



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:07 AM GMT

PDB ID : 3HAO  
Title : Crystal structure of bacteriorhodopsin mutant L94A crystallized from bicelles  
Authors : Joh, N.H.; Yang, D.; Bowie, J.U.  
Deposited on : 2009-05-02  
Resolution : 2.49 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](mailto: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.

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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

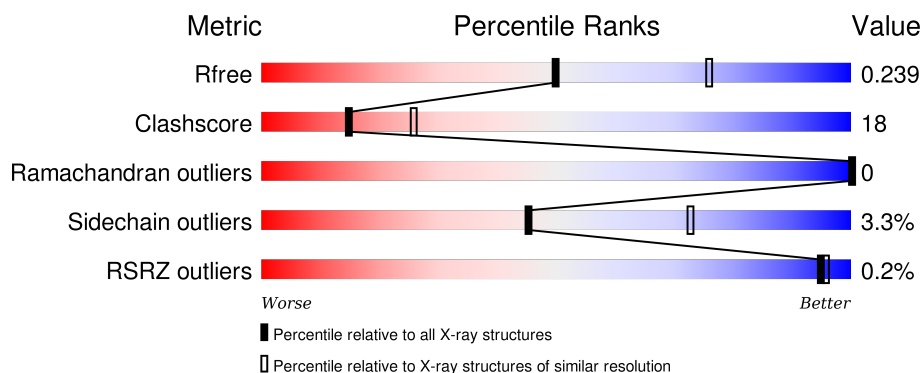
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.49 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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  $\geq 3$ , 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	249	 63% 25% •• 9%
1	B	249	 56% 27% 6% • 9%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3598 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.

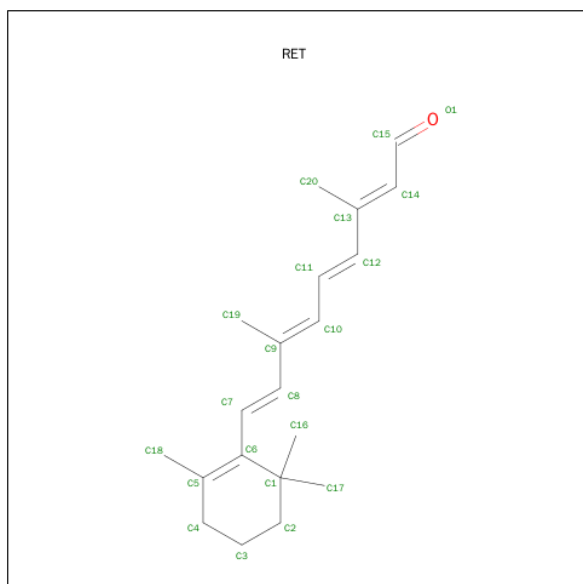
- Molecule 1 is a protein called Bacteriorhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1746	1173	267	297	9			
1	B	226	Total	C	N	O	S	0	0	0
			1746	1173	267	297	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	94	ALA	LEU	ENGINEERED	UNP P02945
B	94	ALA	LEU	ENGINEERED	UNP P02945

- Molecule 2 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>O).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			20	20		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C 20 20	0	0

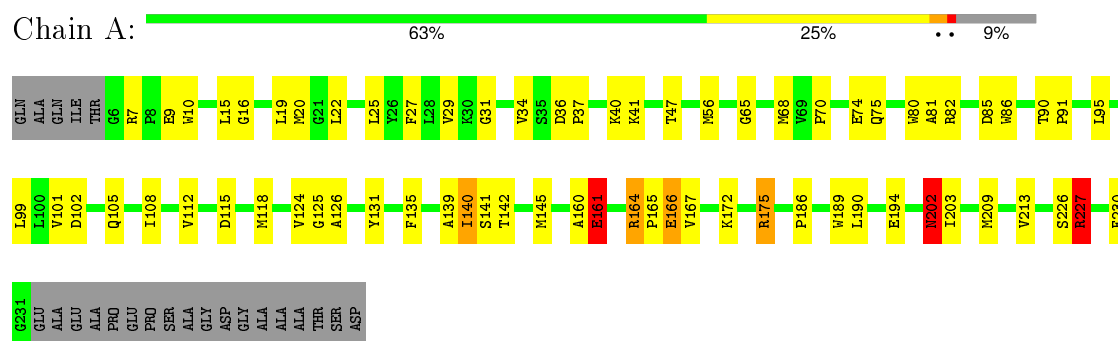
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	39	Total O 39 39	0	0
3	B	27	Total O 27 27	0	0

