



wwPDB X-ray Structure Validation Summary Report i

Mar 1, 2014 – 12:20 AM GMT

PDB ID : 3BPR
Title : Crystal structure of catalytic domain of the proto-oncogene tyrosine-protein kinase MER in complex with inhibitor C52
Authors : Walker, J.R.; Huang, X.; Finerty Jr, P.J.; Weigelt, J.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Dhe-Paganon, S.; Structural Genomics Consortium (SGC)
Deposited on : 2007-12-19
Resolution : 2.80 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

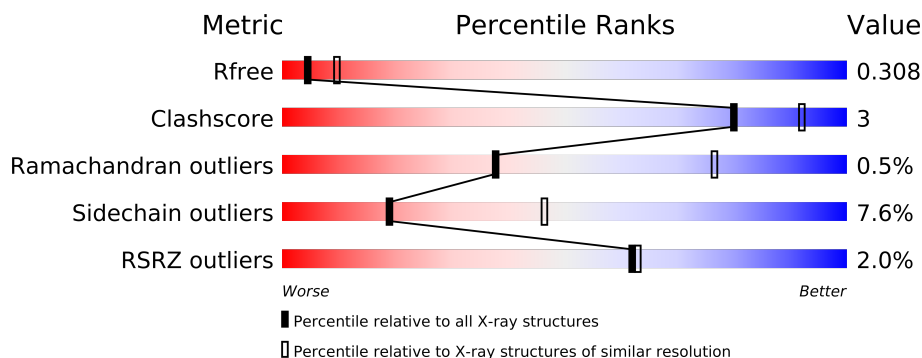
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	313	
1	B	313	
1	C	313	
1	D	313	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8399 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Proto-oncogene tyrosine-protein kinase MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	2	0
			2027	1299	332	375	21			
1	B	256	Total	C	N	O	S	0	2	0
			2012	1289	336	368	19			
1	C	259	Total	C	N	O	S	0	4	0
			2073	1326	348	379	20			
1	D	259	Total	C	N	O	S	0	3	0
			2057	1316	345	376	20			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	552	MET	-	EXPRESSION TAG	UNP Q12866
A	553	GLY	-	EXPRESSION TAG	UNP Q12866
A	554	SER	-	EXPRESSION TAG	UNP Q12866
A	555	SER	-	EXPRESSION TAG	UNP Q12866
A	556	HIS	-	EXPRESSION TAG	UNP Q12866
A	557	HIS	-	EXPRESSION TAG	UNP Q12866
A	558	HIS	-	EXPRESSION TAG	UNP Q12866
A	559	HIS	-	EXPRESSION TAG	UNP Q12866
A	560	HIS	-	EXPRESSION TAG	UNP Q12866
A	561	HIS	-	EXPRESSION TAG	UNP Q12866
A	562	SER	-	EXPRESSION TAG	UNP Q12866
A	563	SER	-	EXPRESSION TAG	UNP Q12866
A	564	GLY	-	EXPRESSION TAG	UNP Q12866
A	565	LEU	-	EXPRESSION TAG	UNP Q12866
A	566	VAL	-	EXPRESSION TAG	UNP Q12866
A	567	PRO	-	EXPRESSION TAG	UNP Q12866
A	568	ARG	-	EXPRESSION TAG	UNP Q12866
A	569	GLY	-	EXPRESSION TAG	UNP Q12866
B	552	MET	-	EXPRESSION TAG	UNP Q12866
B	553	GLY	-	EXPRESSION TAG	UNP Q12866
B	554	SER	-	EXPRESSION TAG	UNP Q12866

