



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 27, 2026 – 05:54 PM EDT

PDB ID : 2Q4U / pdb_00002q4u
Title : Ensemble refinement of the crystal structure of an EF-hand protein from *Danio rerio* Dr.36843
Authors : Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on : 2007-05-31
Resolution : 2.10 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

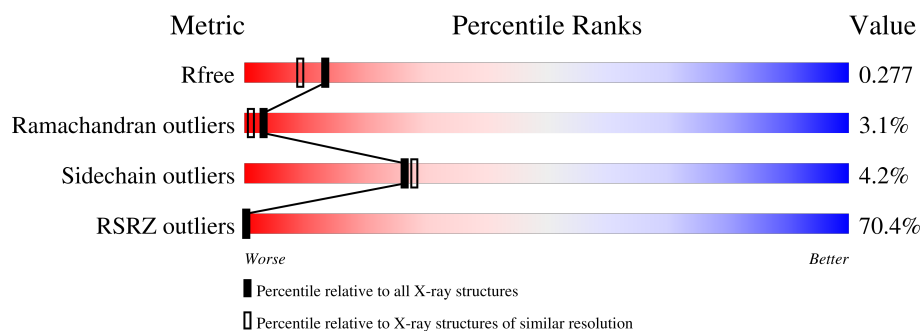
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



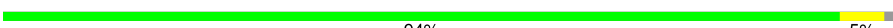
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	1-A	272	67% 94% 5%
1	10-A	272	94%
1	11-A	272	93% 6%
1	12-A	272	94% 6%
1	13-A	272	92% 7%
1	14-A	272	92% 7%
1	15-A	272	93% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	16-A	272	 92% 7% .
1	2-A	272	 92% 7% .
1	3-A	272	 94% 5% .
1	4-A	272	 94% 5% .
1	5-A	272	 94% 5% .
1	6-A	272	 92% 7% .
1	7-A	272	 93% 7% .
1	8-A	272	 93% 6% .
1	9-A	272	 91% 8% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 39088 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 Protein Zgc:100843.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	1-A	270	Total	C	N	O	S	Se	0	0	0
			2203	1402	374	414	3	10			
1	2-A	270	Total	C	N	O	S	Se	0	0	0
			2203	1402	374	414	3	10			
1	3-A	270	Total	C	N	O	S	Se	0	0	0
			2203	1402	374	414	3	10			
1	4-A	270	Total	C	N	O	S	Se	0	0	0
			2203	1402	374	414	3	10			
1	5-A	270	Total	C	N	O	S	Se	0	0	0
			2203	1402	374	414	3	10			
1	6-A	270	Total	C	N	O	S	Se	0	0	0
			2203	1402	374	414	3	10			
1	7-A	270	Total	C	N	O	S	Se	0	0	0
			2203	1402	374	414	3	10			
1	8-A	270	Total	C	N	O	S	Se	0	0	0
			2203	1402	374	414	3	10			
1	9-A	270	Total	C	N	O	S	Se	0	0	0
			2203	1402	374	414	3	10			
1	10-A	270	Total	C	N	O	S	Se	0	0	0
			2203	1402	374	414	3	10			
1	11-A	270	Total	C	N	O	S	Se	0	0	0
			2203	1402	374	414	3	10			
1	12-A	270	Total	C	N	O	S	Se	0	0	0
			2203	1402	374	414	3	10			
1	13-A	270	Total	C	N	O	S	Se	0	0	0
			2203	1402	374	414	3	10			
1	14-A	270	Total	C	N	O	S	Se	0	0	0
			2203	1402	374	414	3	10			
1	15-A	270	Total	C	N	O	S	Se	0	0	0
			2203	1402	374	414	3	10			
1	16-A	270	Total	C	N	O	S	Se	0	0	0
			2203	1402	374	414	3	10			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q5XJX1
A	40	MSE	MET	modified residue	UNP Q5XJX1
A	63	MSE	MET	modified residue	UNP Q5XJX1
A	82	MSE	MET	modified residue	UNP Q5XJX1
A	107	MSE	MET	modified residue	UNP Q5XJX1
A	153	MSE	MET	modified residue	UNP Q5XJX1
A	154	MSE	MET	modified residue	UNP Q5XJX1
A	186	MSE	MET	modified residue	UNP Q5XJX1
A	225	MSE	MET	modified residue	UNP Q5XJX1
A	226	MSE	MET	modified residue	UNP Q5XJX1
A	251	MSE	MET	modified residue	UNP Q5XJX1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1-A	240	Total O 240 240	0	0
2	2-A	240	Total O 240 240	0	0
2	3-A	240	Total O 240 240	0	0
2	4-A	240	Total O 240 240	0	0
2	5-A	240	Total O 240 240	0	0
2	6-A	240	Total O 240 240	0	0
2	7-A	240	Total O 240 240	0	0
2	8-A	240	Total O 240 240	0	0
2	9-A	240	Total O 240 240	0	0
2	10-A	240	Total O 240 240	0	0
2	11-A	240	Total O 240 240	0	0
2	12-A	240	Total O 240 240	0	0
2	13-A	240	Total O 240 240	0	0

