



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 02:35 PM EDT

PDB ID : 6UV0  
Title : Crystal structure of apo core domain of RNA helicase DDX17  
Authors : Ngo, T.D.; Partin, A.C.; Nam, Y.  
Deposited on : 2019-11-01  
Resolution : 2.60 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)

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<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>.

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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
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

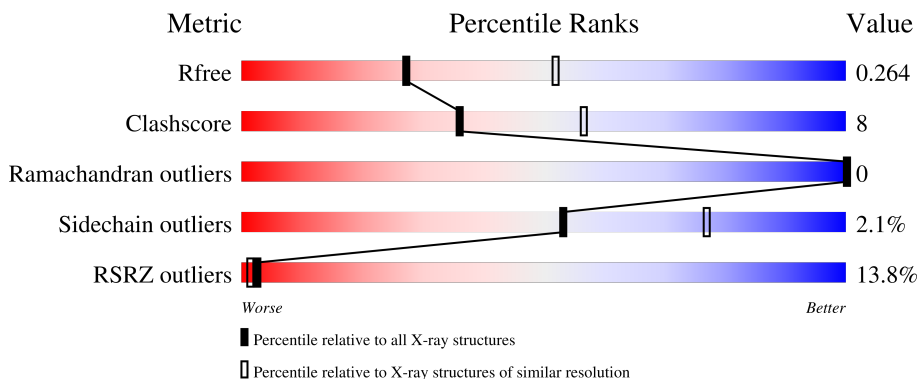
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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  $\geq 3$ , 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	448	
1	B	448	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6761 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 Probable ATP-dependent RNA helicase DDX17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3401	2150	598	631	22			
1	B	405	Total	C	N	O	S	0	0	0
			3261	2065	576	599	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	SER	-	expression tag	UNP Q92841
A	31	GLY	-	expression tag	UNP Q92841
B	30	SER	-	expression tag	UNP Q92841
B	31	GLY	-	expression tag	UNP Q92841

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

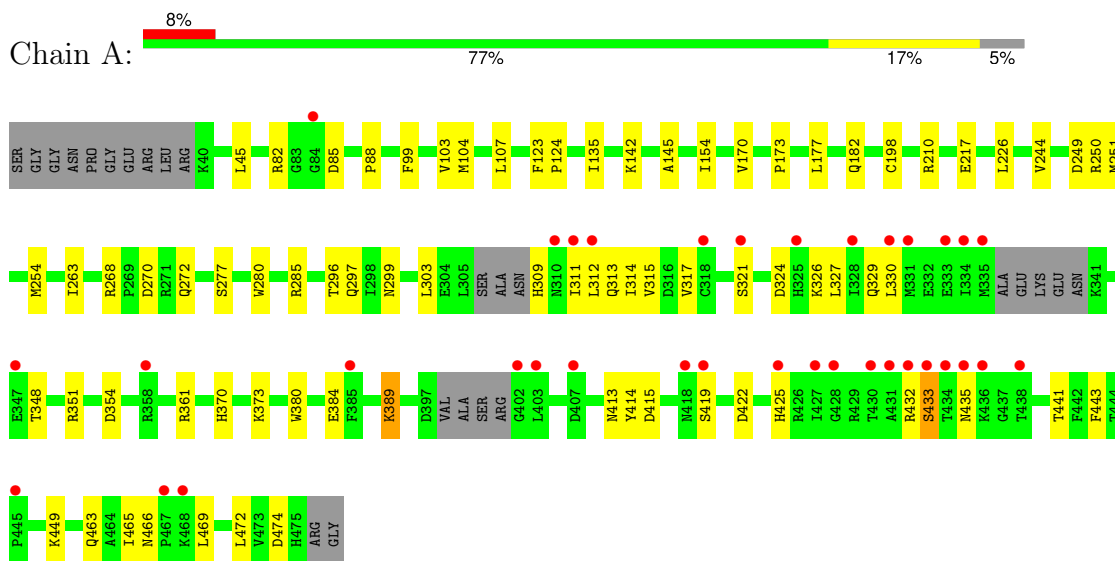
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total	O	0	0
			51	51		
3	B	47	Total	O	0	0
			47	47		

