



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2016 – 06:03 PM EDT

PDB ID : 5DZR
Title : Structure of RNA Helicase FRH a Critical Component of the Neurospora
Crassa Circadian Clock
Authors : Conrad, K.S.; Crane, B.C.
Deposited on : 2015-09-26
Resolution : 3.16 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
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)	:	rb-20027939

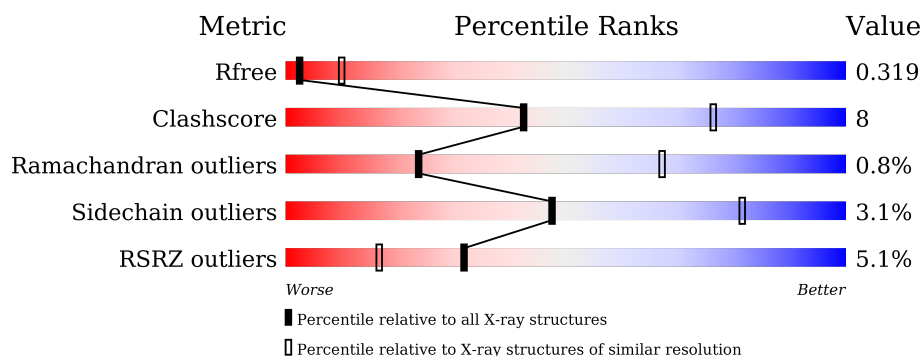
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.16 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	1112 (3.20-3.12)
Clashscore	102246	1249 (3.20-3.12)
Ramachandran outliers	100387	1222 (3.20-3.12)
Sidechain outliers	100360	1221 (3.20-3.12)
RSRZ outliers	91569	1117 (3.20-3.12)

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. 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	993	<div> <div>5%</div> <div>74%</div> <div>21%</div> <div>..</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7697 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.

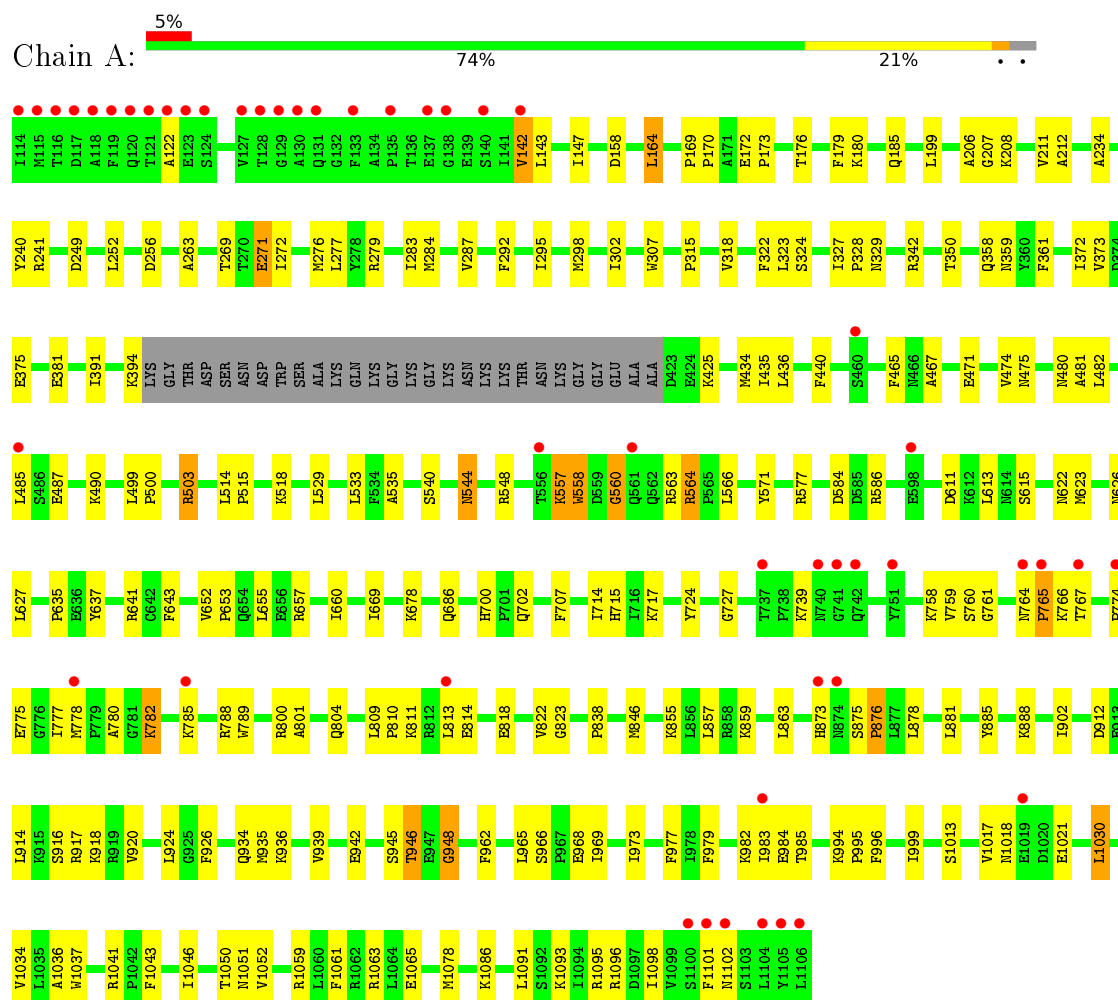
- Molecule 1 is a protein called FRQ-interacting RNA helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	965	7697	4905	1323	1427	42	0	0	0

