

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Mol	Chain	Length	Quality of chain
1	K	170	54%37%5%
2	B	186	54%34%9%
2	D	186	56%35%7%
2	F	186	43%49%5%
2	H	186	54%39%
2	J	186	49%41%6%
2	L	186	46%39%11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16581 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1292	814	235	236	7			
1	C	161	Total	C	N	O	S	0	0	0
			1245	786	227	225	7			
1	E	168	Total	C	N	O	S	0	0	0
			1292	814	235	236	7			
1	G	161	Total	C	N	O	S	0	0	0
			1245	786	227	225	7			
1	I	168	Total	C	N	O	S	0	0	0
			1292	814	235	236	7			
1	K	161	Total	C	N	O	S	0	0	0
			1245	786	227	225	7			

- Molecule 2 is a protein called tRNA-splicing endonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1412	903	247	259	3			
2	D	184	Total	C	N	O	S	0	0	0
			1442	919	254	265	4			
2	F	180	Total	C	N	O	S	0	0	0
			1412	903	247	259	3			
2	H	184	Total	C	N	O	S	0	0	0
			1442	919	254	265	4			
2	J	180	Total	C	N	O	S	0	0	0
			1412	903	247	259	3			
2	L	184	Total	C	N	O	S	0	0	0
			1442	919	254	265	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total 35	O 35	0	0
3	B	40	Total 40	O 40	0	0
3	C	36	Total 36	O 36	0	0
3	D	45	Total 45	O 45	0	0
3	E	33	Total 33	O 33	0	0
3	F	41	Total 41	O 41	0	0
3	G	21	Total 21	O 21	0	0
3	H	32	Total 32	O 32	0	0
3	I	38	Total 38	O 38	0	0
3	J	23	Total 23	O 23	0	0
3	K	28	Total 28	O 28	0	0
3	L	36	Total 36	O 36	0	0

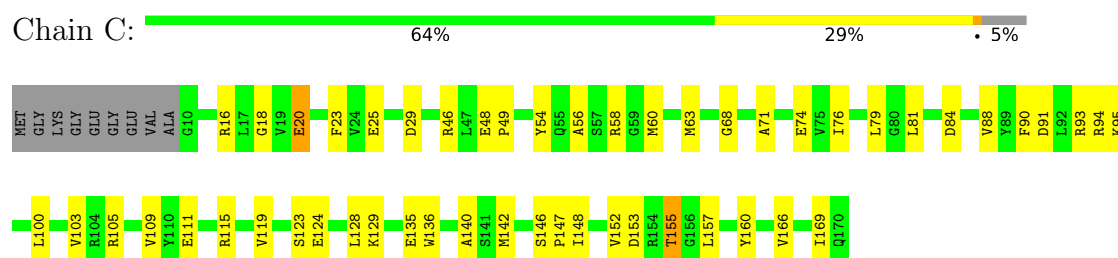
3 Residue-property plots

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: Putative uncharacterized protein



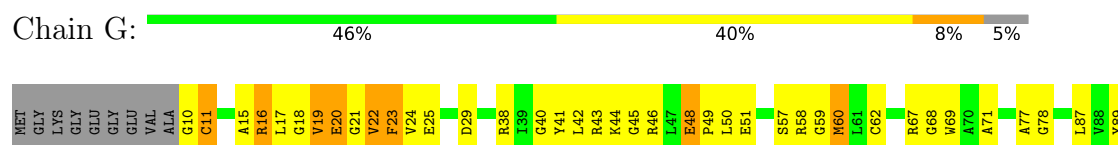
• Molecule 1: Putative uncharacterized protein



• Molecule 1: Putative uncharacterized protein



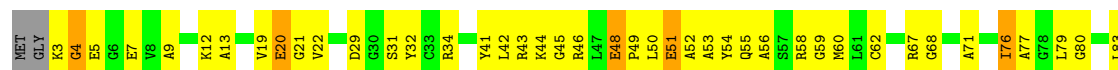
• Molecule 1: Putative uncharacterized protein





• Molecule 1: Putative uncharacterized protein

Chain I: 49% 46% ..



