



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 3, 2024 – 01:21 PM JST

PDB ID : 5WTJ
Title : Crystal structure of an endonuclease
Authors : Liu, L.; Wang, Y.
Deposited on : 2016-12-13
Resolution : 3.50 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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

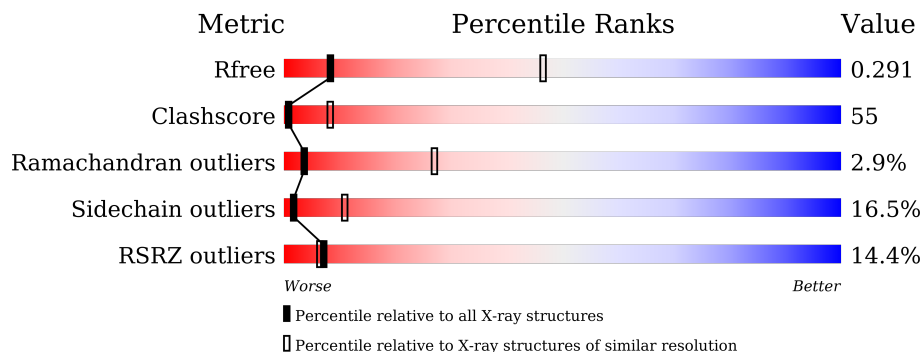
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1094 (3.56-3.44)
Clashscore	180529	1045 (3.54-3.46)
Ramachandran outliers	177936	1032 (3.54-3.46)
Sidechain outliers	177891	1033 (3.54-3.46)
RSRZ outliers	164620	1093 (3.56-3.44)

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	1397	<div> <div>7%</div> <div>30%</div> <div>33%</div> <div>9%</div> <div>•</div> <div>27%</div> </div>
1	B	1397	<div> <div>14%</div> <div>32%</div> <div>31%</div> <div>9%</div> <div>•</div> <div>28%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15952 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 CRISPR-associated endoribonuclease C2c2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1019	Total	C	N	O	S	Se	0	0	0
			8013	5109	1350	1538	5	11			
1	B	1012	Total	C	N	O	S	Se	0	0	0
			7938	5055	1326	1541	6	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1390	LEU	-	expression tag	UNP P0DOC6
A	1391	GLU	-	expression tag	UNP P0DOC6
A	1392	HIS	-	expression tag	UNP P0DOC6
A	1393	HIS	-	expression tag	UNP P0DOC6
A	1394	HIS	-	expression tag	UNP P0DOC6
A	1395	HIS	-	expression tag	UNP P0DOC6
A	1396	HIS	-	expression tag	UNP P0DOC6
A	1397	HIS	-	expression tag	UNP P0DOC6
B	1390	LEU	-	expression tag	UNP P0DOC6
B	1391	GLU	-	expression tag	UNP P0DOC6
B	1392	HIS	-	expression tag	UNP P0DOC6
B	1393	HIS	-	expression tag	UNP P0DOC6
B	1394	HIS	-	expression tag	UNP P0DOC6
B	1395	HIS	-	expression tag	UNP P0DOC6
B	1396	HIS	-	expression tag	UNP P0DOC6
B	1397	HIS	-	expression tag	UNP P0DOC6

