



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 28, 2026 – 11:44 PM UTC

PDB ID : 2CX4 / pdb_00002cx4
Title : Crystal structure of a bacterioferritin comigratory protein peroxiredoxin from the *Aeropyrum pernix* K1 (form-2 crystal)
Authors : Mizohata, E.; Murayama, K.; Idaka, M.; Tatsuguchi, A.; Terada, T.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-06-27
Resolution : 2.30 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
Mogul : 2022.3.0, CSD as543be (2022)
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

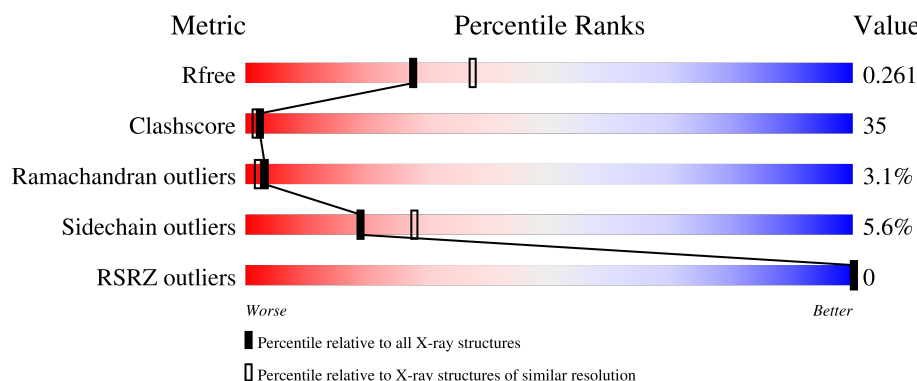
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



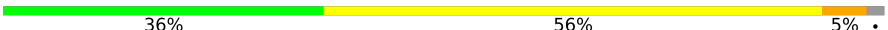
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	164	43% 49% 5% ..
1	B	164	32% 59% 6% ..
1	C	164	36% 58% ..
1	D	164	42% 50% 5% .
1	E	164	41% 51% 5% .

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Mol	Chain	Length	Quality of chain
1	F	164	 36% 56% 5% •
1	G	164	 36% 55% 7% •
1	H	164	 33% 57% 8% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10735 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 bacterioferritin comigratory protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	Se	0	0	0
			1293	837	213	238	3	2			
1	B	160	Total	C	N	O	S	Se	0	0	0
			1289	835	212	237	3	2			
1	C	161	Total	C	N	O	S	Se	0	0	0
			1293	837	213	238	3	2			
1	D	160	Total	C	N	O	S	Se	0	0	0
			1289	835	212	237	3	2			
1	E	161	Total	C	N	O	S	Se	0	0	0
			1293	837	213	238	3	2			
1	F	160	Total	C	N	O	S	Se	0	0	0
			1289	835	212	237	3	2			
1	G	161	Total	C	N	O	S	Se	0	0	0
			1293	837	213	238	3	2			
1	H	160	Total	C	N	O	S	Se	0	0	0
			1289	835	212	237	3	2			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	GB 14601861
A	60	MSE	MET	modified residue	GB 14601861
A	118	MSE	MET	modified residue	GB 14601861
B	1	MSE	MET	modified residue	GB 14601861
B	60	MSE	MET	modified residue	GB 14601861
B	118	MSE	MET	modified residue	GB 14601861
C	1	MSE	MET	modified residue	GB 14601861
C	60	MSE	MET	modified residue	GB 14601861
C	118	MSE	MET	modified residue	GB 14601861
D	1	MSE	MET	modified residue	GB 14601861
D	60	MSE	MET	modified residue	GB 14601861
D	118	MSE	MET	modified residue	GB 14601861
E	1	MSE	MET	modified residue	GB 14601861

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Chain	Residue	Modelled	Actual	Comment	Reference
E	60	MSE	MET	modified residue	GB 14601861
E	118	MSE	MET	modified residue	GB 14601861
F	1	MSE	MET	modified residue	GB 14601861
F	60	MSE	MET	modified residue	GB 14601861
F	118	MSE	MET	modified residue	GB 14601861
G	1	MSE	MET	modified residue	GB 14601861
G	60	MSE	MET	modified residue	GB 14601861
G	118	MSE	MET	modified residue	GB 14601861
H	1	MSE	MET	modified residue	GB 14601861
H	60	MSE	MET	modified residue	GB 14601861
H	118	MSE	MET	modified residue	GB 14601861

