



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 23, 2024 – 04:12 PM JST

PDB ID : 8Y0C
Title : Crystal structure of FnCas12a in complex with pre-crRNA and 18nt target DNA
Authors : Chen, J.; Liu, L.
Deposited on : 2024-01-22
Resolution : 3.45 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	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

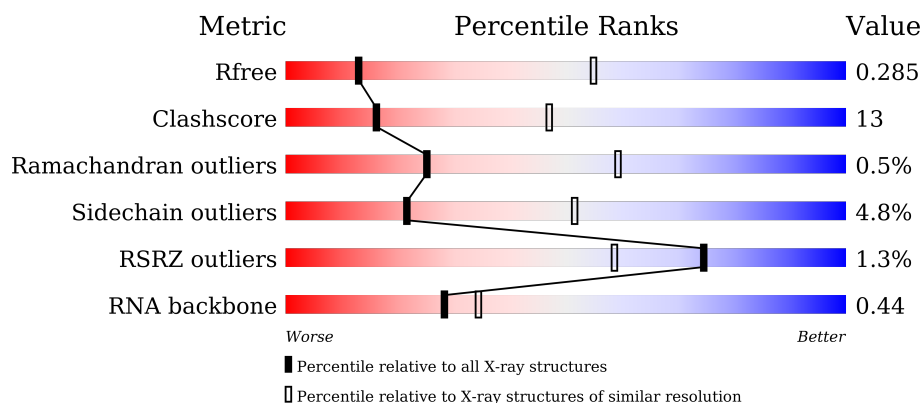
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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}	164625	1597 (3.52-3.40)
Clashscore	180529	1041 (3.50-3.42)
Ramachandran outliers	177936	1026 (3.50-3.42)
Sidechain outliers	177891	1027 (3.50-3.42)
RSRZ outliers	164620	1596 (3.52-3.40)
RNA backbone	3690	1057 (3.92-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	B	58	
2	C	27	
3	D	11	
4	A	1300	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12057 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 RNA chain called RNA (42-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	42	Total	C	N	O	P	0	0	0
			890	400	155	294	41			

- Molecule 2 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	27	Total	C	N	O	P	0	0	0
			550	265	95	163	27			

- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*GP*TP*CP*CP*TP*TP*AP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	11	Total	C	N	O	P	0	0	0
			221	107	34	69	11			

- Molecule 4 is a protein called CRISPR-associated endonuclease Cas12a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1260	Total	C	N	O	S	0	0	0
			10392	6681	1711	1978	22			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1006	ALA	GLU	conflict	UNP A0Q7Q2

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Mg	0	0
			2	2		

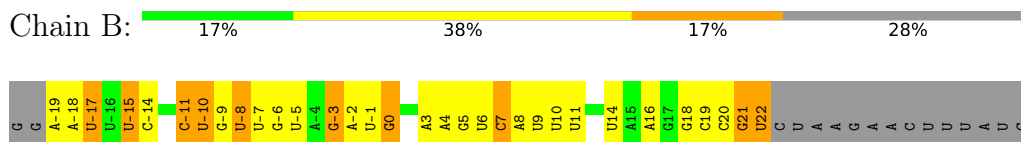
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		

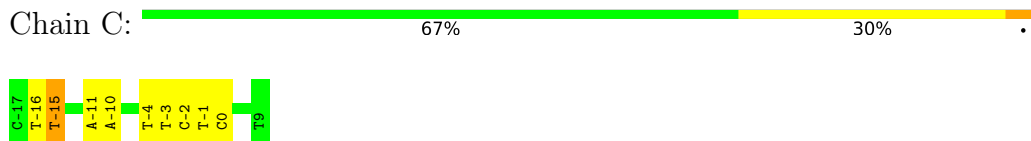
3 Residue-property plots

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: RNA (42-MER)



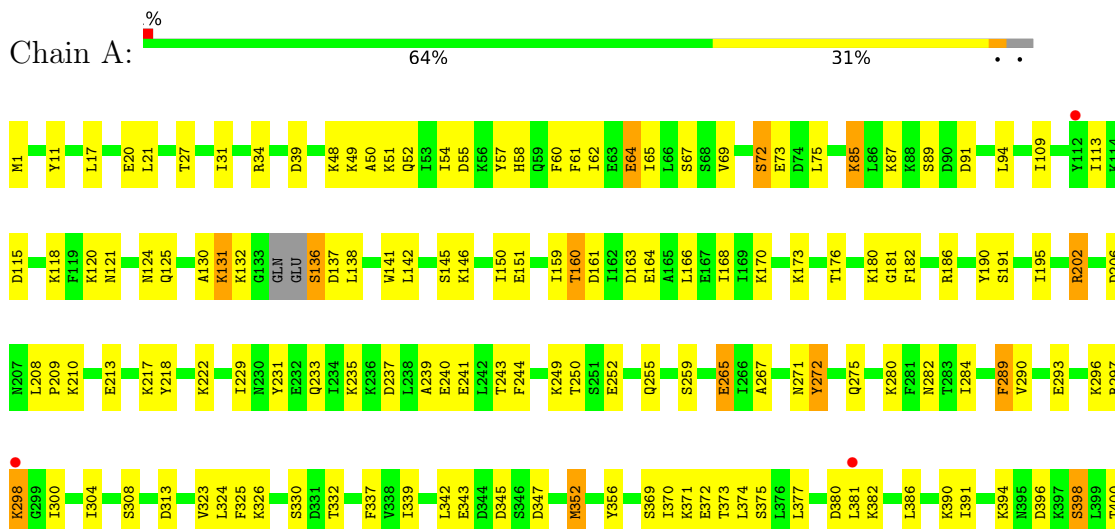
- Molecule 2: DNA (27-MER)