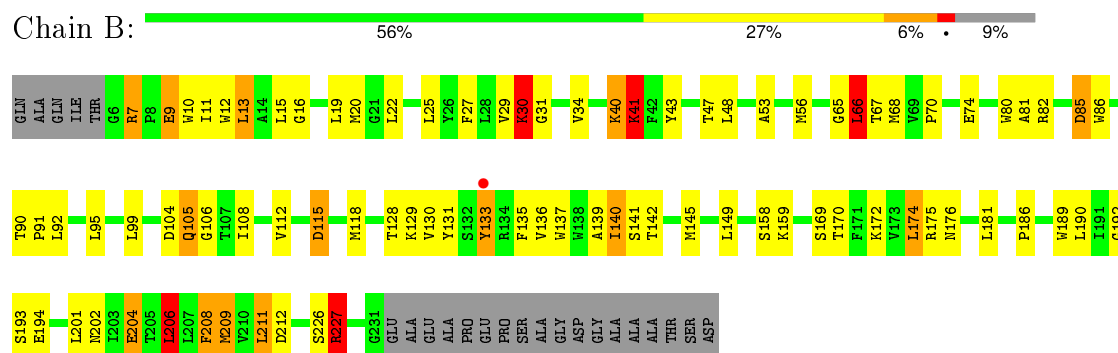
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Bacteriorhodopsin



#### • Molecule 1: Bacteriorhodopsin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.56Å 108.71Å 56.19Å 90.00° 114.03° 90.00°	Depositor
Resolution (Å)	30.00 – 2.49 29.60 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.00-2.49) 95.6 (29.60-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.82 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.209 , 0.245 0.206 , 0.239	Depositor DCC
$R_{free}$ test set	907 reflections (5.77%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 44.4	EDS
Estimated twinning fraction	0.500 for -h,-k,h+l 0.437 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.500 for -h,-k,h+l	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 16633 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3598	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	1.26	28/1794 (1.6%)	1.13	28/2450 (1.1%)
1	B	2.17	100/1794 (5.6%)	1.34	35/2450 (1.4%)
All	All	1.77	128/3588 (3.6%)	1.24	63/4900 (1.3%)