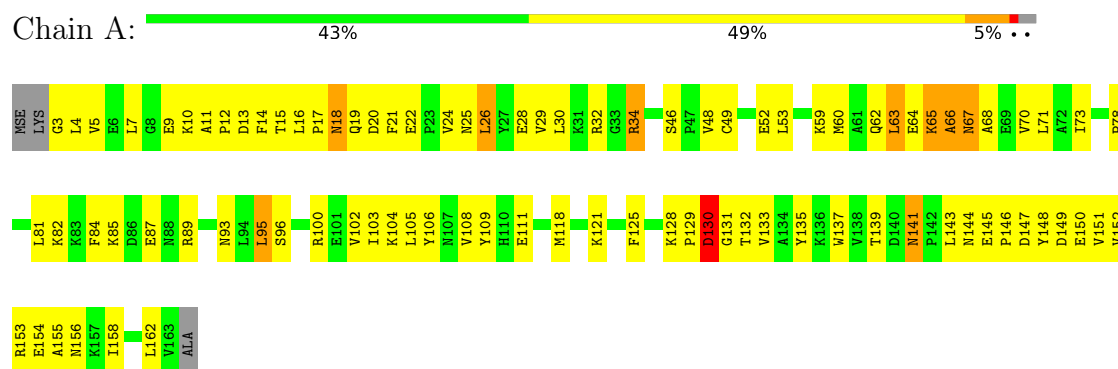
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	56	Total O 56 56	0	0
2	B	78	Total O 78 78	0	0
2	C	56	Total O 56 56	0	0
2	D	36	Total O 36 36	0	0
2	E	41	Total O 41 41	0	0
2	F	47	Total O 47 47	0	0
2	G	62	Total O 62 62	0	0
2	H	31	Total O 31 31	0	0

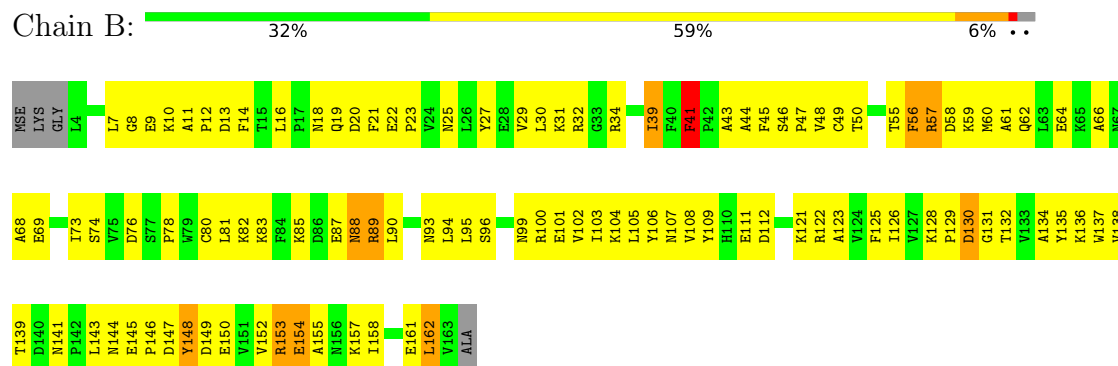
3 Residue-property plots

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.