Continued on next page...

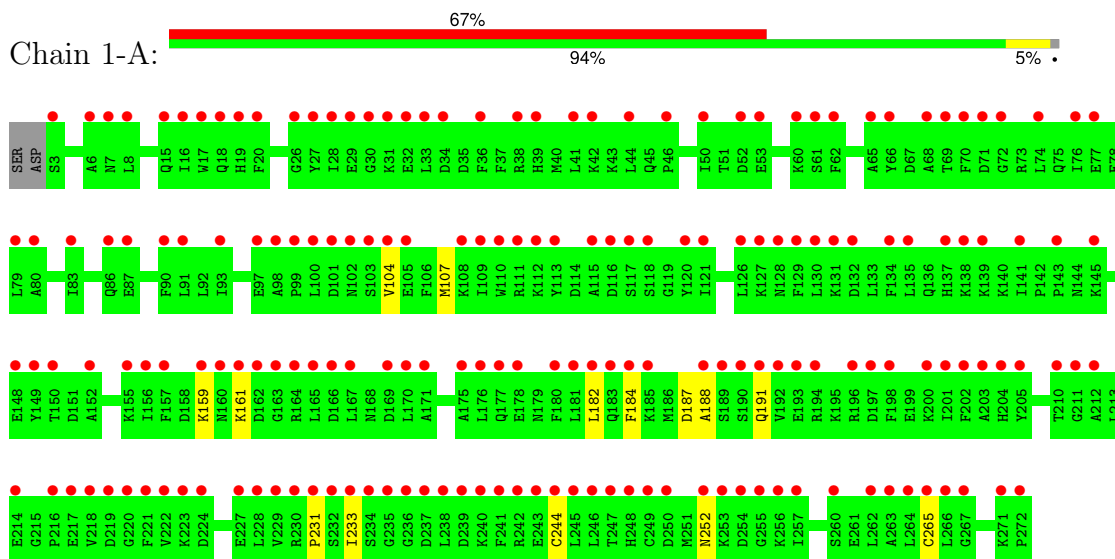
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	14-A	240	Total 240	O 240	0	0
2	15-A	240	Total 240	O 240	0	0
2	16-A	240	Total 240	O 240	0	0

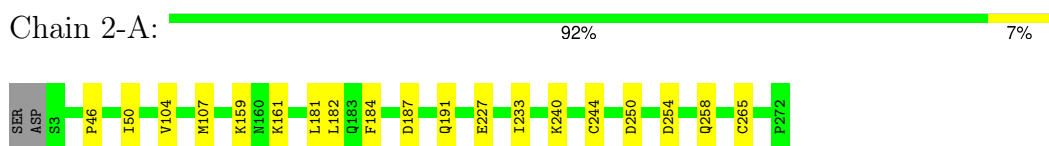
3 Residue-property plots

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.