3 Residue-property plots

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: FRQ-interacting RNA helicase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.80Å 107.75Å 125.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.83 – 3.16 81.83 – 3.16	Depositor EDS
% Data completeness (in resolution range)	96.7 (81.83-3.16) 81.6 (81.83-3.16)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.19Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.264 , 0.325 0.255 , 0.319	Depositor DCC
R_{free} test set	766 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	83.0	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 67.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7697	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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 [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	0.23	0/7844	0.43	3/10593 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	503	ARG	NE-CZ-NH1	-7.23	116.68	120.30
1	A	164	LEU	CA-CB-CG	6.55	130.36	115.30
1	A	948	GLY	N-CA-C	-5.76	98.69	113.10

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	7697	0	7781	129	0
All	All	7697	0	7781	129	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 8.

All (129) 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:A:717:LYS:HB3	1:A:800:ARG:HG3	1.64	0.77
1:A:564:ARG:HH11	1:A:564:ARG:HG2	1.50	0.75
1:A:372:ILE:HG22	1:A:373:VAL:HG23	1.73	0.70
1:A:983:ILE:HG12	1:A:1052:VAL:HG22	1.75	0.68
1:A:199:LEU:HA	1:A:322:PHE:HB2	1.78	0.66
1:A:241:ARG:NH2	1:A:1102:ASN:O	2.29	0.65
1:A:1065:GLU:OE2	1:A:1095:ARG:NH1	2.30	0.65
1:A:295:ILE:HG12	1:A:324:SER:HB2	1.82	0.62
1:A:474:VAL:HG21	1:A:503:ARG:HA	1.80	0.62
1:A:212:ALA:HB2	1:A:323:LEU:HD11	1.82	0.62
1:A:1036:ALA:HB1	1:A:1041:ARG:HD3	1.82	0.61
1:A:946:THR:HG21	1:A:977:PHE:HB3	1.83	0.60
1:A:966:SER:HB2	1:A:969:ILE:HD13	1.82	0.60
1:A:968:GLU:OE2	1:A:1093:LYS:NZ	2.35	0.59
1:A:916:SER:OG	1:A:1013:SER:O	2.19	0.59
1:A:939:VAL:HG11	1:A:1078:MET:HG3	1.85	0.59
1:A:627:LEU:HD13	1:A:635:PRO:HA	1.84	0.59
1:A:724:TYR:CD2	1:A:759:VAL:HG11	2.38	0.58
1:A:945:SER:O	1:A:1063:ARG:NH2	2.36	0.57
1:A:147:ILE:HA	1:A:350:THR:HG22	1.87	0.57
1:A:435:ILE:HB	1:A:440:PHE:HB2	1.85	0.57
1:A:295:ILE:HD13	1:A:322:PHE:HB3	1.87	0.57
1:A:764:ASN:O	1:A:766:LYS:N	2.37	0.57
1:A:724:TYR:HD2	1:A:759:VAL:HG11	1.69	0.56
