



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 04:20 PM EDT

PDB ID : 2HBJ  
Title : Structure of the yeast nuclear exosome component, Rrp6p, reveals an interplay between the active site and the HRDC domain  
Authors : Midtgaard, S.F.; Assenholt, J.; Jonstrup, A.T.; Van, L.B.; Jensen, T.H.; Brodersen, D.E.  
Deposited on : unknown  
Resolution : 2.10 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)

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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

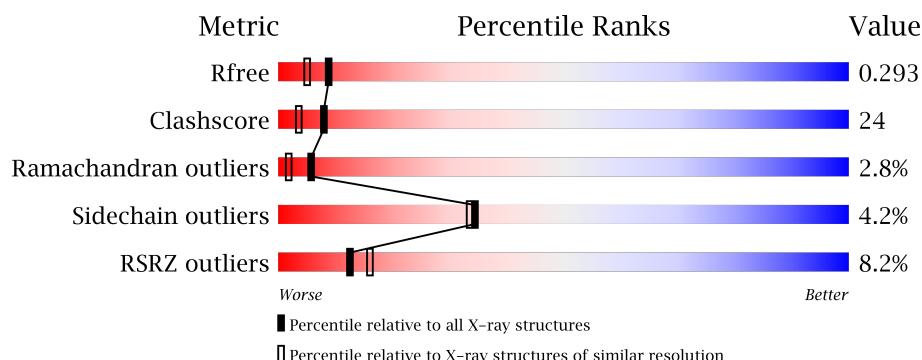
# 1 Overall quality at a glance

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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	410	<div> <div>8%</div> <div>60%</div> <div>30%</div> <div>5%</div> <div>5%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3417 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 Exosome complex exonuclease RRP6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3216	2058	552	598	8			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	GLY	-	CLONING ARTIFACT	UNP Q12149
A	128	MET	-	CLONING ARTIFACT	UNP Q12149
A	361	ALA	TYR	ENGINEERED	UNP Q12149

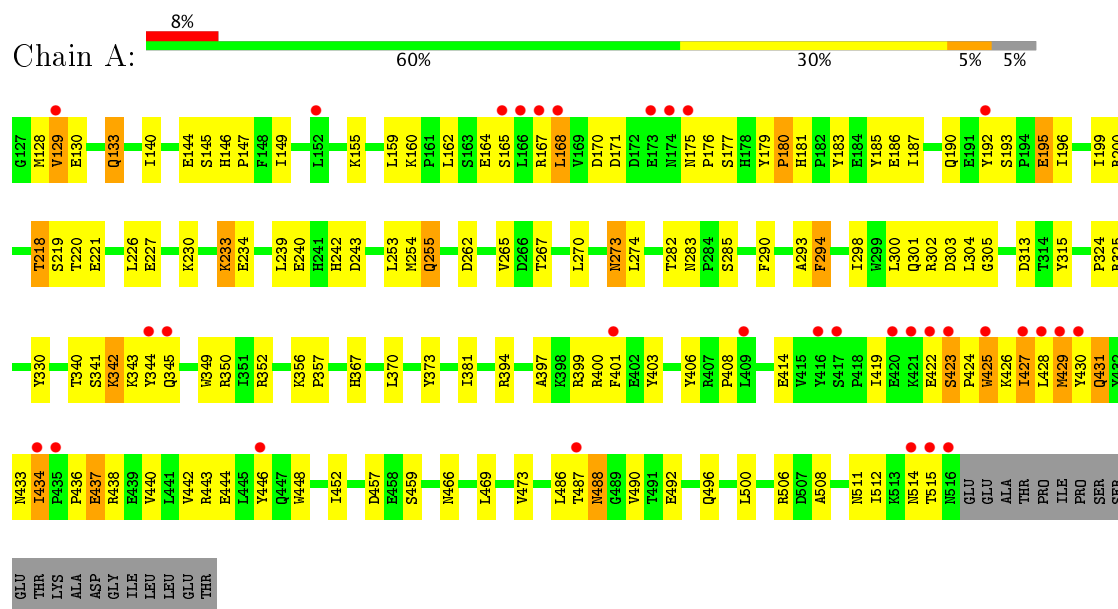
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	201	Total	O	0	0
			201	201		