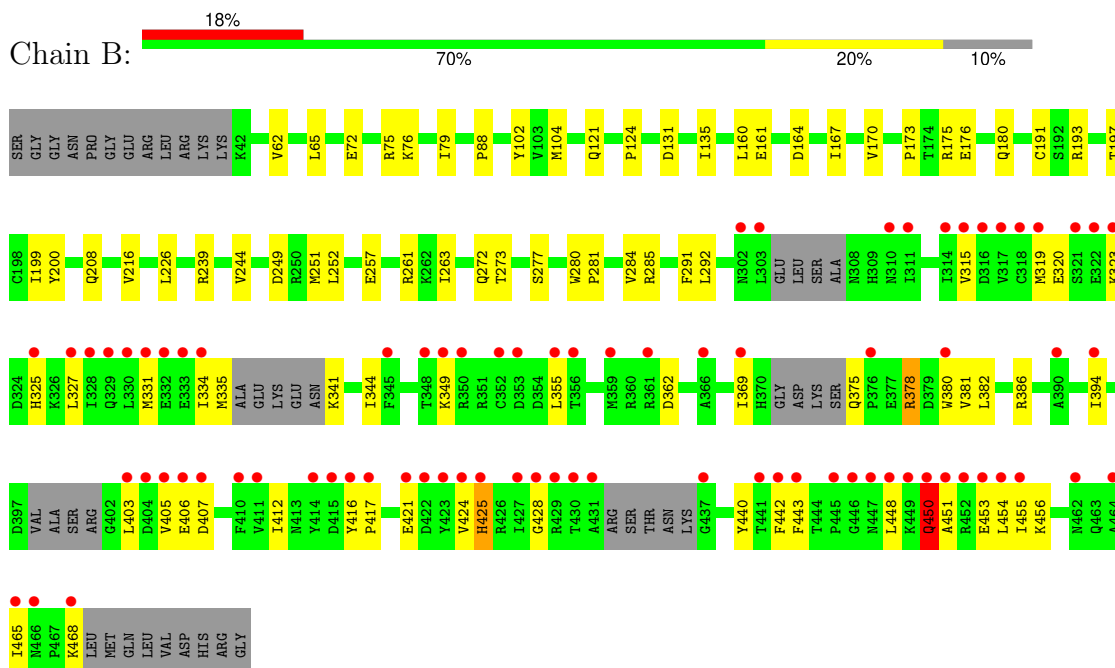
### 3 Residue-property plots

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: Probable ATP-dependent RNA helicase DDX17



- Molecule 1: Probable ATP-dependent RNA helicase DDX17



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.65Å 97.81Å 154.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 2.60 48.91 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.91-2.60) 99.4 (48.91-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.66 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.213 , 0.260 0.218 , 0.264	Depositor DCC
$R_{free}$ test set	1998 reflections (6.22%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.2	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 57.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6761	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MG

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	0.25	0/3471	0.43	0/4696
1	B	0.26	0/3328	0.45	0/4500
All	All	0.25	0/6799	0.44	0/9196

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	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	425	HIS	Peptide
1	B	450	GLN	Peptide

### 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	3401	0	3374	43	1
1	B	3261	0	3243	63	1
2	A	1	0	0	0	0
3	A	51	0	0	6	0
3	B	47	0	0	3	0
All	All	6761	0	6617	106	1