1:A:715:HIS:HB3	1:A:801:ALA:HB3	1.87	0.56
1:A:540:SER:O	1:A:577:ARG:NH2	2.38	0.56
1:A:1065:GLU:HG3	1:A:1091:LEU:HD11	1.88	0.55
1:A:778:MET:O	1:A:780:ALA:N	2.39	0.55
1:A:302:ILE:HG12	1:A:558:TRP:HH2	1.71	0.55
1:A:611:ASP:N	1:A:611:ASP:OD1	2.38	0.55
1:A:813:LEU:HD21	1:A:822:VAL:HG21	1.89	0.54
1:A:279:ARG:NH1	1:A:942:GLU:OE2	2.40	0.54
1:A:804:GLN:HB2	1:A:838:PRO:HB2	1.89	0.54
1:A:240:TYR:CG	1:A:252:LEU:HD23	2.43	0.54
1:A:358:GLN:NE2	1:A:375:GLU:OE2	2.41	0.54
1:A:809:LEU:HD12	1:A:810:PRO:HD2	1.91	0.53
1:A:548:ARG:NE	1:A:584:ASP:OD1	2.37	0.53
1:A:878:LEU:HD13	1:A:881:LEU:HD12	1.91	0.53
1:A:934:GLN:HG3	1:A:935:MET:H	1.73	0.52
1:A:474:VAL:HG12	1:A:529:LEU:HB3	1.89	0.52
1:A:717:LYS:HD2	1:A:800:ARG:HE	1.74	0.52
1:A:760:SER:O	1:A:777:ILE:N	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:LEU:HD23	1:A:1098:ILE:HD11	1.92	0.52
1:A:315:PRO:HB2	1:A:318:VAL:HG23	1.92	0.52
1:A:482:LEU:HD11	1:A:490:LYS:HD2	1.91	0.52
1:A:298:MET:HG3	1:A:307:TRP:HB2	1.92	0.51
1:A:789:TRP:CD1	1:A:823:GLY:HA3	2.45	0.51
1:A:185:GLN:NE2	1:A:206:ALA:O	2.44	0.50
1:A:760:SER:OG	1:A:761:GLY:N	2.42	0.50
1:A:302:ILE:HG12	1:A:558:TRP:CH2	2.47	0.50
1:A:985:THR:HB	1:A:1050:THR:HG22	1.93	0.49
1:A:358:GLN:OE1	1:A:586:ARG:NH1	2.44	0.49
1:A:669:ILE:O	1:A:888:LYS:NZ	2.45	0.49
1:A:515:PRO:HA	1:A:518:LYS:HG2	1.95	0.49
1:A:914:LEU:HG	1:A:918:LYS:HE2	1.95	0.48
1:A:185:GLN:NE2	1:A:207:GLY:O	2.47	0.48
1:A:487:GLU:HG2	1:A:490:LYS:HE2	1.96	0.48
1:A:707:PHE:CZ	1:A:846:MET:HA	2.49	0.48
1:A:361:PHE:HB2	1:A:372:ILE:HD13	1.96	0.48
1:A:1037:TRP:CH2	1:A:1096:ARG:HD2	2.49	0.48
1:A:234:ALA:HB2	1:A:1059:ARG:HH21	1.78	0.47
1:A:1043:PHE:HA	1:A:1046:ILE:HD12	1.96	0.47
1:A:515:PRO:HB2	1:A:1101:PHE:CE1	2.50	0.47
1:A:269:THR:HG22	1:A:271:GLU:H	1.80	0.47
1:A:962:PHE:O	1:A:1086:LYS:NZ	2.46	0.47
1:A:924:LEU:HD23	1:A:926:PHE:HE1	1.79	0.47
1:A:637:TYR:CZ	1:A:641:ARG:HD2	2.50	0.46
1:A:342:ARG:HH12	1:A:641:ARG:HH11	1.62	0.46
1:A:1030:LEU:HD21	1:A:1061:PHE:HE1	1.81	0.46
1:A:240:TYR:CD2	1:A:252:LEU:HD23	2.51	0.46
1:A:1018:ASN:HB2	1:A:1021:GLU:HG3	1.98	0.46
1:A:994:LYS:HB3	1:A:995:PRO:HD3	1.98	0.46
1:A:564:ARG:NH1	1:A:564:ARG:HG2	2.24	0.45
1:A:249:ASP:O	1:A:263:ALA:HB1	2.17	0.45
1:A:269:THR:HB	1:A:272:ILE:HG12	1.99	0.45
1:A:544:ASN:ND2	1:A:544:ASN:O	2.50	0.45
1:A:678:LYS:HG2	1:A:885:TYR:HE2	1.82	0.45
1:A:359:ASN:OD1	1:A:571:TYR:OH	2.33	0.44