### 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 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: Exosome complex exonuclease RRP6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.14Å 110.14Å 80.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	55.06 – 2.10 95.38 – 2.07	Depositor EDS
% Data completeness (in resolution range)	93.6 (55.06-2.10) 92.9 (95.38-2.07)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 2.07Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.232 , 0.292 0.233 , 0.293	Depositor DCC
$R_{free}$ test set	3087 reflections (9.97%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 58.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3417	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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](#)

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	0.41	0/3296	0.63	0/4479

There are no bond length outliers.

There are no bond angle outliers.

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	3216	0	3205	153	0
2	A	201	0	0	8	0
All	All	3417	0	3205	153	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 24.

All (153) 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:167:ARG:HG3	1:A:168:LEU:H	1.24	0.98
1:A:273:ASN:N	1:A:273:ASN:HD22	1.56	0.97
1:A:426:LYS:HE2	1:A:443:ARG:HG3	1.46	0.96
1:A:422:GLU:HB3	1:A:466:ASN:HD21	1.29	0.95

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:PRO:HG2	1:A:429:MET:HB2	1.51	0.92
1:A:273:ASN:H	1:A:273:ASN:HD22	0.99	0.91
1:A:437:GLU:HB2	1:A:512:ILE:HD12	1.56	0.87
1:A:422:GLU:CB	1:A:466:ASN:HD21	1.90	0.85
1:A:422:GLU:HB3	1:A:466:ASN:ND2	1.91	0.84
1:A:423:SER:HB3	1:A:428:LEU:HB3	1.60	0.81
1:A:273:ASN:N	1:A:273:ASN:ND2	2.24	0.81
1:A:302:ARG:NH1	1:A:303:ASP:OD1	2.15	0.80
1:A:301:GLN:NE2	1:A:401:PHE:H	1.79	0.80
1:A:218:THR:HG22	1:A:221:GLU:H	1.47	0.78
1:A:273:ASN:H	1:A:273:ASN:ND2	1.80	0.78
1:A:427:ILE:HG23	1:A:434:ILE:HD12	1.65	0.77
1:A:167:ARG:O	1:A:168:LEU:HB2	1.83	0.77
1:A:167:ARG:HG3	1:A:168:LEU:N	2.00	0.74
1:A:302:ARG:HH11	1:A:302:ARG:HG2	1.52	0.74
1:A:294:PHE:HB2	1:A:399:ARG:NH1	2.03	0.74
1:A:167:ARG:CG	1:A:168:LEU:H	2.00	0.72
1:A:438:ARG:O	1:A:442:VAL:HG23	1.90	0.72
1:A:167:ARG:HH12	1:A:180:PRO:HG3	1.57	0.70
1:A:422:GLU:CG	1:A:466:ASN:HD21	2.04	0.70
1:A:175:ASN:HD22	1:A:408:PRO:HB3	1.57	0.70
1:A:183:TYR:HD1	1:A:186:GLU:HG3	1.57	0.69
1:A:159:LEU:HD11	1:A:190:GLN:HG3	1.75	0.69
1:A:429:MET:C	1:A:431:GLN:H	1.96	0.68
1:A:167:ARG:NH1	1:A:180:PRO:HG3	2.09	0.67
1:A:426:LYS:HE2	1:A:443:ARG:CG	2.22	0.67
1:A:128:MET:HE1	1:A:130:GLU:HB2	1.77	0.66
1:A:342:LYS:HA	1:A:345:GLN:OE1	1.96	0.66