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 (106) 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:320:GLU:O	1:B:323:LYS:HB2	1.72	0.87
1:A:474:ASP:OD1	3:A:901:HOH:O	1.94	0.84
1:B:320:GLU:O	1:B:323:LYS:CB	2.27	0.81
1:B:315:VAL:HG11	1:B:454:LEU:HD11	1.63	0.81
1:B:424:VAL:HG13	1:B:425:HIS:HD2	1.46	0.80
1:A:272:GLN:OE1	3:A:902:HOH:O	2.06	0.74
1:A:419:SER:HG	1:A:422:ASP:H	1.37	0.72
1:B:450:GLN:HG2	1:B:453:GLU:HG3	1.72	0.71
1:B:272:GLN:OE1	3:B:501:HOH:O	2.10	0.70
1:B:382:LEU:HD13	1:B:403:LEU:HG	1.75	0.68
1:B:175:ARG:NH1	1:B:176:GLU:OE2	2.28	0.67
1:B:425:HIS:HA	1:B:428:GLY:H	1.60	0.66
1:A:351:ARG:HA	1:A:354:ASP:HB2	1.78	0.66
1:B:443:PHE:HE2	1:B:451:ALA:HB2	1.60	0.65
1:A:315:VAL:O	1:A:466:ASN:ND2	2.30	0.65
1:B:197:THR:HB	1:B:216:VAL:HG11	1.78	0.64
1:B:104:MET:SD	3:B:537:HOH:O	2.55	0.64
1:B:180:GLN:OE1	3:B:502:HOH:O	2.15	0.64
1:A:469:LEU:HA	1:A:472:LEU:HD12	1.81	0.62
1:A:182:GLN:HG3	1:A:198:CYS:HB2	1.82	0.61
1:B:443:PHE:CE2	1:B:451:ALA:HB2	2.35	0.61
1:A:422:ASP:HA	1:A:425:HIS:CE1	2.36	0.61
1:B:102:TYR:HB2	1:B:191:CYS:HB3	1.83	0.61
1:A:154:ILE:HD13	1:A:217:GLU:HB3	1.83	0.60
1:A:297:GLN:NE2	1:A:299:ASN:OD1	2.35	0.60
1:A:173:PRO:HB3	1:A:251:MET:HG2	1.86	0.58
1:B:72:GLU:OE1	1:B:75:ARG:NH2	2.37	0.58
1:B:320:GLU:O	1:B:323:LYS:HB3	2.03	0.57
1:B:193:ARG:O	1:B:193:ARG:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:ILE:HG13	1:B:440:TYR:HB2	1.87	0.56
1:A:327:LEU:HD22	1:A:414:TYR:CD1	2.40	0.56
1:B:405:VAL:HG12	1:B:406:GLU:H	1.70	0.56
1:B:344:ILE:HA	1:B:412:ILE:O	2.05	0.55
1:A:326:LYS:O	1:A:329:GLN:HB2	2.06	0.55
1:A:312:LEU:HG	1:A:314:ILE:HG12	1.88	0.55
1:B:273:THR:HB	1:B:292:LEU:HD23	1.89	0.55
1:B:79:ILE:HD13	1:B:121:GLN:HB2	1.90	0.53
1:A:413:ASN:HB2	1:A:441:THR:HG22	1.90	0.53
1:B:175:ARG:HG3	1:B:200:TYR:CD1	2.44	0.53
1:B:424:VAL:HG13	1:B:425:HIS:CD2	2.36	0.53
1:A:433:SER:O	1:A:435:ASN:ND2	2.42	0.52
1:B:421:GLU:HA	1:B:424:VAL:HG12	1.90	0.52
1:B:261:ARG:HG2	1:B:291:PHE:HZ	1.75	0.52
1:B:280:TRP:CE2	1:B:285:ARG:HG2	2.45	0.52
1:B:355:LEU:HD12	1:B:394:ILE:HD13	1.91	0.51
1:B:448:LEU:HG	1:B:451:ALA:HB3	1.91	0.51
1:A:303:LEU:HD12	1:A:432:ARG:HG3	1.92	0.51
1:B:453:GLU:HA	1:B:456:LYS:HE3	1.92	0.51
1:A:311:ILE:HA	3:A:916:HOH:O	2.09	0.51
1:A:413:ASN:HD22	1:A:441:THR:HG22	1.76	0.51
1:A:226:LEU:HD23	1:A:263:ILE:HD13	1.93	0.50
1:A:173:PRO:HD2	1:A:177:LEU:HD23	1.94	0.50