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Chain	Residue	Modelled	Actual	Comment	Reference
B	555	SER	-	EXPRESSION TAG	UNP Q12866
B	556	HIS	-	EXPRESSION TAG	UNP Q12866
B	557	HIS	-	EXPRESSION TAG	UNP Q12866
B	558	HIS	-	EXPRESSION TAG	UNP Q12866
B	559	HIS	-	EXPRESSION TAG	UNP Q12866
B	560	HIS	-	EXPRESSION TAG	UNP Q12866
B	561	HIS	-	EXPRESSION TAG	UNP Q12866
B	562	SER	-	EXPRESSION TAG	UNP Q12866
B	563	SER	-	EXPRESSION TAG	UNP Q12866
B	564	GLY	-	EXPRESSION TAG	UNP Q12866
B	565	LEU	-	EXPRESSION TAG	UNP Q12866
B	566	VAL	-	EXPRESSION TAG	UNP Q12866
B	567	PRO	-	EXPRESSION TAG	UNP Q12866
B	568	ARG	-	EXPRESSION TAG	UNP Q12866
B	569	GLY	-	EXPRESSION TAG	UNP Q12866
C	552	MET	-	EXPRESSION TAG	UNP Q12866
C	553	GLY	-	EXPRESSION TAG	UNP Q12866
C	554	SER	-	EXPRESSION TAG	UNP Q12866
C	555	SER	-	EXPRESSION TAG	UNP Q12866
C	556	HIS	-	EXPRESSION TAG	UNP Q12866
C	557	HIS	-	EXPRESSION TAG	UNP Q12866
C	558	HIS	-	EXPRESSION TAG	UNP Q12866
C	559	HIS	-	EXPRESSION TAG	UNP Q12866
C	560	HIS	-	EXPRESSION TAG	UNP Q12866
C	561	HIS	-	EXPRESSION TAG	UNP Q12866
C	562	SER	-	EXPRESSION TAG	UNP Q12866
C	563	SER	-	EXPRESSION TAG	UNP Q12866
C	564	GLY	-	EXPRESSION TAG	UNP Q12866
C	565	LEU	-	EXPRESSION TAG	UNP Q12866
C	566	VAL	-	EXPRESSION TAG	UNP Q12866
C	567	PRO	-	EXPRESSION TAG	UNP Q12866
C	568	ARG	-	EXPRESSION TAG	UNP Q12866
C	569	GLY	-	EXPRESSION TAG	UNP Q12866
D	552	MET	-	EXPRESSION TAG	UNP Q12866
D	553	GLY	-	EXPRESSION TAG	UNP Q12866
D	554	SER	-	EXPRESSION TAG	UNP Q12866
D	555	SER	-	EXPRESSION TAG	UNP Q12866
D	556	HIS	-	EXPRESSION TAG	UNP Q12866
D	557	HIS	-	EXPRESSION TAG	UNP Q12866
D	558	HIS	-	EXPRESSION TAG	UNP Q12866
D	559	HIS	-	EXPRESSION TAG	UNP Q12866
D	560	HIS	-	EXPRESSION TAG	UNP Q12866

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Chain	Residue	Modelled	Actual	Comment	Reference
D	561	HIS	-	EXPRESSION TAG	UNP Q12866
D	562	SER	-	EXPRESSION TAG	UNP Q12866
D	563	SER	-	EXPRESSION TAG	UNP Q12866
D	564	GLY	-	EXPRESSION TAG	UNP Q12866
D	565	LEU	-	EXPRESSION TAG	UNP Q12866
D	566	VAL	-	EXPRESSION TAG	UNP Q12866
D	567	PRO	-	EXPRESSION TAG	UNP Q12866
D	568	ARG	-	EXPRESSION TAG	UNP Q12866
D	569	GLY	-	EXPRESSION TAG	UNP Q12866

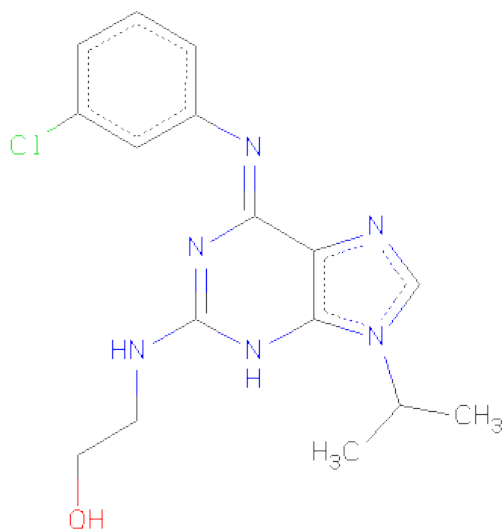
- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0

- Molecule 4 is 2-(2-HYDROXYETHYLAMINO)-6-(3-CHLOROANILINO)-9-ISOPROPYL PURINE (three-letter code: OLP) (formula: C₁₆H₁₉ClN₆O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			24	16	1	6	1		
4	B	1	Total	C	Cl	N	O	0	0
			24	16	1	6	1		
4	C	1	Total	C	Cl	N	O	0	0
			24	16	1	6	1		
4	D	1	Total	C	Cl	N	O	0	0
			24	16	1	6	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total	O	0	0
			39	39		
5	B	31	Total	O	0	0
			31	31		
5	C	32	Total	O	0	0
			32	32		
5	D	29	Total	O	0	0
			29	29		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.00Å 91.70Å 120.75Å 90.00° 94.06° 90.00°	Depositor
Resolution (Å)	47.30 – 2.80 47.29 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.30-2.80) 98.7 (47.29-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.274 , 0.301 0.280 , 0.308	Depositor DCC
R_{free} test set	1889 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 37227 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8399	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.20 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3674e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLP, NA, CL

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	0.52	0/2068	0.62	0/2803
1	B	0.53	0/2052	0.63	0/2778
1	C	0.53	0/2114	0.62	0/2857
1	D	0.53	0/2098	0.63	0/2836
All	All	0.53	0/8332	0.62	0/11274