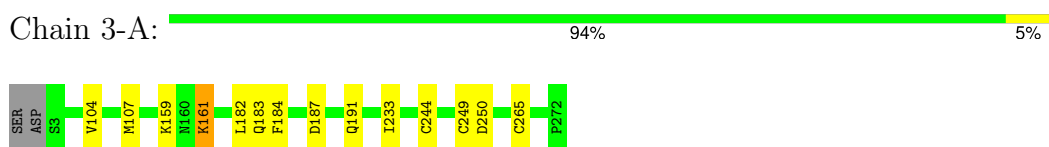
• Molecule 1: Protein Zgc:100843



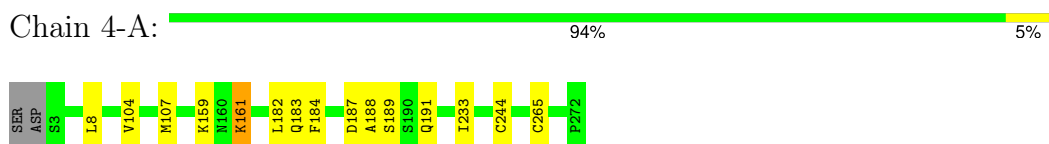
• Molecule 1: Protein Zgc:100843



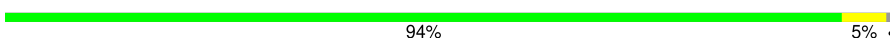
• Molecule 1: Protein Zgc:100843



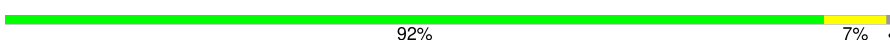
• Molecule 1: Protein Zgc:100843



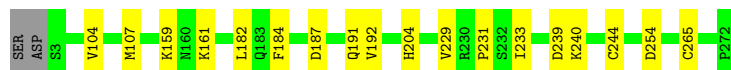
• Molecule 1: Protein Zgc:100843

Chain 5-A:  94% 5%

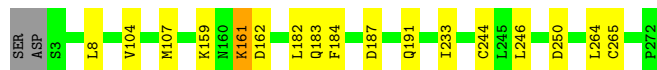
• Molecule 1: Protein Zgc:100843

Chain 6-A:  92% 7%

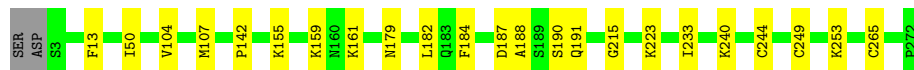
• Molecule 1: Protein Zgc:100843

Chain 7-A:  93% 7%

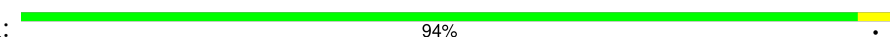
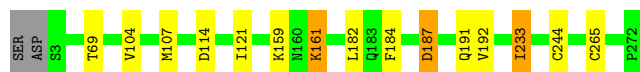
• Molecule 1: Protein Zgc:100843

Chain 8-A:  93% 6%

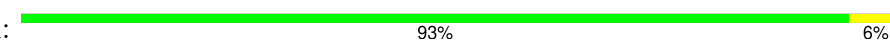
• Molecule 1: Protein Zgc:100843

Chain 9-A:  91% 8%

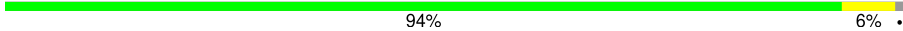
• Molecule 1: Protein Zgc:100843

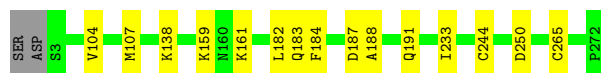
Chain 10-A:  94% 5%

• Molecule 1: Protein Zgc:100843

Chain 11-A:  93% 6%

• Molecule 1: Protein Zgc:100843

Chain 12-A:  94% 6% .