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
1	A	0	3

All (128) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	140	ILE	CA-CB	-14.14	1.22	1.54
1	B	204	GLU	CD-OE1	-13.47	1.10	1.25
1	B	9	GLU	CD-OE2	-13.10	1.11	1.25
1	A	175	ARG	CZ-NH2	-13.02	1.16	1.33
1	A	230	PHE	CE2-CZ	-12.67	1.13	1.37
1	A	175	ARG	CZ-NH1	-12.61	1.16	1.33
1	B	105	GLN	C-O	-12.22	1.00	1.23
1	A	161	GLU	CD-OE1	-12.18	1.12	1.25
1	B	43	TYR	CD1-CE1	-12.13	1.21	1.39
1	A	230	PHE	CE1-CZ	-12.08	1.14	1.37
1	B	82	ARG	C-O	-11.82	1.00	1.23
1	B	82	ARG	CZ-NH1	-11.76	1.17	1.33
1	B	204	GLU	CD-OE2	-11.70	1.12	1.25
1	A	140	ILE	C-O	-11.51	1.01	1.23
1	B	43	TYR	CD2-CE2	-11.01	1.22	1.39
1	B	9	GLU	CD-OE1	-10.97	1.13	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	208	PHE	CE2-CZ	-10.74	1.17	1.37
1	B	133	TYR	CE1-CZ	-10.43	1.25	1.38
1	B	208	PHE	CG-CD1	-10.31	1.23	1.38
1	B	211	LEU	CG-CD2	-10.14	1.14	1.51
1	B	174	LEU	CG-CD1	-9.99	1.14	1.51
1	B	133	TYR	CD1-CE1	-9.68	1.24	1.39
1	B	41	LYS	C-O	-9.47	1.05	1.23
1	B	12	TRP	CG-CD1	-9.40	1.23	1.36
1	B	7	ARG	CZ-NH2	-9.35	1.20	1.33
1	B	208	PHE	C-O	-9.32	1.05	1.23
1	B	41	LYS	CE-NZ	-9.24	1.25	1.49
1	B	7	ARG	CZ-NH1	-9.15	1.21	1.33
1	B	172	LYS	C-O	-9.02	1.06	1.23
1	B	174	LEU	C-O	-8.92	1.06	1.23
1	B	85	ASP	N-CA	-8.91	1.28	1.46
1	B	43	TYR	C-O	-8.90	1.06	1.23
1	B	169	SER	C-O	-8.84	1.06	1.23
1	B	11	ILE	CB-CG2	-8.80	1.25	1.52
1	B	208	PHE	CD2-CE2	-8.69	1.21	1.39
1	B	172	LYS	CB-CG	-8.68	1.29	1.52
1	B	174	LEU	N-CA	-8.65	1.29	1.46
1	B	9	GLU	C-O	-8.57	1.07	1.23
1	B	85	ASP	CG-OD1	-8.57	1.05	1.25
1	B	82	ARG	CZ-NH2	-8.54	1.22	1.33
1	A	164	ARG	C-O	-8.52	1.07	1.23
1	B	115	ASP	C-O	-8.49	1.07	1.23
1	B	66	LEU	C-O	-8.47	1.07	1.23
1	B	12	TRP	CD2-CE2	-8.44	1.31	1.41
1	A	230	PHE	CG-CD2	-8.41	1.26	1.38
1	A	175	ARG	C-O	-8.22	1.07	1.23
1	B	172	LYS	CE-NZ	-8.22	1.28	1.49
1	B	204	GLU	C-O	-8.18	1.07	1.23
1	B	85	ASP	CG-OD2	-8.09	1.06	1.25
1	B	140	ILE	C-O	-7.96	1.08	1.23
1	B	43	TYR	CE1-CZ	-7.91	1.28	1.38
1	A	166	GLU	CD-OE1	-7.86	1.17	1.25
1	A	230	PHE	CD1-CE1	-7.77	1.23	1.39
1	B	11	ILE	C-O	-7.37	1.09	1.23
1	B	140	ILE	CB-CG2	-7.36	1.30	1.52
1	B	172	LYS	CD-CE	-7.30	1.32	1.51
1	B	133	TYR	CG-CD1	-7.22	1.29	1.39
1	A	166	GLU	CD-OE2	-7.18	1.17	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	30	LYS	CB-CG	-7.18	1.33	1.52
1	B	209	MET	C-O	-7.14	1.09	1.23
1	B	68	MET	CG-SD	-7.11	1.62	1.81