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2027	0	0	6	0
1	B	2012	0	0	7	0
1	C	2073	0	0	4	0
1	D	2057	0	0	5	0
2	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	24	0	19	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	19	2	0
4	C	24	0	19	2	0
4	D	24	0	19	4	0
5	A	39	0	0	2	0
5	B	31	0	0	1	0
5	C	32	0	0	1	0
5	D	29	0	0	0	0
All	All	8399	0	76	28	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

The worst 5 of 28 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:674:MET:O	4:A:900:OLP:HAG	1.78	0.84
1:D:674:MET:O	4:D:900:OLP:HAG	1.86	0.76
1:B:728:ASN:ND2	5:B:128:HOH:O	2.20	0.74
1:A:675:LYS:O	4:A:900:OLP:HAE	1.90	0.71
1:D:675:LYS:O	4:D:900:OLP:HAE	1.95	0.66

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	255/313 (82%)	239 (94%)	14 (6%)	2 (1%)	27	65
1	B	248/313 (79%)	234 (94%)	13 (5%)	1 (0%)	43	80
1	C	253/313 (81%)	234 (92%)	18 (7%)	1 (0%)	43	80
1	D	254/313 (81%)	236 (93%)	17 (7%)	1 (0%)	43	80
All	All	1010/1252 (81%)	943 (93%)	62 (6%)	5 (0%)	38	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	598	PHE
1	B	598	PHE
1	D	598	PHE
1	C	598	PHE
1	A	692	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	214/280 (76%)	196 (92%)	18 (8%)	16	41
1	B	215/280 (77%)	199 (93%)	16 (7%)	20	48
1	C	224/280 (80%)	204 (91%)	20 (9%)	14	38
1	D	223/280 (80%)	208 (93%)	15 (7%)	23	55
All	All	876/1120 (78%)	807 (92%)	69 (8%)	19	44

5 of 69 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	811	ASP
1	C	662	GLN
1	D	744	LEU
1	B	824	ASP
1	C	598	PHE

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

5.3.3 RNA ⓘ

There are no RNA chains 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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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$
4	OLP	A	900	-	26,26,26	1.39	2 (7%)	33,36,36	4.15	6 (18%)
4	OLP	B	900	-	26,26,26	1.49	3 (11%)	33,36,36	4.72	8 (24%)
4	OLP	C	900	-	26,26,26	1.41	4 (15%)	33,36,36	4.26	10 (30%)
4	OLP	D	900	-	26,26,26	1.46	2 (7%)	33,36,36	4.42	6 (18%)

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
4	OLP	A	900	-	-	0/10/12/12	0/1/3/3
4	OLP	B	900	-	-	0/10/12/12	0/1/3/3
4	OLP	C	900	-	-	0/10/12/12	0/1/3/3
4	OLP	D	900	-	-	0/10/12/12	0/1/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	900	OLP	CAR-N6	-4.48	1.34	1.42
4	B	900	OLP	CAR-N6	-4.09	1.35	1.42
4	A	900	OLP	CAR-N6	-3.83	1.35	1.42
4	C	900	OLP	CAR-N6	-3.38	1.36	1.42
4	A	900	OLP	C4-N9	-3.11	1.32	1.38

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	B	900	OLP	N3-C4-N9	25.34	135.39	126.41
4	D	900	OLP	N3-C4-N9	23.70	134.81	126.41
4	C	900	OLP	N3-C4-N9	22.64	134.44	126.41
4	A	900	OLP	N3-C4-N9	22.22	134.29	126.41
4	B	900	OLP	C8-N9-C4	4.66	110.46	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	261/313 (83%)	0.06	4 (1%) 70 71	41, 58, 90, 117	0
1	B	256/313 (81%)	0.07	6 (2%) 57 58	38, 56, 86, 109	0
1	C	259/313 (82%)	0.12	4 (1%) 70 71	35, 55, 83, 106	0
1	D	259/313 (82%)	0.13	7 (2%) 52 52	38, 56, 89, 133	0
All	All	1035/1252 (82%)	0.09	21 (2%) 62 63	35, 57, 88, 133	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	622	LYS	3.6
1	A	621	MET	3.5
1	B	659	MET	3.2
1	A	690	THR	3.2
1	B	622	LYS	3.0

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 carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	OLP	B	900	24/24	0.21	0.07	49,53,57,59	0
4	OLP	C	900	24/24	0.21	0.04	47,52,56,59	0
4	OLP	D	900	24/24	0.21	-0.17	44,52,58,62	0
4	OLP	A	900	24/24	0.20	-0.19	46,49,53,57	0
3	CL	C	133	1/1	0.18	-0.93	43,43,43,43	0
2	NA	B	1	1/1	0.10	-1.94	35,35,35,35	0
3	CL	D	134	1/1	0.14	-3.02	32,32,32,32	0

6.5 Other polymers

There are no such residues in this entry.