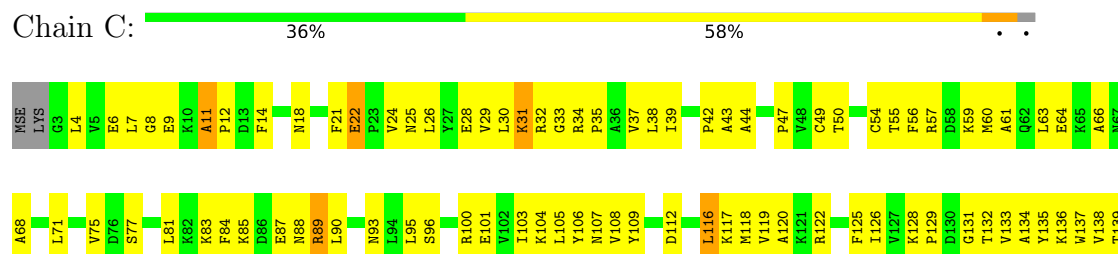
• Molecule 1: bacterioferritin comigratory protein



• Molecule 1: bacterioferritin comigratory protein



• Molecule 1: bacterioferritin comigratory protein





- Molecule 1: bacterioferritin comigratory protein

Chain D: 42% 50% 5% .



- Molecule 1: bacterioferritin comigratory protein

Chain E: 41% 51% 5% .



- Molecule 1: bacterioferritin comigratory protein

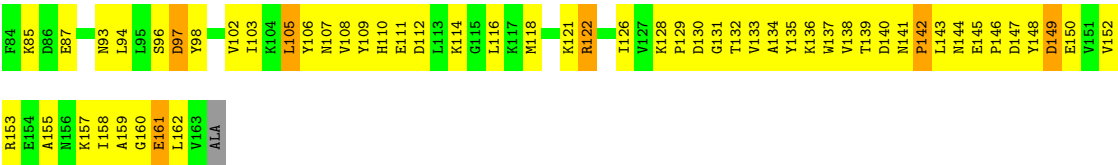
Chain F: 36% 56% 5% .



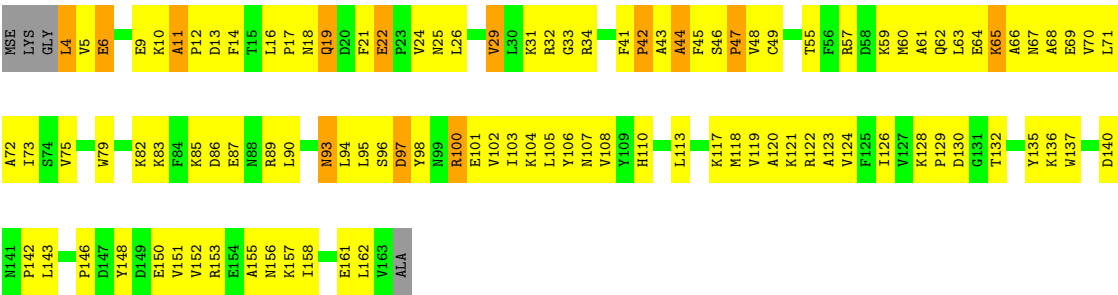
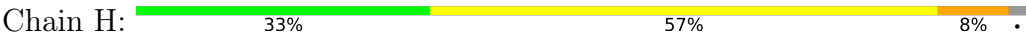
- Molecule 1: bacterioferritin comigratory protein

Chain G: 36% 55% 7% .





● Molecule 1: bacterioferritin comigratory protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	132.48Å 132.48Å 106.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.32 – 2.30 46.32 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.6 (46.32-2.30) 95.2 (46.32-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.203 , 0.263 0.211 , 0.261	Depositor DCC
R_{free} test set	6351 reflections (4.41%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.691	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.479 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10735	wwPDB-VP
Average B, all atoms (Å ²)	48.0	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 85.79 % 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 1.1361e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.44	0/1320	0.89	3/1787 (0.2%)
1	B	0.44	0/1316	0.90	4/1782 (0.2%)
1	C	0.48	0/1320	0.90	2/1787 (0.1%)
1	D	0.45	0/1316	0.88	3/1782 (0.2%)
1	E	0.45	0/1320	0.91	3/1787 (0.2%)
1	F	0.47	0/1316	0.89	1/1782 (0.1%)
1	G	0.47	0/1320	0.83	2/1787 (0.1%)
1	H	0.45	0/1316	0.89	3/1782 (0.2%)
All	All	0.46	0/10544	0.89	21/14276 (0.1%)

There are no bond length outliers.