1:A:558:TRP:CZ2	1:A:560:GLY:HA3	2.52	0.44
1:A:652:VAL:HG13	1:A:653:PRO:HD3	2.00	0.44
1:A:814:GLU:N	1:A:818:GLU:OE2	2.46	0.44
1:A:283:ILE:O	1:A:287:VAL:HG23	2.17	0.44
1:A:292:PHE:HB3	1:A:307:TRP:HZ3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:ALA:O	1:A:471:GLU:N	2.50	0.44
1:A:329:ASN:HD21	1:A:613:LEU:HB3	1.81	0.44
1:A:857:LEU:HD12	1:A:857:LEU:HA	1.85	0.44
1:A:142:VAL:HA	1:A:143:LEU:HA	1.75	0.44
1:A:499:LEU:HB3	1:A:500:PRO:HD3	2.01	0.43
1:A:637:TYR:O	1:A:641:ARG:HG3	2.18	0.43
1:A:984:GLU:HB2	1:A:1051:ASN:ND2	2.33	0.43
1:A:615:SER:HB2	1:A:643:PHE:HD2	1.83	0.43
1:A:962:PHE:HA	1:A:965:LEU:HD12	2.00	0.43
1:A:657:ARG:HA	1:A:660:ILE:HG12	2.01	0.43
1:A:917:ARG:O	1:A:920:VAL:HG22	2.19	0.43
1:A:700:HIS:HD2	1:A:702:GLN:HB2	1.84	0.43
1:A:622:ASN:OD1	1:A:626:ASN:ND2	2.52	0.43
1:A:342:ARG:HH12	1:A:641:ARG:NH1	2.17	0.43
1:A:984:GLU:HB2	1:A:1051:ASN:HD21	1.82	0.43
1:A:208:LYS:O	1:A:211:VAL:HG12	2.19	0.43
1:A:487:GLU:O	1:A:490:LYS:HG2	2.19	0.42
1:A:436:LEU:HD22	1:A:465:PHE:CE1	2.54	0.42
1:A:875:SER:HA	1:A:876:PRO:HD3	1.89	0.42
1:A:965:LEU:HD13	1:A:973:ILE:HD12	2.01	0.42
1:A:855:LYS:O	1:A:859:LYS:HG2	2.20	0.42
1:A:515:PRO:HA	1:A:518:LYS:HE3	2.01	0.42
1:A:758:LYS:HA	1:A:788:ARG:O	2.19	0.42
1:A:533:LEU:HD22	1:A:535:ALA:HB2	2.02	0.41
1:A:765:PRO:HG2	1:A:774:PRO:HB3	2.02	0.41
1:A:480:ASN:OD1	1:A:481:ALA:N	2.53	0.41
1:A:1030:LEU:O	1:A:1034:VAL:HG12	2.20	0.41
1:A:686:GLN:HB3	1:A:863:LEU:HD21	2.02	0.41
1:A:778:MET:HB3	1:A:778:MET:HE2	1.88	0.41
1:A:176:THR:O	1:A:179:PHE:HB2	2.21	0.41
1:A:394:LYS:HA	1:A:394:LYS:HD3	1.81	0.41
1:A:936:LYS:O	1:A:939:VAL:HG22	2.21	0.41
1:A:172:GLU:HA	1:A:173:PRO:HD3	1.84	0.41
1:A:342:ARG:HH22	1:A:641:ARG:HH12	1.68	0.41
1:A:655:LEU:HD23	1:A:902:ILE:HG12	2.02	0.41
1:A:996:PHE:O	1:A:999:ILE:HG13	2.21	0.41
1:A:499:LEU:O	1:A:503:ARG:HG3	2.21	0.41
1:A:514:LEU:HA	1:A:515:PRO:HD3	1.96	0.41
1:A:169:PRO:HA	1:A:170:PRO:HD3	1.99	0.40
1:A:557:LYS:HE3	1:A:564:ARG:HD2	2.04	0.40
1:A:158:ASP:N	1:A:158:ASP:OD1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:HD23	1:A:284:MET:HG3	2.03	0.40
1:A:327:ILE:HA	1:A:328:PRO:HD3	1.91	0.40
1:A:782:LYS:HG2	1:A:785:LYS:HB2	2.03	0.40
1:A:272:ILE:O	1:A:276:MET:HG3	2.22	0.40
1:A:714:ILE:O	1:A:727:GLY:N	2.55	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	961/993 (97%)	911 (95%)	42 (4%)	8 (1%)	24 67