1:A:181:HIS:HE1	1:A:397:ALA:O	1.79	0.66
1:A:428:LEU:O	1:A:428:LEU:HD12	1.96	0.66
1:A:511:ASN:O	1:A:515:THR:HG23	1.97	0.65
1:A:262:ASP:OD2	1:A:367:HIS:HD2	1.80	0.64
1:A:128:MET:CE	1:A:130:GLU:HB2	2.27	0.64
1:A:167:ARG:HH11	1:A:167:ARG:HG2	1.61	0.63
1:A:175:ASN:HD22	1:A:408:PRO:CB	2.12	0.63
1:A:431:GLN:HA	1:A:434:ILE:HD11	1.81	0.62
1:A:186:GLU:CD	1:A:186:GLU:H	2.02	0.60
1:A:298:ILE:HG23	1:A:401:PHE:HB2	1.82	0.60
1:A:302:ARG:HG2	1:A:302:ARG:NH1	2.17	0.60
1:A:424:PRO:HD3	1:A:430:TYR:CE2	2.37	0.59
1:A:431:GLN:C	1:A:433:ASN:H	2.04	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:TRP:NE1	1:A:426:LYS:HG3	2.17	0.58
1:A:305:GLY:HA2	2:A:560:HOH:O	2.04	0.58
1:A:488:ASN:HB3	2:A:575:HOH:O	2.03	0.58
1:A:254:MET:HE2	1:A:300:LEU:HD21	1.86	0.58
1:A:192:TYR:HB3	1:A:196:ILE:HG21	1.84	0.58
1:A:193:SER:O	1:A:196:ILE:HG22	2.04	0.57
1:A:340:THR:HG22	1:A:341:SER:N	2.18	0.57
1:A:218:THR:HG23	2:A:665:HOH:O	2.05	0.56
1:A:167:ARG:O	1:A:168:LEU:CB	2.54	0.56
1:A:226:LEU:O	1:A:230:LYS:HG3	2.05	0.56
1:A:356:LYS:N	1:A:357:PRO:HD2	2.22	0.54
1:A:424:PRO:HG2	1:A:429:MET:H	1.71	0.54
1:A:242:HIS:CD2	1:A:350:ARG:HD3	2.43	0.53
1:A:506:ARG:HD2	2:A:559:HOH:O	2.07	0.53
1:A:302:ARG:HD3	1:A:401:PHE:CZ	2.44	0.53
1:A:301:GLN:HE22	1:A:401:PHE:H	1.54	0.53
1:A:492:GLU:O	1:A:496:GLN:HG3	2.08	0.53
1:A:344:TYR:OH	1:A:357:PRO:HB2	2.08	0.53
1:A:140:ILE:HG12	1:A:457:ASP:OD2	2.09	0.53
1:A:302:ARG:HD3	1:A:401:PHE:CE2	2.44	0.52
1:A:187:ILE:O	1:A:394:ARG:HD2	2.09	0.52
1:A:486:LEU:O	1:A:488:ASN:N	2.42	0.51
1:A:508:ALA:O	1:A:512:ILE:HG12	2.10	0.51
1:A:155:LYS:HG3	1:A:183:TYR:CZ	2.45	0.51
1:A:239:LEU:HD23	1:A:254:MET:HG3	1.93	0.51
1:A:424:PRO:O	1:A:425:TRP:C	2.50	0.50
1:A:512:ILE:HB	2:A:718:HOH:O	2.10	0.50
1:A:140:ILE:HD12	1:A:140:ILE:O	2.11	0.50
1:A:352:ARG:HD3	2:A:668:HOH:O	2.11	0.50
1:A:144:GLU:CD	1:A:403:TYR:HB3	2.32	0.50
1:A:427:ILE:HD13	1:A:442:VAL:HG21	1.93	0.50
1:A:426:LYS:CE	1:A:443:ARG:HG3	2.30	0.50
1:A:160:LYS:HG3	1:A:164:GLU:OE1	2.11	0.49
1:A:423:SER:HA	1:A:430:TYR:CE2	2.47	0.49
1:A:340:THR:HG22	1:A:341:SER:H	1.76	0.49
1:A:424:PRO:CG	1:A:429:MET:H	2.25	0.49
1:A:167:ARG:NH1	1:A:167:ARG:HG2	2.26	0.49
1:A:218:THR:HG22	1:A:220:THR:N	2.27	0.49
1:A:425:TRP:CD1	1:A:426:LYS:HG3	2.48	0.49
1:A:426:LYS:O	1:A:427:ILE:C	2.52	0.49
1:A:429:MET:CE	1:A:429:MET:HA	2.43	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:MET:HB3	1:A:265:VAL:HB	1.95	0.48
1:A:429:MET:C	1:A:431:GLN:N	2.66	0.48
1:A:442:VAL:O	1:A:446:TYR:HD2	1.95	0.48
1:A:164:GLU:O	1:A:167:ARG:NH1	2.47	0.48
1:A:514:ASN:O	1:A:515:THR:C	2.50	0.48
1:A:419:ILE:HG23	2:A:725:HOH:O	2.14	0.47
1:A:128:MET:HG3	1:A:129:VAL:N	2.29	0.47
1:A:423:SER:HA	1:A:430:TYR:HE2	1.79	0.47