1	B	133	TYR	C-O	-7.10	1.09	1.23
1	A	126	ALA	N-CA	-6.96	1.32	1.46
1	B	40	LYS	CG-CD	-6.96	1.28	1.52
1	B	208	PHE	CE1-CZ	-6.94	1.24	1.37
1	B	41	LYS	N-CA	-6.92	1.32	1.46
1	B	206	LEU	C-O	-6.90	1.10	1.23
1	A	160	ALA	C-N	-6.85	1.18	1.34
1	B	40	LYS	C-O	-6.81	1.10	1.23
1	A	101	VAL	C-N	6.72	1.49	1.34
1	B	41	LYS	CD-CE	-6.72	1.34	1.51
1	B	12	TRP	C-O	-6.71	1.10	1.23
1	B	175	ARG	C-N	-6.71	1.18	1.34
1	B	115	ASP	C-N	-6.69	1.21	1.33
1	A	166	GLU	CA-CB	-6.68	1.39	1.53
1	B	13	LEU	C-O	-6.68	1.10	1.23
1	A	172	LYS	CA-CB	-6.67	1.39	1.53
1	A	105	GLN	C-N	-6.64	1.21	1.33
1	B	12	TRP	CD1-NE1	-6.64	1.26	1.38
1	B	66	LEU	CG-CD2	-6.63	1.27	1.51
1	B	9	GLU	CG-CD	-6.60	1.42	1.51
1	B	30	LYS	C-N	-6.57	1.21	1.33
1	B	169	SER	N-CA	-6.47	1.33	1.46
1	B	174	LEU	CG-CD2	-6.45	1.28	1.51
1	B	209	MET	CG-SD	-6.44	1.64	1.81
1	A	202	ASN	CA-CB	-6.42	1.36	1.53
1	B	176	ASN	N-CA	-6.40	1.33	1.46
1	B	82	ARG	N-CA	-6.35	1.33	1.46
1	B	133	TYR	CB-CG	-6.31	1.42	1.51
1	B	82	ARG	NE-CZ	-6.29	1.24	1.33
1	B	172	LYS	CG-CD	-6.25	1.31	1.52
1	B	172	LYS	CA-CB	-6.12	1.40	1.53
1	B	9	GLU	CB-CG	-6.09	1.40	1.52
1	B	66	LEU	C-N	-6.09	1.20	1.34
1	B	40	LYS	N-CA	-5.98	1.34	1.46
1	B	158	SER	CB-OG	-5.96	1.34	1.42
1	B	209	MET	SD-CE	-5.95	1.44	1.77
1	A	202	ASN	CG-ND2	-5.89	1.18	1.32
1	A	126	ALA	C-O	-5.88	1.12	1.23
1	B	12	TRP	CZ3-CH2	-5.87	1.30	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	85	ASP	CB-CG	-5.86	1.39	1.51
1	B	209	MET	C-N	-5.82	1.20	1.34
1	A	172	LYS	CD-CE	-5.82	1.36	1.51
1	B	159	LYS	N-CA	-5.81	1.34	1.46
1	B	105	GLN	C-N	-5.78	1.22	1.33
1	B	7	ARG	C-O	-5.72	1.12	1.23
1	B	133	TYR	CZ-OH	-5.66	1.28	1.37
1	B	30	LYS	CD-CE	-5.66	1.37	1.51
1	A	161	GLU	C-O	-5.62	1.12	1.23
1	A	164	ARG	CA-CB	-5.61	1.41	1.53
1	A	102	ASP	C-O	-5.59	1.12	1.23
1	B	30	LYS	C-O	-5.58	1.12	1.23
1	B	43	TYR	CG-CD2	-5.55	1.31	1.39
1	B	133	TYR	N-CA	-5.53	1.35	1.46
1	B	115	ASP	N-CA	-5.48	1.35	1.46
1	A	164	ARG	CB-CG	-5.41	1.38	1.52
1	B	169	SER	CB-OG	-5.34	1.35	1.42
1	B	204	GLU	N-CA	-5.28	1.35	1.46
1	B	227	ARG	CB-CG	-5.20	1.38	1.52
1	A	230	PHE	CD2-CE2	-5.16	1.28	1.39
1	B	43	TYR	CZ-OH	-5.12	1.29	1.37
1	B	82	ARG	CD-NE	-5.11	1.37	1.46
1	B	7	ARG	CB-CG	-5.10	1.38	1.52
1	B	208	PHE	N-CA	-5.09	1.36	1.46
1	A	125	GLY	C-O	-5.08	1.15	1.23
1	B	211	LEU	CG-CD1	-5.06	1.33	1.51
1	B	115	ASP	CG-OD2	-5.06	1.13	1.25
1	B	129	LYS	C-O	-5.00	1.13	1.23