• Molecule 1: Protein Zgc:100843

Chain 13-A:  92% 7% .



• Molecule 1: Protein Zgc:100843

Chain 14-A:  92% 7% ..



• Molecule 1: Protein Zgc:100843

Chain 15-A:  93% 6% ..



• Molecule 1: Protein Zgc:100843

Chain 16-A:  92% 7% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	47.88Å 52.75Å 114.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.17 – 2.10 44.17 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (44.17-2.10) 98.8 (44.17-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.154 , 0.242 0.186 , 0.277	Depositor DCC
R_{free} test set	885 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.02 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	39088	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.07% 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

5.1 Standard geometry

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	1-A	0.22	0/2235	0.27	0/2976
1	2-A	0.22	0/2235	0.27	0/2976
1	3-A	0.22	0/2235	0.27	0/2976
1	4-A	0.22	0/2235	0.27	0/2976
1	5-A	0.22	0/2235	0.27	0/2976
1	6-A	0.22	0/2235	0.27	0/2976
1	7-A	0.22	0/2235	0.27	0/2976
1	8-A	0.22	0/2235	0.27	0/2976
1	9-A	0.22	0/2235	0.27	0/2976
1	10-A	0.22	0/2235	0.27	0/2976
1	11-A	0.22	0/2235	0.27	0/2976
1	12-A	0.22	0/2235	0.27	0/2976
1	13-A	0.22	0/2235	0.27	0/2976
1	14-A	0.22	0/2235	0.27	0/2976
1	15-A	0.22	0/2235	0.27	0/2976
1	16-A	0.22	0/2235	0.27	0/2976
All	All	0.22	0/35760	0.27	0/47616

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	16-A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	16-A	27	TYR	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	1-A	2203	0	2186	0	0
1	2-A	2203	0	2186	0	0
1	3-A	2203	0	2186	0	0
1	4-A	2203	0	2186	0	0
1	5-A	2203	0	2186	0	0
1	6-A	2203	0	2186	0	0
1	7-A	2203	0	2186	0	0
1	8-A	2203	0	2186	0	0
1	9-A	2203	0	2186	0	0
1	10-A	2203	0	2186	0	0
1	11-A	2203	0	2186	0	0
1	12-A	2203	0	2186	0	0
1	13-A	2203	0	2186	0	0
1	14-A	2203	0	2186	0	0
1	15-A	2203	0	2186	0	0
1	16-A	2203	0	2186	0	0
2	1-A	240	0	0	0	0
2	2-A	240	0	0	0	0
2	3-A	240	0	0	0	0
2	4-A	240	0	0	0	0
2	5-A	240	0	0	0	0
2	6-A	240	0	0	0	0
2	7-A	240	0	0	0	0
2	8-A	240	0	0	0	0
2	9-A	240	0	0	0	0
2	10-A	240	0	0	0	0
2	11-A	240	0	0	0	0
2	12-A	240	0	0	0	0
2	13-A	240	0	0	0	0
2	14-A	240	0	0	0	0
2	15-A	240	0	0	0	0
2	16-A	240	0	0	0	0
All	All	39088	0	34976	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	1-A	268/272 (98%)	234 (87%)	30 (11%)	4 (2%)	8	4
1	2-A	268/272 (98%)	243 (91%)	16 (6%)	9 (3%)	3	1
1	3-A	268/272 (98%)	239 (89%)	24 (9%)	5 (2%)	6	3
1	4-A	268/272 (98%)	245 (91%)	17 (6%)	6 (2%)	5	2
1	5-A	268/272 (98%)	244 (91%)	18 (7%)	6 (2%)	5	2
1	6-A	268/272 (98%)	236 (88%)	22 (8%)	10 (4%)	2	1
1	7-A	268/272 (98%)	225 (84%)	35 (13%)	8 (3%)	3	1
1	8-A	268/272 (98%)	240 (90%)	20 (8%)	8 (3%)	3	1
1	9-A	268/272 (98%)	227 (85%)	28 (10%)	13 (5%)	1	0
1	10-A	268/272 (98%)	228 (85%)	32 (12%)	8 (3%)	3	1
1	11-A	268/272 (98%)	238 (89%)	22 (8%)	8 (3%)	3	1
1	12-A	268/272 (98%)	238 (89%)	25 (9%)	5 (2%)	6	3
1	13-A	268/272 (98%)	235 (88%)	23 (9%)	10 (4%)	2	1
1	14-A	268/272 (98%)	211 (79%)	44 (16%)	13 (5%)	1	0
1	15-A	268/272 (98%)	225 (84%)	33 (12%)	10 (4%)	2	1
1	16-A	268/272 (98%)	235 (88%)	22 (8%)	11 (4%)	2	0
All	All	4288/4352 (98%)	3743 (87%)	411 (10%)	134 (3%)	3	1