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	19	GLN	N-CA-C	-7.32	104.22	113.01
1	F	28	GLU	N-CA-C	-7.17	103.46	111.28
1	G	28	GLU	N-CA-C	-6.22	104.50	111.28
1	B	56	PHE	N-CA-C	-5.90	106.62	113.88
1	A	66	ALA	N-CA-C	-5.76	106.42	113.50

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	1293	0	1302	83	0
1	B	1289	0	1299	115	0
1	C	1293	0	1301	99	0
1	D	1289	0	1300	90	0
1	E	1293	0	1303	79	0
1	F	1289	0	1298	94	0
1	G	1293	0	1301	102	0
1	H	1289	0	1300	90	0
2	A	56	0	0	4	0
2	B	78	0	0	4	0
2	C	56	0	0	4	0
2	D	36	0	0	1	0
2	E	41	0	0	0	0
2	F	47	0	0	3	0
2	G	62	0	0	0	0
2	H	31	0	0	1	0
All	All	10735	0	10404	735	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 35.

The worst 5 of 735 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:D:62:GLN:HB3	1:D:152:VAL:HG11	1.38	1.05
1:B:55:THR:HG22	1:B:56:PHE:H	1.21	1.01
1:C:139:THR:HG21	1:C:144:ASN:HB3	1.44	0.99
1:F:100:ARG:NH2	2:F:187:HOH:O	1.99	0.94
1:C:18:ASN:HD21	1:C:22:GLU:HB3	1.34	0.92

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	159/164 (97%)	134 (84%)	21 (13%)	4 (2%)	4	3
1	B	158/164 (96%)	128 (81%)	25 (16%)	5 (3%)	3	2
1	C	159/164 (97%)	129 (81%)	26 (16%)	4 (2%)	4	3
1	D	158/164 (96%)	132 (84%)	24 (15%)	2 (1%)	9	10
1	E	159/164 (97%)	132 (83%)	22 (14%)	5 (3%)	3	2
1	F	158/164 (96%)	134 (85%)	20 (13%)	4 (2%)	4	3
1	G	159/164 (97%)	124 (78%)	26 (16%)	9 (6%)	1	0
1	H	158/164 (96%)	132 (84%)	20 (13%)	6 (4%)	2	1
All	All	1268/1312 (97%)	1045 (82%)	184 (14%)	39 (3%)	3	2

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	4	LEU
1	G	9	GLU
1	H	44	ALA
1	A	17	PRO
1	B	148	TYR

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	141/140 (101%)	131 (93%)	10 (7%)	13	19
1	B	141/140 (101%)	130 (92%)	11 (8%)	11	16
1	C	141/140 (101%)	135 (96%)	6 (4%)	26	39
1	D	141/140 (101%)	133 (94%)	8 (6%)	18	27
1	E	141/140 (101%)	134 (95%)	7 (5%)	22	33
1	F	141/140 (101%)	134 (95%)	7 (5%)	22	33
1	G	141/140 (101%)	134 (95%)	7 (5%)	22	33
1	H	141/140 (101%)	134 (95%)	7 (5%)	22	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1128/1120 (101%)	1065 (94%)	63 (6%)	19	28

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	19	GLN
1	G	149	ASP
1	E	4	LEU
1	G	140	ASP
1	H	22	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	93	ASN
1	G	107	ASN
1	F	141	ASN
1	G	25	ASN
1	G	144	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	159/164 (96%)	-1.40	0 100 100	28, 48, 73, 79	0
1	B	158/164 (96%)	-1.34	0 100 100	30, 51, 67, 73	0
1	C	159/164 (96%)	-1.37	0 100 100	28, 48, 65, 84	0
1	D	158/164 (96%)	-1.38	0 100 100	28, 48, 67, 88	0
1	E	159/164 (96%)	-1.40	0 100 100	23, 49, 65, 74	0
1	F	158/164 (96%)	-1.39	0 100 100	26, 46, 66, 82	0
1	G	159/164 (96%)	-1.37	0 100 100	25, 50, 72, 78	0
1	H	158/164 (96%)	-1.41	0 100 100	26, 45, 73, 82	0
All	All	1268/1312 (96%)	-1.38	0 100 100	23, 48, 70, 88	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.