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	13	LEU	CB-CG-CD1	10.15	128.25	111.00
1	A	227	ARG	NE-CZ-NH1	-9.83	115.39	120.30
1	A	164	ARG	NE-CZ-NH1	9.61	125.10	120.30
1	A	161	GLU	O-C-N	-9.42	107.63	122.70
1	B	174	LEU	CA-CB-CG	9.17	136.38	115.30
1	A	227	ARG	NE-CZ-NH2	8.84	124.72	120.30
1	B	66	LEU	CB-CG-CD2	-8.34	96.83	111.00
1	B	30	LYS	CD-CE-NZ	8.16	130.46	111.70
1	A	166	GLU	N-CA-CB	8.06	125.11	110.60
1	B	176	ASN	CB-CA-C	-7.96	94.47	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	LEU	CB-CG-CD2	7.91	124.44	111.00
1	A	164	ARG	NH1-CZ-NH2	-7.74	110.88	119.40
1	A	160	ALA	C-N-CA	7.69	140.93	121.70
1	B	211	LEU	CA-CB-CG	7.69	132.99	115.30
1	B	85	ASP	CB-CG-OD1	7.63	125.17	118.30
1	A	164	ARG	CG-CD-NE	7.61	127.78	111.80
1	B	204	GLU	OE1-CD-OE2	-7.36	114.46	123.30
1	A	164	ARG	NE-CZ-NH2	7.11	123.85	120.30
1	A	101	VAL	C-N-CA	-7.10	103.94	121.70
1	A	164	ARG	CB-CG-CD	7.01	129.83	111.60
1	B	172	LYS	CD-CE-NZ	-7.01	95.58	111.70
1	A	227	ARG	CA-CB-CG	6.92	128.62	113.40
1	A	227	ARG	CG-CD-NE	6.84	126.17	111.80
1	B	206	LEU	CA-CB-CG	6.79	130.92	115.30
1	B	85	ASP	OD1-CG-OD2	-6.60	110.76	123.30
1	A	227	ARG	CB-CG-CD	6.58	128.72	111.60
1	A	175	ARG	CG-CD-NE	6.58	125.61	111.80
1	A	161	GLU	CB-CA-C	6.56	123.53	110.40
1	A	226	SER	C-N-CA	6.54	138.04	121.70
1	A	161	GLU	OE1-CD-OE2	-6.35	115.68	123.30
1	B	208	PHE	O-C-N	-6.32	112.59	122.70
1	B	40	LYS	CD-CE-NZ	6.28	126.14	111.70
1	B	7	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	172	LYS	CB-CA-C	-6.20	98.01	110.40
1	B	174	LEU	CB-CA-C	6.16	121.90	110.20
1	B	11	ILE	CG1-CB-CG2	-6.11	97.96	111.40
1	B	169	SER	N-CA-CB	-6.04	101.44	110.50
1	B	209	MET	CA-C-O	5.96	132.61	120.10
1	B	68	MET	CG-SD-CE	5.89	109.62	100.20
1	B	169	SER	CB-CA-C	5.76	121.04	110.10
1	A	172	LYS	O-C-N	-5.75	113.50	122.70
1	B	140	ILE	CB-CA-C	-5.72	100.16	111.60
1	B	41	LYS	CA-C-N	5.71	129.75	117.20
1	B	9	GLU	OE1-CD-OE2	-5.70	116.46	123.30
1	B	41	LYS	CA-C-O	-5.68	108.17	120.10
1	A	125	GLY	CA-C-O	-5.63	110.46	120.60
1	A	227	ARG	CB-CA-C	-5.60	99.20	110.40
1	B	174	LEU	CA-C-O	-5.52	108.50	120.10
1	B	105	GLN	CA-C-N	5.50	127.20	116.20
1	A	175	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	B	9	GLU	CG-CD-OE1	5.33	128.96	118.30
1	A	124	VAL	C-N-CA	5.31	133.45	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ALA	CB-CA-C	5.27	118.00	110.10
1	B	7	ARG	CD-NE-CZ	5.22	130.91	123.60
1	B	66	LEU	O-C-N	-5.20	114.38	122.70
1	B	174	LEU	CB-CG-CD2	5.20	119.83	111.00
1	B	174	LEU	CB-CG-CD1	5.17	119.79	111.00
1	B	40	LYS	CA-C-N	5.16	128.56	117.20
1	B	206	LEU	CB-CG-CD1	5.11	119.69	111.00
1	A	105	GLN	CA-C-N	5.10	126.40	116.20
1	A	161	GLU	N-CA-CB	5.08	119.75	110.60
1	A	164	ARG	CD-NE-CZ	5.08	130.72	123.60
1	B	66	LEU	CA-C-O	5.04	130.68	120.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	ILE	Mainchain
1	A	161	GLU	Mainchain
1	A	202	ASN	Sidechain