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	765	PRO
1	A	142	VAL
1	A	560	GLY
1	A	876	PRO
1	A	739	LYS
1	A	948	GLY
1	A	122	ALA
1	A	775	GLU

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	843/867 (97%)	817 (97%)	26 (3%)	47 81

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	LEU
1	A	180	LYS
1	A	256	ASP
1	A	271	GLU
1	A	381	GLU
1	A	391	ILE
1	A	425	LYS
1	A	434	MET
1	A	475	ASN
1	A	544	ASN
1	A	557	LYS
1	A	558	TRP
1	A	563	ARG
1	A	564	ARG
1	A	566	LEU
1	A	623	MET
1	A	767	THR
1	A	782	LYS
1	A	811	LYS
1	A	873	HIS
1	A	912	ASP
1	A	946	THR
1	A	979	PHE
1	A	982	LYS
1	A	1017	VAL
1	A	1030	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	475	ASN

5.3.3 RNA ⓘ

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](#)

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

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	965/993 (97%)	0.39	49 (5%) 32 17	53, 88, 135, 166	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	GLY	8.0
1	A	121	THR	7.7
1	A	115	MET	7.1
1	A	122	ALA	6.9
1	A	119	PHE	6.7
1	A	114	ILE	6.0
1	A	130	ALA	5.7
1	A	124	SER	5.5
1	A	1104	LEU	5.0
1	A	1100	SER	4.5
1	A	118	ALA	4.4
1	A	874	ASN	4.4
1	A	128	THR	4.2
1	A	1101	PHE	4.0
1	A	127	VAL	3.8
1	A	135	PRO	3.6
1	A	123	GLU	3.6
1	A	983	ILE	3.6
1	A	785	LYS	3.4
1	A	873	HIS	3.4
1	A	1105	TYR	3.4
1	A	117	ASP	3.3
1	A	561	GLN	3.3
1	A	774	PRO	3.3
1	A	1106	LEU	3.3
1	A	120	GLN	3.2
1	A	140	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	116	THR	3.1
1	A	131	GLN	2.9
1	A	741	GLY	2.9
1	A	765	PRO	2.9
1	A	133	PHE	2.6
1	A	142	VAL	2.6
1	A	1102	ASN	2.5
1	A	460	SER	2.5
1	A	764	ASN	2.5
1	A	485	LEU	2.5
1	A	556	THR	2.4
1	A	1019	GLU	2.4
1	A	813	LEU	2.3
1	A	767	THR	2.3
1	A	138	GLY	2.3
1	A	737	THR	2.3
1	A	751	TYR	2.2
1	A	742	GLN	2.2
1	A	778	MET	2.2
1	A	598	GLU	2.1
1	A	740	ASN	2.0
1	A	137	GLU	2.0

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 carbohydrates 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.