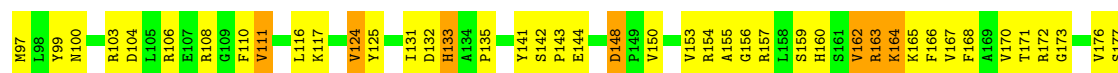
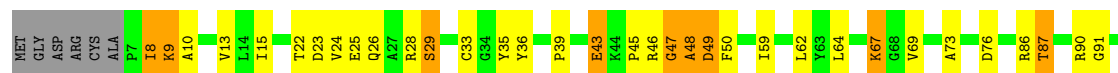
• Molecule 1: Putative uncharacterized protein

Chain K: 54% 37% .. 5%



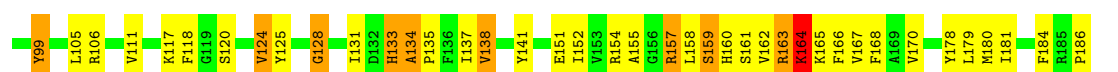
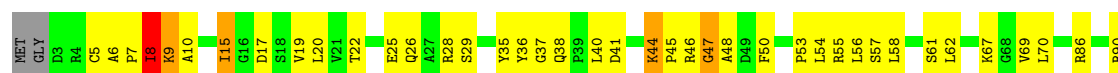
• Molecule 2: tRNA-splicing endonuclease

Chain B: 54% 34% 9% .

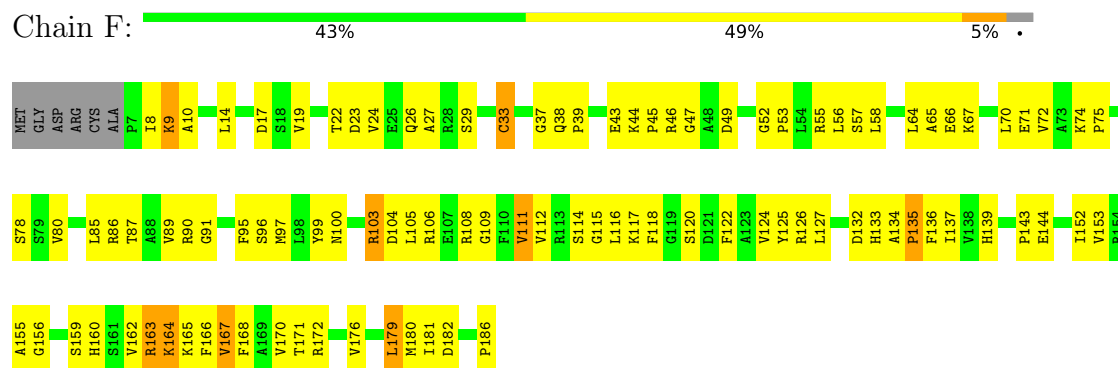


• Molecule 2: tRNA-splicing endonuclease

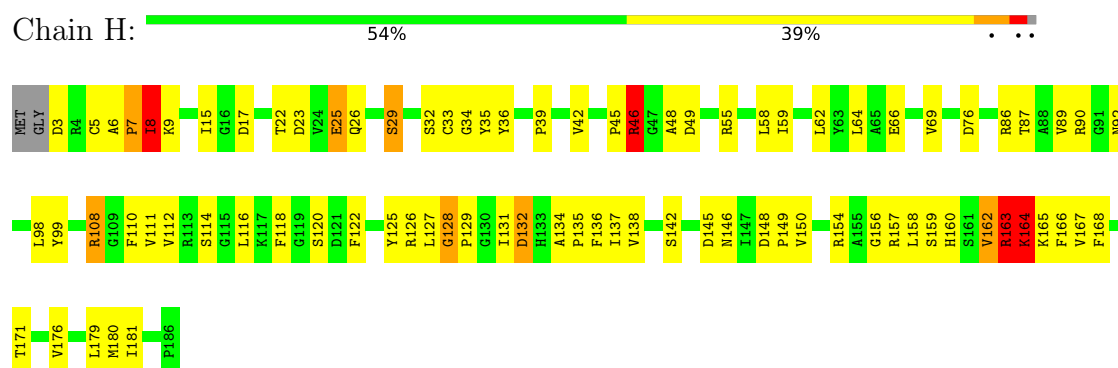
Chain D: 56% 35% 7% ..