## 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	1746	0	1798	50	0
1	B	1746	0	1799	76	0
2	A	20	0	27	5	0
2	B	20	0	27	6	0
3	A	39	0	0	0	0
3	B	27	0	0	2	0
All	All	3598	0	3651	127	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 18.

All (127) 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:B:145:MET:O	1:B:149:LEU:HD23	1.25	1.32
1:B:145:MET:O	1:B:149:LEU:CD2	1.77	1.31
1:B:30:LYS:HA	1:B:30:LYS:HE3	1.48	0.92
1:B:142:THR:HB	3:B:259:HOH:O	1.68	0.92
1:B:9:GLU:H	1:B:9:GLU:CD	1.77	0.86
1:B:145:MET:O	1:B:149:LEU:HD22	1.84	0.78
1:B:9:GLU:HB3	1:B:202:ASN:HA	1.66	0.76
1:B:192:GLY:HA3	1:B:204:GLU:OE2	1.87	0.74
1:B:227:ARG:H	1:B:227:ARG:NE	1.86	0.74
1:A:164:ARG:HE	1:A:167:VAL:HG23	1.51	0.74
1:B:128:THR:HG21	1:B:133:TYR:HB3	1.69	0.73
1:B:91:PRO:HD3	1:B:115:ASP:OD1	1.89	0.73
1:A:36:ASP:O	1:A:40:LYS:HG3	1.89	0.72
1:B:193:SER:H	1:B:204:GLU:CD	1.92	0.71
1:B:137:TRP:HA	1:B:140:ILE:HD12	1.70	0.71
1:B:193:SER:N	1:B:204:GLU:OE1	2.22	0.70
1:A:164:ARG:NE	1:A:167:VAL:HG23	2.06	0.70
1:B:112:VAL:O	1:B:115:ASP:HB3	1.93	0.69
1:B:139:ALA:O	1:B:142:THR:HG22	1.93	0.69
1:A:139:ALA:O	1:A:142:THR:HG22	1.93	0.68
1:B:53:ALA:HA	1:B:85:ASP:OD2	1.93	0.68
1:B:149:LEU:N	1:B:149:LEU:HD22	2.10	0.66
1:A:164:ARG:HD2	1:A:166:GLU:HB3	1.76	0.66
1:B:145:MET:C	1:B:149:LEU:HD23	2.14	0.66
1:B:206:LEU:HD22	1:B:206:LEU:O	1.96	0.66
1:B:34:VAL:CG1	1:B:40:LYS:HG2	2.27	0.65
1:A:9:GLU:OE1	1:A:9:GLU:N	2.23	0.65
1:A:34:VAL:HG13	1:A:40:LYS:HG2	1.79	0.65
1:B:65:GLY:HA3	1:B:81:ALA:HB2	1.79	0.63
1:A:65:GLY:HA3	1:A:81:ALA:HB2	1.79	0.63
1:B:9:GLU:OE1	1:B:9:GLU:N	2.30	0.62
1:A:186:PRO:HB3	2:A:301:RET:H183	1.80	0.62
1:B:149:LEU:H	1:B:149:LEU:HD22	1.65	0.62
1:B:30:LYS:CE	1:B:30:LYS:HA	2.21	0.62
1:B:186:PRO:HB3	2:B:301:RET:H183	1.80	0.61
1:B:31:GLY:O	1:B:34:VAL:HG12	2.00	0.61
1:B:34:VAL:HG13	1:B:40:LYS:CG	2.31	0.61
1:A:31:GLY:O	1:A:34:VAL:HG12	2.00	0.61
1:B:136:VAL:O	1:B:140:ILE:CD1	2.49	0.60
1:B:130:VAL:O	1:B:133:TYR:HB2	2.01	0.60
1:B:10:TRP:HA	1:B:13:LEU:HD12	1.84	0.60
1:A:164:ARG:HG3	1:A:165:PRO:N	2.11	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:VAL:O	1:B:140:ILE:HD12	2.02	0.59
1:B:227:ARG:H	1:B:227:ARG:HE	1.51	0.58
1:B:140:ILE:HG22	1:B:140:ILE:O	1.96	0.57
1:B:149:LEU:CD2	1:B:149:LEU:H	2.19	0.56
1:A:202:ASN:OD1	1:A:203:ILE:N	2.38	0.55
1:A:90:THR:OG1	1:A:91:PRO:CD	2.55	0.55
1:B:90:THR:OG1	1:B:91:PRO:CD	2.55	0.55
1:B:7:ARG:HH21	1:B:201:LEU:HD23	1.72	0.54
1:B:56:MET:HG3	1:B:85:ASP:HB2	1.88	0.54
1:B:170:THR:HG22	1:B:174:LEU:HD12	1.89	0.53
1:A:164:ARG:HG3	1:A:165:PRO:CD	2.39	0.53
1:B:66:LEU:HG	1:B:67:THR:N	2.24	0.53
1:B:226:SER:HA	1:B:227:ARG:NH2	2.24	0.52
1:B:34:VAL:HG13	1:B:40:LYS:HG3	1.92	0.52
1:A:37:PRO:O	1:A:41:LYS:HG2	2.10	0.52
1:B:86:TRP:CD1	2:B:301:RET:H14	2.45	0.52
1:B:193:SER:N	1:B:204:GLU:OE2	2.43	0.52
1:A:166:GLU:CG	1:A:166:GLU:O	2.54	0.52