- Molecule 3: DNA (5'-D(P*AP*GP*TP*CP*CP*TP*TP*TP*AP*CP*T)-3')



- Molecule 4: CRISPR-associated endonuclease Cas12a



K1221	THR	A1137	L1052	K956	K954	R755	M633	K496	D401
GLY	A1138	R1053	R1054	T960	S861	Y762	K636	L499	L402
THR	K1141	A1054	Y1055	R964	V862	K763	I640	D409	S403
GLU	T1142	Y1055	P1060	D965	I863	F766	D643	Y506	Y410
LEU	T1143	Y1055	F1061	S966	K869	E767	K644	Q423	Q423
Y1228	I1144	P1060	E1062	A967	D870	T774	A645	G510	GLN
L1229	R1150	E1062	T1063	R968	K871	D775	K646	K511	ILE
S1230	L1151	T1063	F1064	K972	R872	S776	K647	K512	ALA
S1231	F1154	F1064	K1065	K973	D876	V777	K650	D513	PRO
P1232	R1155	K1065	K1066	K974	K877	Q780	I657	L514	LYS
P1233	N1156	K1066	M1067	H975	F873	G781	I657	L515	ASN
A1234	SER	G1068	K1068	N976	F879	K782	I657	SS18	LEU
G1238	ASP	K1069	Q1070	K978	F880	K667	K667	AS19	ASP
F1241	LYS	Q1070	L1071	K984	I884	Y784	L785	E520	ASN
D1242	ASN	G1072	I1073	L985	T885	L785	P670	L529	PRO
S1243	HIS	I1073	L985	N986	I886	Y789	S675	T533	LYS
P1247	TRP	I1073	S986	Q987	N887	N790	I679	L536	GLU
P1248	D1164	T1165	Q987	V988	K896	F793	P684	F543	LEU
N1249	T1165	R1166	D1007	L1008	D898	R800	L689	D550	ALA
M1250	R1166	L1174	L1008	ASN	L902	P801	R690	A552	LYS
D1253	L1174	L1085	ASN	PHE	K905	L803	I691	K557	K444
A1254	L1178	C1086	P1087	GLY	K906	L803	I691	D558	T445
D1255	T1183	V1088	T1089	F1012	E906	H804	K693	E559	K457
A1256	T1183	T1089	T1089	F1012	K907	H804	K693	N574	L450
N1257	F1184	Y1099	Y1099	K1013	K907	H804	K693	I575	E461
G1258	Y1185	E1100	E1100	R1014	V911	N816	S695	Y585	E462
A1259	E1100	S1101	S1101	GLY	V911	L817	S695	K597	F463
Y1260	S1101	V1102	V1102	ARG	S915	Q818	T696	L598	N464
H1261	V1102	S1103	S1103	PHE	I916	D819	K697	K465	H466
L1267	K1104	K1103	K1103	K1018	I916	V820	Q704	R467	R467
M1268	S1105	S1106	S1106	V1019	R913	V821	E711	D468	D468
L1269	Q1106	E1107	E1107	E1020	H922	Y822	F712	T469	T469
L1270	E1107	F1108	F1108	Y1024	Y925	K823	D716	D470	D470
G1271	E1198	F1109	F1109	L1027	Y926	E827	C717	K471	K471
R1272	S1199	S1110	S1110	L1027	Y926	E827	C717	Q472	Q472
M1276	D1200	K1111	K1111	I1032	Y926	E827	C717	F475	F475
F1203	F1203	F1112	F1112	E1033	V929	A828	I721	A483	A483
F1204	F1204	D1113	D1113	K1034	I935	E529	D722	D616	D616
A1205	A1205	K1114	K1114	L1035	I935	E529	D722	N617	N617
K1206	K1206	I1115	I1115	L1038	D939	Y832	K725	T618	T618
L1207	L1207	C1116	C1116	L1038	D939	Y832	K725	M487	M487
Y1291	Y1291	K1121	K1121	V1039	N942	I637	Q726	I623	I623
F1292	F1292	G1122	G1122	F1040	I943	I637	Q726	D626	D626
E1293	E1293	Y1123	Y1123	K1041	I943	I637	Q726		
F1294	F1294	T1213	T1213	D1042	I944	K940	W734		
V1295	V1295	I1214	I1214	N1043	G945	K940	W734		
Q1296	Q1296	L1216	L1216	E1044	G945	K946	D736		
N1297	N1297	Q1216	Q1216	F1045	D947	K946	D736		
R1298	R1298	M1217	M1217	D1046	R943	A843	T744		
N1299	N1299	R1218	R1218	D1047	M949	A843	T744		
N1300	N1300	N1219	N1219	T1048	K852	R745	Q745		
		S1220	S1220	G1049	N853	R745	Q745		