1:A:159:LEU:HD12	1:A:186:GLU:HA	1.95	0.47
1:A:240:GLU:HG2	1:A:255:GLN:NE2	2.29	0.47
1:A:325:ARG:HB2	1:A:330:TYR:CG	2.50	0.47
1:A:145:SER:O	1:A:146:HIS:HB3	2.15	0.47
1:A:140:ILE:HD11	2:A:714:HOH:O	2.14	0.47
1:A:431:GLN:HA	1:A:434:ILE:CD1	2.43	0.46
1:A:301:GLN:HE22	1:A:400:ARG:HA	1.80	0.46
1:A:175:ASN:HB2	1:A:408:PRO:HB3	1.98	0.46
1:A:324:PRO:HG2	1:A:330:TYR:OH	2.16	0.46
1:A:185:TYR:HB3	1:A:186:GLU:OE2	2.15	0.46
1:A:283:ASN:OD1	1:A:285:SER:HB2	2.16	0.46
1:A:440:VAL:O	1:A:444:GLU:HG3	2.16	0.46
1:A:183:TYR:O	1:A:187:ILE:HG13	2.15	0.45
1:A:199:ILE:HG13	1:A:381:ILE:HG21	1.99	0.45
1:A:431:GLN:HA	1:A:434:ILE:CG1	2.46	0.45
1:A:149:ILE:HG12	1:A:179:TYR:CE2	2.52	0.45
1:A:290:PHE:CB	1:A:293:ALA:HB2	2.46	0.45
1:A:218:THR:CG2	1:A:219:SER:N	2.80	0.45
1:A:341:SER:C	1:A:343:LYS:H	2.20	0.45
1:A:448:TRP:CZ2	1:A:452:ILE:HG13	2.51	0.45
1:A:469:LEU:O	1:A:473:VAL:HG23	2.17	0.45
1:A:370:LEU:O	1:A:373:TYR:HB3	2.17	0.44
1:A:422:GLU:HB3	1:A:466:ASN:CG	2.35	0.44
1:A:428:LEU:HD13	1:A:430:TYR:C	2.37	0.44
1:A:218:THR:CG2	1:A:220:THR:H	2.31	0.44
1:A:270:LEU:O	1:A:274:LEU:HG	2.17	0.44
1:A:262:ASP:OD2	1:A:367:HIS:CD2	2.65	0.44
1:A:431:GLN:C	1:A:433:ASN:N	2.71	0.44
1:A:195:GLU:HB2	1:A:200:ARG:CZ	2.48	0.44
1:A:448:TRP:CE2	1:A:452:ILE:HG13	2.53	0.44
1:A:168:LEU:HD21	1:A:177:SER:OG	2.18	0.44
1:A:349:TRP:O	1:A:352:ARG:NH2	2.51	0.44
1:A:356:LYS:HB2	1:A:357:PRO:CD	2.48	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:PRO:HA	1:A:406:TYR:CD2	2.52	0.44
1:A:274:LEU:HD12	1:A:304:LEU:HD22	1.99	0.43
1:A:437:GLU:HG3	1:A:512:ILE:HG21	2.00	0.43
1:A:253:LEU:HD12	1:A:265:VAL:O	2.18	0.43
1:A:313:ASP:OD1	1:A:315:TYR:HB3	2.17	0.43
1:A:423:SER:OG	1:A:466:ASN:HB3	2.18	0.43
1:A:175:ASN:HD22	1:A:408:PRO:CA	2.32	0.43
1:A:428:LEU:O	1:A:434:ILE:HD11	2.19	0.43
1:A:133:GLN:H	1:A:133:GLN:HE21	1.65	0.43
1:A:162:LEU:O	1:A:165:SER:HB2	2.19	0.42
1:A:267:THR:HG22	1:A:274:LEU:CD1	2.49	0.42
1:A:243:ASP:O	1:A:459:SER:HB3	2.20	0.42
1:A:175:ASN:OD1	1:A:176:PRO:O	2.38	0.42
1:A:183:TYR:CZ	1:A:282:THR:HG21	2.55	0.42
1:A:424:PRO:O	1:A:426:LYS:O	2.38	0.41
1:A:233:LYS:HA	1:A:233:LYS:HD2	1.90	0.41
1:A:274:LEU:HA	1:A:274:LEU:HD23	1.89	0.41
1:A:146:HIS:C	1:A:406:TYR:CE2	2.94	0.41
1:A:183:TYR:CD1	1:A:186:GLU:HG3	2.44	0.41
1:A:342:LYS:C	1:A:344:TYR:H	2.23	0.41
1:A:144:GLU:HG3	1:A:403:TYR:CG	2.56	0.41
1:A:290:PHE:HB3	1:A:293:ALA:HB2	2.03	0.40
1:A:414:GLU:OE1	1:A:414:GLU:N	2.54	0.40
1:A:500:LEU:HD23	1:A:500:LEU:C	2.41	0.40
1:A:430:TYR:O	1:A:431:GLN:C	2.60	0.40
1:A:159:LEU:HB2	1:A:185:TYR:CD2	2.56	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	388/410 (95%)	339 (87%)	38 (10%)	11 (3%)	6 2