1:A:16:GLY:O	1:A:20:MET:HG2	2.10	0.52
1:A:86:TRP:CD1	2:A:301:RET:H14	2.45	0.52
1:B:192:GLY:HA3	1:B:204:GLU:CD	2.31	0.51
1:A:164:ARG:NH2	1:A:227:ARG:O	2.43	0.51
1:B:16:GLY:O	1:B:20:MET:HG2	2.10	0.51
1:B:9:GLU:CD	1:B:9:GLU:N	2.54	0.51
1:B:226:SER:HA	1:B:227:ARG:HH21	1.77	0.50
1:B:34:VAL:HG13	1:B:40:LYS:HG2	1.92	0.50
1:A:145:MET:CE	1:A:186:PRO:HG3	2.42	0.50
1:B:145:MET:CE	1:B:186:PRO:HG3	2.42	0.50
1:B:145:MET:HE1	1:B:186:PRO:HG3	1.94	0.49
1:B:139:ALA:O	1:B:142:THR:CG2	2.60	0.49
1:A:139:ALA:O	1:A:142:THR:CG2	2.60	0.49
1:A:166:GLU:CD	1:A:166:GLU:O	2.51	0.49
1:B:108:ILE:O	1:B:112:VAL:HG23	2.13	0.49
1:A:108:ILE:O	1:A:112:VAL:HG23	2.13	0.49
1:B:104:ASP:O	1:B:106:GLY:N	2.46	0.48
1:A:202:ASN:N	1:A:202:ASN:OD1	2.43	0.47
1:B:142:THR:HA	2:B:301:RET:H182	1.95	0.47
1:A:142:THR:HA	2:A:301:RET:H182	1.95	0.47
1:A:68:MET:HB3	1:A:75:GLN:HG3	1.97	0.47
1:B:149:LEU:CD2	1:B:149:LEU:N	2.75	0.47
1:A:82:ARG:O	1:A:85:ASP:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ARG:HG3	1:A:165:PRO:HD2	1.95	0.46
1:B:211:LEU:O	1:B:212:ASP:C	2.51	0.46
1:B:95:LEU:O	1:B:99:LEU:HG	2.16	0.46
1:A:91:PRO:HD3	1:A:115:ASP:OD1	2.16	0.46
1:A:95:LEU:O	1:A:99:LEU:HG	2.16	0.46
1:A:164:ARG:HE	1:A:167:VAL:CG2	2.27	0.45
1:A:135:PHE:HE1	1:A:190:LEU:HD12	1.81	0.45
1:A:15:LEU:O	1:A:19:LEU:HG	2.16	0.45
1:A:7:ARG:O	1:A:10:TRP:HD1	1.99	0.45
1:B:135:PHE:HE1	1:B:190:LEU:HD12	1.81	0.45
1:B:15:LEU:O	1:B:19:LEU:HG	2.16	0.45
1:A:22:LEU:HA	1:A:22:LEU:HD23	1.79	0.45
1:B:181:LEU:HD22	1:B:211:LEU:HD23	1.99	0.44
1:B:41:LYS:HD3	1:B:99:LEU:HD13	1.99	0.44
1:A:90:THR:OG1	1:A:91:PRO:HD3	2.18	0.43
1:A:145:MET:HE1	1:A:186:PRO:HG3	1.99	0.43
1:B:194:GLU:OE1	1:B:194:GLU:N	2.45	0.43
1:A:56:MET:HG3	1:A:85:ASP:HB2	2.01	0.43
1:A:194:GLU:N	1:A:194:GLU:OE1	2.45	0.43
1:B:90:THR:OG1	1:B:91:PRO:HD3	2.18	0.43
1:B:118:MET:O	1:B:141:SER:OG	2.31	0.43
1:B:22:LEU:HA	1:B:22:LEU:HD23	1.79	0.42
1:A:27:PHE:HB3	1:A:47:THR:OG1	2.19	0.42
1:B:27:PHE:HB3	1:B:47:THR:OG1	2.19	0.42
1:A:118:MET:O	1:A:141:SER:OG	2.31	0.42
1:B:7:ARG:O	1:B:10:TRP:HD1	2.02	0.42
1:B:25:LEU:O	1:B:29:VAL:HG23	2.20	0.42
1:A:209:MET:O	1:A:213:VAL:HG23	2.19	0.42
1:B:145:MET:HG3	2:B:301:RET:H181	2.02	0.42
2:B:301:RET:H42	3:B:259:HOH:O	2.20	0.41
1:A:227:ARG:HD3	1:A:227:ARG:HH11	1.46	0.41
1:A:139:ALA:C	1:A:142:THR:HG22	2.40	0.41
1:A:145:MET:HG3	2:A:301:RET:H181	2.03	0.41
1:A:189:TRP:CD1	2:A:301:RET:H22	2.56	0.41
1:A:25:LEU:O	1:A:29:VAL:HG23	2.20	0.41
1:B:104:ASP:O	1:B:105:GLN:C	2.59	0.41
1:B:189:TRP:CD1	2:B:301:RET:H22	2.56	0.41
1:A:70:PRO:HA	1:A:74:GLU:O	2.21	0.41
1:B:145:MET:SD	1:B:149:LEU:HD21	2.61	0.41
1:B:70:PRO:HA	1:B:74:GLU:O	2.21	0.41
1:A:40:LYS:HE3	1:A:40:LYS:HB3	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:LEU:HD23	1:B:92:LEU:CD1	2.51	0.40
1:B:65:GLY:HA2	1:B:80:TRP:CE2	2.56	0.40
1:A:65:GLY:HA2	1:A:80:TRP:CE2	2.56	0.40