1:A:142:LYS:NZ	3:A:911:HOH:O	2.41	0.49
1:A:380:TRP:O	1:A:384:GLU:HG2	2.13	0.49
1:B:455:ILE:HG23	1:B:465:ILE:HD13	1.95	0.49
1:A:370:HIS:CE1	1:A:373:LYS:HG3	2.48	0.48
1:B:135:ILE:HA	1:B:277:SER:O	2.13	0.48
1:B:199:ILE:HG22	1:B:208:GLN:HB3	1.95	0.48
1:A:210:ARG:NH1	3:A:905:HOH:O	2.29	0.48
1:B:327:LEU:HB3	1:B:331:MET:HE3	1.96	0.48
1:A:280:TRP:CE2	1:A:285:ARG:HG2	2.49	0.48
1:B:167:ILE:HG12	1:B:239:ARG:HG3	1.95	0.48
1:B:160:LEU:HD22	1:B:164:ASP:HB3	1.95	0.48
1:B:315:VAL:HG21	1:B:454:LEU:HD21	1.96	0.48
1:A:45:LEU:HD13	1:A:270:ASP:HB3	1.96	0.47
1:B:451:ALA:O	1:B:455:ILE:HD12	2.15	0.47
1:B:281:PRO:O	1:B:285:ARG:HG3	2.15	0.47
1:B:323:LYS:HE2	1:B:442:PHE:CG	2.49	0.47
1:A:99:PHE:HB2	1:A:104:MET:HG2	1.97	0.47
1:B:88:PRO:HG2	1:B:124:PRO:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:VAL:HG22	1:B:244:VAL:HB	1.98	0.46
1:A:317:VAL:HA	1:A:443:PHE:O	2.15	0.46
1:A:249:ASP:N	1:A:249:ASP:OD1	2.49	0.45
1:A:313:GLN:HB2	1:A:463:GLN:HG3	1.98	0.45
1:B:252:LEU:HD22	1:B:257:GLU:HB2	2.00	0.44
1:B:323:LYS:HE2	1:B:442:PHE:CB	2.48	0.44
1:B:173:PRO:HG3	1:B:251:MET:HG3	1.99	0.44
1:B:341:LYS:NZ	1:B:386:ARG:HA	2.33	0.44
1:A:85:ASP:HB3	1:A:296:THR:HG22	1.98	0.44
1:B:281:PRO:HD2	1:B:284:VAL:HB	1.99	0.44
1:B:369:ILE:HD13	1:B:381:VAL:HG21	2.00	0.44
1:A:88:PRO:HG2	1:A:124:PRO:HB2	2.00	0.44
1:B:72:GLU:CD	1:B:75:ARG:HH22	2.21	0.44
1:B:421:GLU:O	1:B:424:VAL:HG12	2.18	0.44
1:B:375:GLN:HA	1:B:378:ARG:HB3	2.00	0.43
1:B:226:LEU:HD23	1:B:263:ILE:HD13	2.00	0.43
1:A:170:VAL:HG22	1:A:244:VAL:HB	2.00	0.43
1:A:135:ILE:HA	1:A:277:SER:O	2.19	0.43
1:A:348:THR:OG1	1:A:351:ARG:N	2.52	0.43
1:B:76:LYS:HB2	1:B:76:LYS:HE2	1.73	0.43
1:A:82:ARG:NH2	3:A:914:HOH:O	2.48	0.42
1:B:161:GLU:N	1:B:164:ASP:OD2	2.32	0.42
1:B:344:ILE:HD12	1:B:394:ILE:HG12	2.00	0.42
1:B:249:ASP:N	1:B:249:ASP:OD1	2.49	0.42
1:A:465:ILE:HG23	1:A:469:LEU:HD23	2.00	0.42
1:B:349:LYS:HB2	1:B:349:LYS:HE2	1.81	0.42
1:B:131:ASP:HA	1:B:273:THR:O	2.19	0.41
1:B:416:TYR:CD1	1:B:417:PRO:HD2	2.56	0.41
1:A:123:PHE:CE1	1:A:145:ALA:HA	2.55	0.41
1:A:330:LEU:HA	1:A:330:LEU:HD23	1.79	0.41
1:B:334:ILE:O	1:B:335:MET:HG2	2.21	0.41
1:B:468:LYS:HE2	1:B:468:LYS:HB2	1.74	0.41
1:A:103:VAL:O	1:A:107:LEU:HB2	2.22	0.40
1:A:250:ARG:O	1:A:254:MET:HG3	2.21	0.40
1:A:268:ARG:NH2	1:A:270:ASP:OD2	2.46	0.40
1:B:62:VAL:HA	1:B:65:LEU:HD12	2.03	0.40