- Molecule 2: tRNA-splicing endonuclease



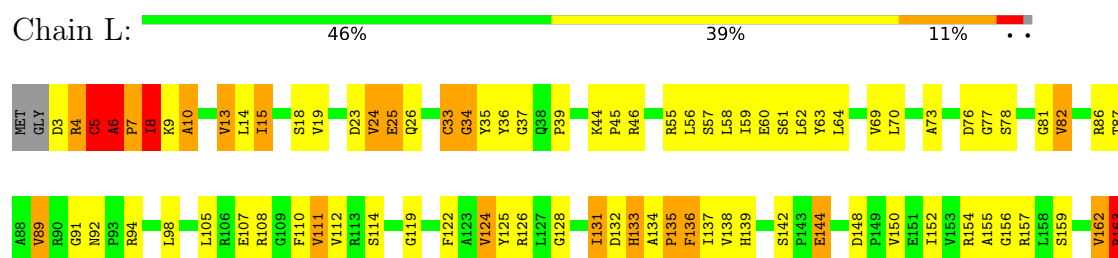
- Molecule 2: tRNA-splicing endonuclease



- Molecule 2: tRNA-splicing endonuclease



- Molecule 2: tRNA-splicing endonuclease



K164	K165	F166	V167	F168	T171	V176	L179	M180	I181	D182	W183	F184	R185	P186
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4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	135.04Å 135.04Å 156.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.24 – 2.80 41.24 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.5 (41.24-2.80) 96.5 (41.24-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.69Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.260 , 0.318 0.260 , 0.315	Depositor DCC
R_{free} test set	4419 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.085 for -h,-k,l 0.315 for h,-h-k,-l 0.085 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16581	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	0/1313	0.98	4/1767 (0.2%)
1	C	0.50	0/1266	0.93	2/1705 (0.1%)
1	E	0.50	0/1313	0.97	2/1767 (0.1%)
1	G	0.57	0/1266	0.96	5/1705 (0.3%)
1	I	0.51	0/1313	0.96	2/1767 (0.1%)
1	K	0.53	0/1266	0.92	4/1705 (0.2%)
2	B	0.61	0/1445	1.04	6/1954 (0.3%)
2	D	0.61	0/1475	1.06	8/1995 (0.4%)
2	F	0.54	0/1445	0.95	3/1954 (0.2%)
2	H	0.59	0/1475	1.07	5/1995 (0.3%)
2	J	0.55	0/1445	0.98	2/1954 (0.1%)
2	L	0.64	0/1475	1.19	11/1995 (0.6%)
All	All	0.56	0/16497	1.01	54/22263 (0.2%)

There are no bond length outliers.

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	33	CYS	N-CA-C	22.75	135.41	111.07
1	E	126	TYR	CA-C-N	11.79	131.91	119.76
1	E	126	TYR	C-N-CA	11.79	131.91	119.76
2	B	48	ALA	N-CA-C	9.75	129.20	114.09
1	I	48	GLU	CA-C-N	7.99	128.42	119.32

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	1292	0	1303	61	0
1	C	1245	0	1258	44	0
1	E	1292	0	1303	73	0
1	G	1245	0	1258	116	0
1	I	1292	0	1303	110	0
1	K	1245	0	1258	59	0
2	B	1412	0	1409	77	0
2	D	1442	0	1433	97	0
2	F	1412	0	1409	97	0
2	H	1442	0	1435	97	0
2	J	1412	0	1409	119	0
2	L	1442	0	1434	158	0
3	A	35	0	0	2	0
3	B	40	0	0	5	0
3	C	36	0	0	2	0
3	D	45	0	0	2	0
3	E	33	0	0	5	0
3	F	41	0	0	9	0
3	G	21	0	0	2	0
3	H	32	0	0	6	0
3	I	38	0	0	11	0
3	J	23	0	0	8	0
3	K	28	0	0	0	0
3	L	36	0	0	15	0
All	All	16581	0	16212	997	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 31.