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	168	LEU
1	A	171	ASP
1	A	423	SER
1	A	425	TRP
1	A	427	ILE
1	A	431	GLN
1	A	487	THR
1	A	170	ASP
1	A	129	VAL
1	A	342	LYS
1	A	436	PRO

### 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	360/377 (96%)	345 (96%)	15 (4%)	34 33

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

Mol	Chain	Res	Type
1	A	133	GLN
1	A	180	PRO
1	A	195	GLU
1	A	218	THR
1	A	227	GLU
1	A	233	LYS
1	A	234	GLU
1	A	255	GLN
1	A	273	ASN
1	A	294	PHE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	429	MET
1	A	434	ILE
1	A	437	GLU
1	A	488	ASN
1	A	490	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	142	ASN
1	A	175	ASN
1	A	181	HIS
1	A	255	GLN
1	A	273	ASN
1	A	301	GLN
1	A	367	HIS
1	A	384	ASN
1	A	433	ASN
1	A	466	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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 ⓘ

### 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	390/410 (95%)	0.64	32 (8%) 12 16	26, 48, 101, 122	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	423	SER	7.5
1	A	166	LEU	7.4
1	A	174	ASN	6.2
1	A	427	ILE	6.0
1	A	425	TRP	5.6
1	A	429	MET	5.4
1	A	409	LEU	5.3
1	A	430	TYR	4.7
1	A	192	TYR	4.6
1	A	435	PRO	3.8
1	A	175	ASN	3.7
1	A	167	ARG	3.7
1	A	422	GLU	3.6
1	A	345	GLN	3.4
1	A	173	GLU	3.3
1	A	344	TYR	3.3
1	A	421	LYS	3.3
1	A	420	GLU	3.1
1	A	487	THR	3.0
1	A	416	TYR	3.0
1	A	417	SER	3.0
1	A	165	SER	3.0
1	A	401	PHE	2.7
1	A	428	LEU	2.7
1	A	446	TYR	2.7
1	A	514	ASN	2.7
1	A	152	LEU	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	516	ASN	2.6
1	A	434	ILE	2.5
1	A	168	LEU	2.4
1	A	129	VAL	2.4
1	A	515	THR	2.1

## 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.