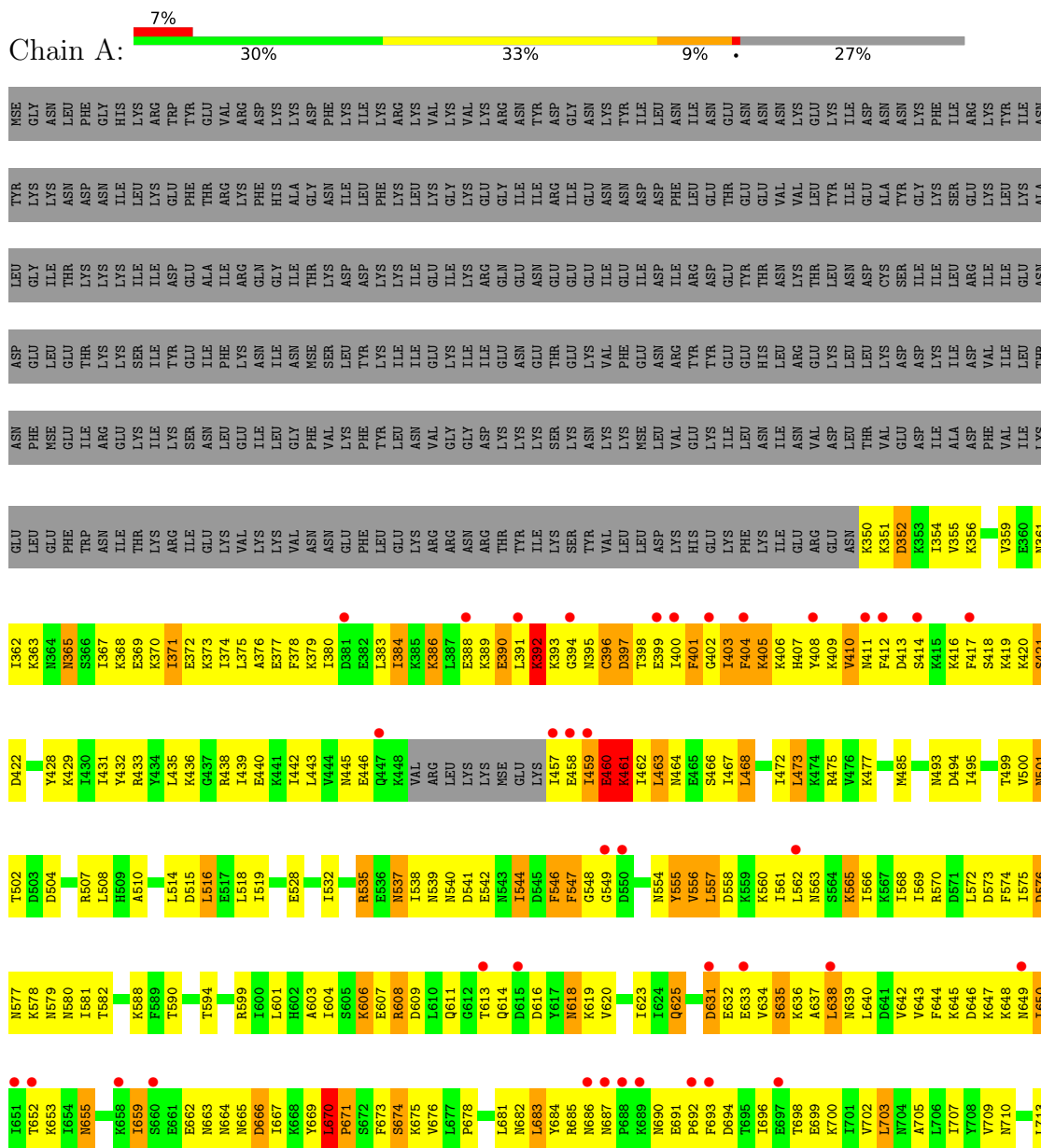
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		