All (1) 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:A:389:LYS:NZ	1:B:406:GLU:OE1[3_554]	2.11	0.09

## 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	416/448 (93%)	400 (96%)	16 (4%)	0	100	100
1	B	393/448 (88%)	375 (95%)	18 (5%)	0	100	100
All	All	809/896 (90%)	775 (96%)	34 (4%)	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	372/393 (95%)	364 (98%)	8 (2%)	52	76
1	B	356/393 (91%)	349 (98%)	7 (2%)	55	78
All	All	728/786 (93%)	713 (98%)	15 (2%)	53	77

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	309	HIS
1	A	321	SER
1	A	324	ASP

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Mol	Chain	Res	Type
1	A	361	ARG
1	A	389	LYS
1	A	415	ASP
1	A	433	SER
1	A	449	LYS
1	B	319	MET
1	B	325	HIS
1	B	362	ASP
1	B	378	ARG
1	B	380	TRP
1	B	407	ASP
1	B	450	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	GLN
1	A	299	ASN
1	A	310	ASN
1	B	310	ASN
1	B	418	ASN
1	B	425	HIS

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 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	424/448 (94%)	0.43	35 (8%) <b>11</b> <b>8</b>	26, 58, 113, 150	0
1	B	405/448 (90%)	0.97	79 (19%) <b>1</b> <b>0</b>	28, 63, 140, 179	0
All	All	829/896 (92%)	0.69	114 (13%) <b>2</b> <b>1</b>	26, 60, 132, 179	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	449	LYS	10.7
1	B	448	LEU	9.5
1	B	315	VAL	8.6
1	B	352	CYS	8.3
1	B	452	ARG	8.3
1	B	442	PHE	8.1
1	B	445	PRO	7.7
1	B	424	VAL	7.4
1	B	431	ALA	6.6
1	B	450	GLN	6.0
1	A	431	ALA	5.9
1	A	318	CYS	5.9
1	A	428	GLY	5.8
1	B	428	GLY	5.7
1	B	348	THR	5.7
1	B	451	ALA	5.4
1	B	318	CYS	5.3
1	B	403	LEU	5.2
1	B	465	ILE	5.1
1	B	359	MET	5.0
1	B	349	LYS	4.9
1	B	446	GLY	4.8
1	A	402	GLY	4.7
1	B	330	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	345	PHE	4.6
1	A	434	THR	4.6
1	A	432	ARG	4.5
1	B	410	PHE	4.5
1	B	414	TYR	4.5
1	B	356	THR	4.4
1	B	328	ILE	4.4
1	B	466	ASN	4.4
1	B	437	GLY	4.2
1	B	443	PHE	4.2
1	B	429	ARG	4.2
1	B	441	THR	4.1
1	B	430	THR	4.1
1	A	311	ILE	4.1
1	B	353	ASP	4.0
1	A	330	LEU	3.9
1	B	355	LEU	3.9
1	A	335	MET	3.6
1	B	454	LEU	3.6
1	A	321	SER	3.5
1	B	415	ASP	3.5
1	B	311	ILE	3.5
1	B	350	ARG	3.4
1	B	394	ILE	3.4
1	B	468	LYS	3.4
1	A	433	SER	3.4
1	B	319	MET	3.4
1	B	464	ALA	3.3
1	B	317	VAL	3.3
1	B	455	ILE	3.3
1	B	331	MET	3.3
1	B	406	GLU	3.3
1	B	421	GLU	3.2
1	B	303	LEU	3.1
1	B	404	ASP	3.1
1	B	447	ASN	3.1
1	B	390	ALA	3.1
1	B	316	ASP	3.1
1	A	418	ASN	3.1
1	A	430	THR	3.0
1	B	425	HIS	3.0
1	B	405	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	323	LYS	2.9
1	B	416	TYR	2.9
1	B	417	PRO	2.9
1	B	329	GLN	2.8
1	B	427	ILE	2.8
1	A	435	ASN	2.7
1	B	333	GLU	2.7
1	A	385	PHE	2.7
1	A	445	PRO	2.7
1	A	438	THR	2.6
1	B	321	SER	2.6
1	B	361	ARG	2.6
1	B	422	ASP	2.6
1	B	366	ALA	2.6
1	B	411	VAL	2.5
1	B	302	ASN	2.5
1	A	427	ILE	2.5
1	B	327	LEU	2.5
1	A	419	SER	2.5
1	B	380	TRP	2.5
1	A	467	PRO	2.4
1	B	334	ILE	2.4
1	B	369	ILE	2.4
1	A	403	LEU	2.4
1	A	84	GLY	2.4
1	A	468	LYS	2.4
1	A	325	HIS	2.4
1	A	334	ILE	2.3
1	A	407	ASP	2.3
1	B	332	GLU	2.3
1	A	331	MET	2.3
1	A	333	GLU	2.2
1	B	423	TYR	2.2
1	B	322	GLU	2.2
1	A	436	LYS	2.2
1	A	312	LEU	2.2
1	A	310	ASN	2.2
1	B	407	ASP	2.2
1	B	314	ILE	2.2
1	B	453	GLU	2.2
1	A	425	HIS	2.1
1	A	358	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	310	ASN	2.1
1	A	328	ILE	2.1
1	A	347	GLU	2.1
1	B	325	HIS	2.0
1	B	462	ASN	2.0
1	B	376	PRO	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 monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	A	800	1/1	0.98	0.25	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.