5 of 134 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	182	LEU
1	1-A	188	ALA
1	2-A	50	ILE
1	2-A	227	GLU
1	2-A	250	ASP

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	1-A	238/230 (104%)	228 (96%)	10 (4%)	26	28
1	2-A	238/230 (104%)	228 (96%)	10 (4%)	26	28
1	3-A	238/230 (104%)	228 (96%)	10 (4%)	26	28
1	4-A	238/230 (104%)	228 (96%)	10 (4%)	26	28
1	5-A	238/230 (104%)	228 (96%)	10 (4%)	26	28
1	6-A	238/230 (104%)	228 (96%)	10 (4%)	26	28
1	7-A	238/230 (104%)	228 (96%)	10 (4%)	26	28
1	8-A	238/230 (104%)	228 (96%)	10 (4%)	26	28
1	9-A	238/230 (104%)	228 (96%)	10 (4%)	26	28
1	10-A	238/230 (104%)	228 (96%)	10 (4%)	26	28
1	11-A	238/230 (104%)	228 (96%)	10 (4%)	26	28
1	12-A	238/230 (104%)	228 (96%)	10 (4%)	26	28
1	13-A	238/230 (104%)	228 (96%)	10 (4%)	26	28
1	14-A	238/230 (104%)	228 (96%)	10 (4%)	26	28
1	15-A	238/230 (104%)	228 (96%)	10 (4%)	26	28
1	16-A	238/230 (104%)	228 (96%)	10 (4%)	26	28
All	All	3808/3680 (104%)	3648 (96%)	160 (4%)	26	28

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	12-A	187	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	15-A	161	LYS
1	12-A	265	CYS
1	14-A	104	VAL
1	16-A	104	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
1	10-A	183	GLN
1	13-A	160	ASN
1	10-A	270	HIS
1	12-A	7	ASN
1	13-A	248	HIS

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 ⓘ

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 [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	1-A	260/272 (95%)	2.99	183 (70%) 0 0	1, 2, 3, 4	260 (100%)
1	2-A	0/272	-	-	-	-
1	3-A	0/272	-	-	-	-
1	4-A	0/272	-	-	-	-
1	5-A	0/272	-	-	-	-
1	6-A	0/272	-	-	-	-
1	7-A	0/272	-	-	-	-
1	8-A	0/272	-	-	-	-
1	9-A	0/272	-	-	-	-
1	10-A	0/272	-	-	-	-
1	11-A	0/272	-	-	-	-
1	12-A	0/272	-	-	-	-
1	13-A	0/272	-	-	-	-
1	14-A	0/272	-	-	-	-
1	15-A	0/272	-	-	-	-
1	16-A	0/272	-	-	-	-
All	All	260/4352 (5%)	2.99	183 (70%) 0 0	1, 2, 3, 4	260 (100%)

The worst 5 of 183 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	231	PRO	10.9
1	1-A	229	VAL	9.7
1	1-A	70	PHE	9.2
1	1-A	184	PHE	8.1
1	1-A	246	LEU	8.0

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.