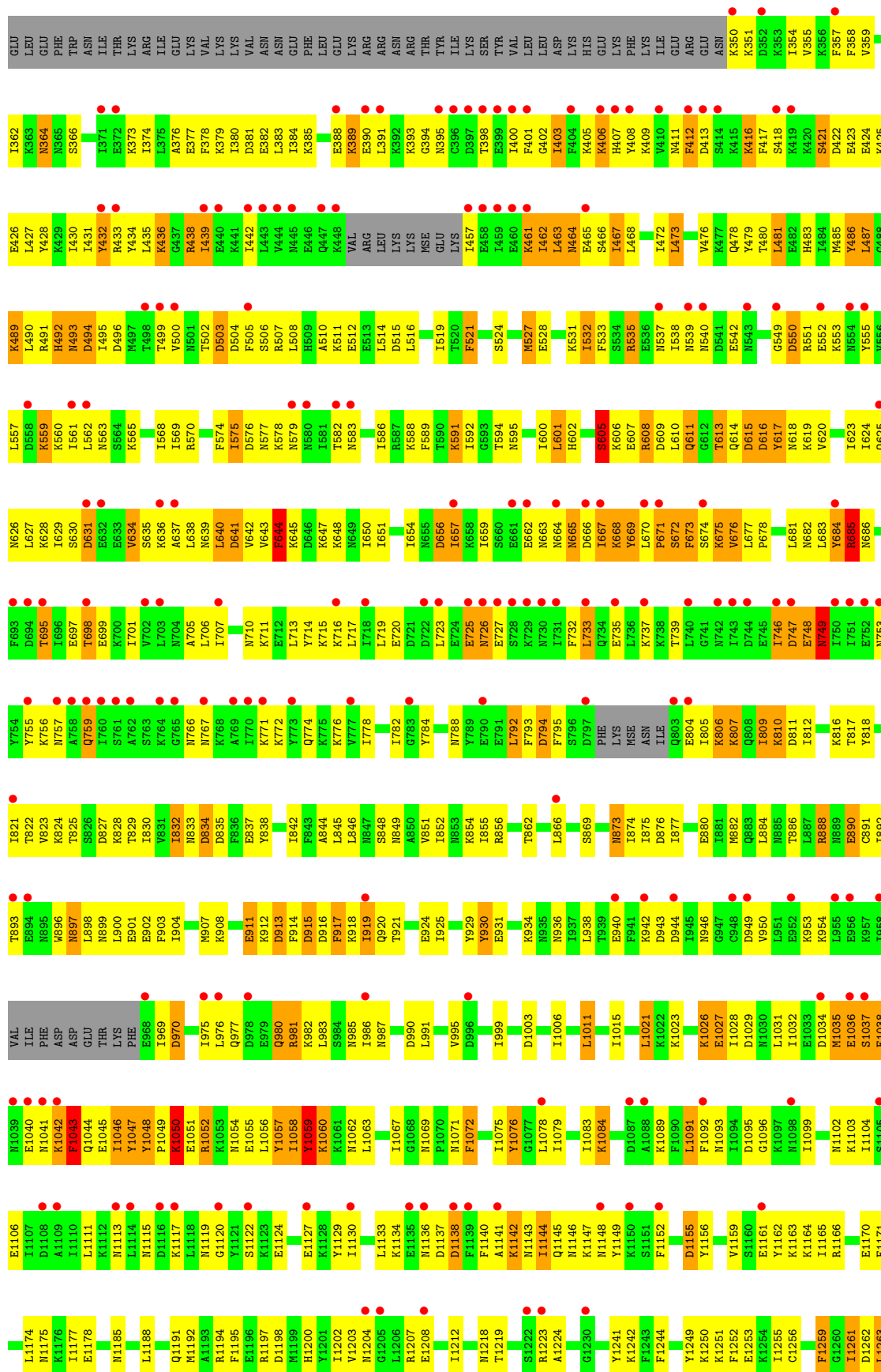
3 Residue-property plots

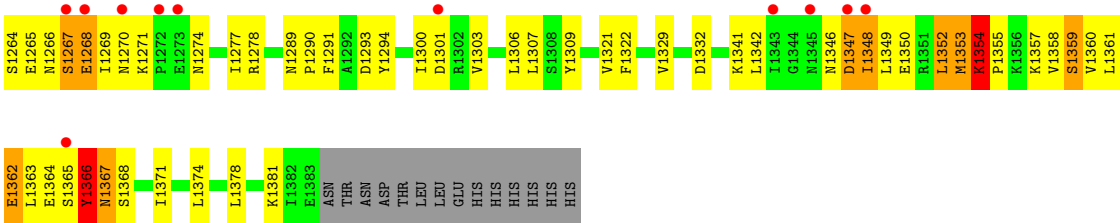
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CRISPR-associated endoribonuclease C2c2