The worst 5 of 997 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:L:5:CYS:HB2	2:L:33:CYS:SG	1.46	1.51
2:L:5:CYS:CB	2:L:33:CYS:SG	2.05	1.44
2:D:8:ILE:HG22	2:D:9:LYS:CB	1.65	1.25
2:D:8:ILE:HG22	2:D:9:LYS:CD	1.68	1.22
2:D:8:ILE:CA	2:D:9:LYS:HB2	1.63	1.22

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	166/170 (98%)	154 (93%)	10 (6%)	2 (1%)	10	34
1	C	159/170 (94%)	149 (94%)	8 (5%)	2 (1%)	9	31
1	E	166/170 (98%)	154 (93%)	12 (7%)	0	100	100
1	G	159/170 (94%)	142 (89%)	15 (9%)	2 (1%)	9	31
1	I	166/170 (98%)	148 (89%)	15 (9%)	3 (2%)	6	23
1	K	159/170 (94%)	146 (92%)	12 (8%)	1 (1%)	21	51
2	B	178/186 (96%)	166 (93%)	8 (4%)	4 (2%)	5	19
2	D	182/186 (98%)	158 (87%)	16 (9%)	8 (4%)	2	7
2	F	178/186 (96%)	157 (88%)	16 (9%)	5 (3%)	4	14
2	H	182/186 (98%)	163 (90%)	13 (7%)	6 (3%)	3	11
2	J	178/186 (96%)	158 (89%)	15 (8%)	5 (3%)	4	14
2	L	182/186 (98%)	148 (81%)	25 (14%)	9 (5%)	1	6
All	All	2055/2136 (96%)	1843 (90%)	165 (8%)	47 (2%)	5	18

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	162	VAL
2	D	9	LYS
2	F	162	VAL
2	H	8	ILE
2	J	164	LYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	130/131 (99%)	121 (93%)	9 (7%)	14	41
1	C	126/131 (96%)	122 (97%)	4 (3%)	34	70
1	E	130/131 (99%)	121 (93%)	9 (7%)	14	41
1	G	126/131 (96%)	115 (91%)	11 (9%)	9	30
1	I	130/131 (99%)	126 (97%)	4 (3%)	35	70
1	K	126/131 (96%)	117 (93%)	9 (7%)	13	39
2	B	151/155 (97%)	135 (89%)	16 (11%)	6	22
2	D	154/155 (99%)	146 (95%)	8 (5%)	21	53
2	F	151/155 (97%)	142 (94%)	9 (6%)	17	47
2	H	154/155 (99%)	138 (90%)	16 (10%)	7	22
2	J	151/155 (97%)	137 (91%)	14 (9%)	8	27
2	L	154/155 (99%)	137 (89%)	17 (11%)	6	20
All	All	1683/1716 (98%)	1557 (92%)	126 (8%)	12	37

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	20	GLU
2	L	5	CYS
2	H	29	SER
2	L	4	ARG
2	L	89	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	146	ASN
2	H	146	ASN
2	H	133	HIS
1	I	144	ASN
2	B	146	ASN

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	168/170 (98%)	-1.36	0 100 100	37, 66, 99, 109	0
1	C	161/170 (94%)	-1.39	0 100 100	39, 66, 88, 93	0
1	E	168/170 (98%)	-1.31	0 100 100	41, 68, 93, 112	0
1	G	161/170 (94%)	-1.29	0 100 100	45, 77, 98, 105	0
1	I	168/170 (98%)	-1.27	0 100 100	45, 81, 99, 108	0
1	K	161/170 (94%)	-1.29	0 100 100	43, 73, 96, 102	0
2	B	180/186 (96%)	-1.41	0 100 100	39, 54, 81, 104	0
2	D	184/186 (98%)	-1.37	0 100 100	43, 61, 91, 104	0
2	F	180/186 (96%)	-1.35	0 100 100	46, 65, 86, 102	0
2	H	184/186 (98%)	-1.38	0 100 100	44, 58, 85, 106	0
2	J	180/186 (96%)	-1.30	0 100 100	48, 63, 86, 97	0
2	L	184/186 (98%)	-1.28	0 100 100	45, 69, 88, 111	0
All	All	2079/2136 (97%)	-1.34	0 100 100	37, 66, 94, 112	0

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.