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	224/249 (90%)	219 (98%)	5 (2%)	0	100	100
1	B	224/249 (90%)	216 (96%)	8 (4%)	0	100	100
All	All	448/498 (90%)	435 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	180/194 (93%)	176 (98%)	4 (2%)	60	84
1	B	180/194 (93%)	172 (96%)	8 (4%)	35	60
All	All	360/388 (93%)	348 (97%)	12 (3%)	45	73

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	TYR
1	A	161	GLU
1	A	175	ARG
1	A	227	ARG
1	B	30	LYS
1	B	41	LYS
1	B	66	LEU
1	B	131	TYR
1	B	206	LEU
1	B	208	PHE
1	B	209	MET
1	B	227	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	B	75	GLN
1	B	76	ASN

### 5.3.3 RNA [i](#)

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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	$\# Z  > 2$
2	RET	A	301	1	19,20,21	2.46	4 (21%)	27,27,28	2.85	14 (51%)
2	RET	B	301	1	19,20,21	2.46	4 (21%)	27,27,28	2.85	14 (51%)

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
2	RET	A	301	1	-	0/13/30/31	0/1/1/1
2	RET	B	301	1	-	0/13/30/31	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	RET	C17-C1	2.33	1.58	1.53
2	B	301	RET	C17-C1	2.33	1.58	1.53
2	B	301	RET	C2-C1	2.39	1.59	1.54
2	A	301	RET	C2-C1	2.40	1.59	1.54
2	A	301	RET	C5-C6	5.58	1.43	1.34
2	B	301	RET	C5-C6	5.59	1.43	1.34
2	B	301	RET	C1-C6	7.40	1.64	1.53
2	A	301	RET	C1-C6	7.40	1.64	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	RET	C8-C9-C10	-4.94	111.03	118.98
2	B	301	RET	C8-C9-C10	-4.87	111.14	118.98
2	A	301	RET	C10-C11-C12	-4.54	109.28	123.13
2	B	301	RET	C10-C11-C12	-4.54	109.28	123.13
2	A	301	RET	C11-C10-C9	-3.96	121.48	127.20
2	B	301	RET	C11-C10-C9	-3.92	121.53	127.20
2	A	301	RET	C7-C6-C5	-3.77	112.73	121.37
2	B	301	RET	C7-C6-C5	-3.77	112.74	121.37
2	B	301	RET	C12-C13-C14	-2.48	110.84	118.92
2	A	301	RET	C12-C13-C14	-2.47	110.89	118.92
2	B	301	RET	C18-C5-C4	-2.39	108.89	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	RET	C18-C5-C4	-2.38	108.92	113.43
2	B	301	RET	C2-C1-C6	2.58	114.45	110.36
2	A	301	RET	C2-C1-C6	2.59	114.47	110.36
2	A	301	RET	C7-C8-C9	2.90	130.63	126.22
2	B	301	RET	C7-C8-C9	2.97	130.74	126.22
2	B	301	RET	C20-C13-C12	3.01	123.11	118.10
2	A	301	RET	C20-C13-C12	3.05	123.18	118.10
2	B	301	RET	C3-C4-C5	3.13	118.83	113.87
2	A	301	RET	C3-C4-C5	3.13	118.83	113.87
2	B	301	RET	C17-C1-C6	3.26	115.41	110.30
2	A	301	RET	C17-C1-C6	3.26	115.42	110.30
2	B	301	RET	C19-C9-C8	3.63	124.14	118.10
2	A	301	RET	C19-C9-C8	3.68	124.21	118.10
2	B	301	RET	C1-C6-C7	3.84	126.57	115.82
2	A	301	RET	C1-C6-C7	3.84	126.57	115.82
2	A	301	RET	C18-C5-C6	6.26	130.75	124.61
2	B	301	RET	C18-C5-C6	6.30	130.79	124.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	RET	5	0
2	B	301	RET	6	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	226/249 (90%)	-0.39	0 <b>100</b> <b>100</b>	8, 21, 38, 50	0
1	B	226/249 (90%)	-0.38	1 (0%) <b>93</b> <b>93</b>	10, 22, 38, 53	0
All	All	452/498 (90%)	-0.38	1 (0%) <b>95</b> <b>96</b>	8, 21, 39, 53	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	133	TYR	2.8

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	RET	A	301	20/21	0.88	0.16	1.80	20,29,33,33	0
2	RET	B	301	20/21	0.93	0.14	0.73	18,20,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.