4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.66Å 94.23Å 338.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.38 – 3.50 48.38 – 3.50	Depositor EDS
% Data completeness (in resolution range)	81.0 (48.38-3.50) 81.0 (48.38-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.71 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.263 , 0.291 0.263 , 0.291	Depositor DCC
R_{free} test set	1882 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.648	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.053 for k,h,-l	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	15952	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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	A	0.48	2/8117 (0.0%)	0.67	16/10925 (0.1%)
1	B	0.42	2/8038 (0.0%)	0.66	11/10824 (0.1%)
All	All	0.45	4/16155 (0.0%)	0.66	27/21749 (0.1%)

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	2
1	B	0	7
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	671	PRO	N-CD	5.24	1.55	1.47
1	B	1038	GLU	CB-CG	-5.17	1.42	1.52
1	A	1272	PRO	N-CD	5.09	1.54	1.47
1	B	671	PRO	N-CD	5.09	1.54	1.47

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	634	VAL	CB-CA-C	-11.15	90.21	111.40
1	A	997	GLN	CB-CA-C	6.94	124.28	110.40
1	B	1021	LEU	CB-CG-CD1	-6.59	99.80	111.00
1	B	403	ILE	CB-CA-C	-6.57	98.46	111.60
1	A	758	ALA	CB-CA-C	-6.33	100.60	110.10

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1051	GLU	Peptide
1	A	1356	LYS	Peptide
1	B	412	PHE	Peptide
1	B	605	SER	Peptide
1	B	644	PHE	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	A	8013	0	7662	834	3
1	B	7938	0	7580	876	1
2	A	1	0	0	0	0
All	All	15952	0	15242	1710	4

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 55.

The worst 5 of 1710 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:976:LEU:HD23	1:B:977:GLN:N	1.22	1.45
1:A:696:ILE:CB	1:A:699:GLU:HB3	1.55	1.35
1:B:817:THR:CG2	1:B:818:TYR:HA	1.54	1.35
1:B:914:PHE:HA	1:B:915:ASP:CB	1.47	1.34
1:B:914:PHE:CA	1:B:915:ASP:HB2	1.54	1.32

All (4) 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)
1:B:426:GLU:OE1	1:B:1037:SER:OG[4_446]	1.51	0.69
1:A:776:LYS:CB	1:A:1348:ILE:CD1[3_655]	1.91	0.29
1:A:398:THR:CB	1:A:907:MSE:CE[3_655]	2.08	0.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:LYS:CD	1:A:1348:ILE:CD1[3_655]	2.10	0.10

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	1013/1397 (72%)	908 (90%)	79 (8%)	26 (3%)	4	28
1	B	1004/1397 (72%)	888 (88%)	84 (8%)	32 (3%)	3	25
All	All	2017/2794 (72%)	1796 (89%)	163 (8%)	58 (3%)	3	27

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	392	LYS
1	A	410	VAL
1	A	458	GLU
1	A	460	GLU
1	A	461	LYS

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	824/1316 (63%)	681 (83%)	143 (17%)	1	9
1	B	822/1316 (62%)	693 (84%)	129 (16%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1646/2632 (62%)	1374 (84%)	272 (16%)	2 11

5 of 272 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	931	GLU
1	B	1027	GLU
1	B	1244	PHE
1	A	1026	LYS
1	A	1023	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	483	HIS
1	B	1175	ASN
1	B	539	ASN
1	B	1200	HIS
1	B	1062	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	1008/1397 (72%)	0.64	94 (9%) 16 12	2, 42, 106, 153	0
1	B	1002/1397 (71%)	1.18	195 (19%) 4 3	12, 67, 134, 199	0
All	All	2010/2794 (71%)	0.91	289 (14%) 7 6	2, 55, 128, 199	0

The worst 5 of 289 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	500	VAL	6.8
1	B	407	HIS	6.3
1	B	1345	ASN	6.2
1	B	726	ASN	6.0
1	B	396	CYS	5.9

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.