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	124.28Å 124.28Å 268.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.22 – 3.45 47.22 – 3.45	Depositor EDS
% Data completeness (in resolution range)	88.9 (47.22-3.45) 88.8 (47.22-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.216 , 0.285 0.217 , 0.285	Depositor DCC
R_{free} test set	1394 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	12057	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: MG

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	B	0.89	0/995	1.80	36/1548 (2.3%)
2	C	1.15	1/615 (0.2%)	1.17	2/946 (0.2%)
3	D	1.15	1/245 (0.4%)	1.25	1/375 (0.3%)
4	A	0.55	0/10595	0.71	3/14220 (0.0%)
All	All	0.64	2/12450 (0.0%)	0.90	42/17089 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	-3	DT	C3'-O3'	-7.79	1.33	1.44
3	D	0	DC	C3'-O3'	-5.93	1.36	1.44

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	C	C2-N1-C1'	9.34	129.07	118.80
1	B	-10	U	N3-C2-O2	-8.90	115.97	122.20
1	B	4	A	C8-N9-C4	8.30	109.12	105.80
1	B	-11	C	C6-N1-C2	-8.05	117.08	120.30
1	B	-19	A	N1-C6-N6	-7.47	114.12	118.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	789	TYR	Peptide

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	B	890	0	449	17	0
2	C	550	0	308	4	0
3	D	221	0	127	7	0
4	A	10392	0	10350	289	1
5	B	2	0	0	0	0
6	A	2	0	0	1	0
All	All	12057	0	11234	301	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 13.

The worst 5 of 301 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)
4:A:371:LYS:HE2	4:A:489:PHE:HB3	1.47	0.93
1:B:19:C:N3	1:B:21:G:N2	2.20	0.89
4:A:518:SER:O	6:A:1401:HOH:O	1.95	0.85
4:A:960:ILE:HG22	4:A:977:ILE:HD12	1.63	0.81
2:C:0:DC:H4'	4:A:827:GLU:HG3	1.63	0.81

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)
4:A:72:SER:OG	4:A:1046:ASP:OD1[5_454]	2.11	0.09

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
4	A	1246/1300 (96%)	1185 (95%)	55 (4%)	6 (0%)	25 59

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	574	ASN
4	A	160	THR
4	A	626	ASP
4	A	1013	LYS
4	A	1137	ALA

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
4	A	1144/1183 (97%)	1089 (95%)	55 (5%)	21 51

5 of 55 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	746	ARG
4	A	854	LYS
4	A	1298	ARG
4	A	1130	TYR
4	A	755	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such

sidechains are listed below:

Mol	Chain	Res	Type
4	A	843	HIS
4	A	901	ASN
4	A	1043	ASN
4	A	617	ASN
4	A	77	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	41/58 (70%)	6 (14%)	2 (4%)

5 of 6 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	-10	U
1	B	-9	G
1	B	-7	U
1	B	-6	G
1	B	21	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	-10	U
1	B	0	G

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](#)

Of 2 ligands modelled in this entry, 2 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 [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	B	42/58 (72%)	-0.74	0 100 100	19, 27, 101, 139	0
2	C	27/27 (100%)	-0.63	0 100 100	21, 39, 70, 98	0
3	D	11/11 (100%)	-0.61	0 100 100	33, 38, 78, 95	0
4	A	1260/1300 (96%)	-0.20	18 (1%) 73 57	14, 44, 112, 152	0
All	All	1340/1396 (95%)	-0.23	18 (1%) 74 59	14, 43, 112, 152	0

The worst 5 of 18 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	1207	LEU	5.3
4	A	1203	PHE	3.7
4	A	1213	THR	2.9
4	A	1214	ILE	2.9
4	A	298	LYS	2.7

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 monosaccharides 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(\AA^2)	Q<0.9
5	MG	B	101	1/1	0.95	0.28	2,2,2,2	0
5	MG	B	102	1/1	0.96	0.20	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.