Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:28 AM GMT

PDB ID	:	2HBK
Title	:	Structure of the yeast nuclear exosome component, Rrp6p, reveals an interplay between the active site and the HRDC domain; Protein in complex with Mn
Authors	:	Midtgaard, S.F.; Assenholt, J.; Jonstrup, A.T.; Van, L.B.; Jensen, T.H.; Brodersen, D.E.
Deposited on	:	2006-06-14
Resolution	:	2.25 Å(reported)

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

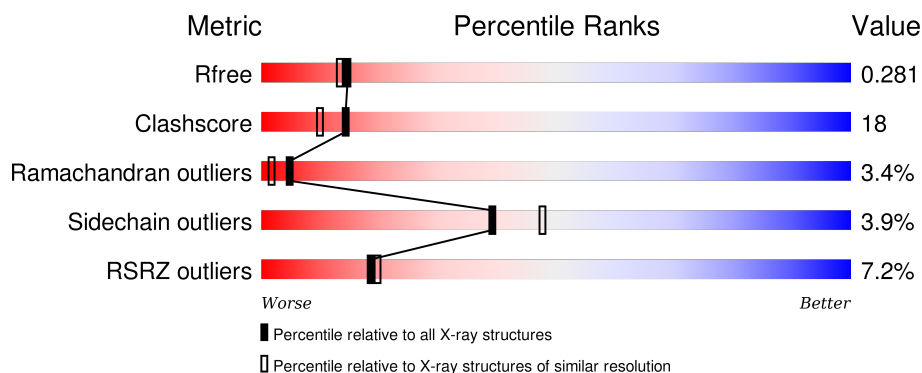|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
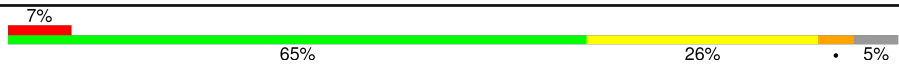*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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	Percentile Ranks	Value
Rfree		0.281
Clashscore		18
Ramachandran outliers		3.4%
Sidechain outliers		3.9%
RSRZ outliers		7.2%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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 <=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	7% · · · 65% · · · 26% · 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3470 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 3216	C 2058	N 552	O 598	S 8	0	0	0

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 MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Mn 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	252	Total 252	O 252	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: Exosome complex exonuclease RRP6
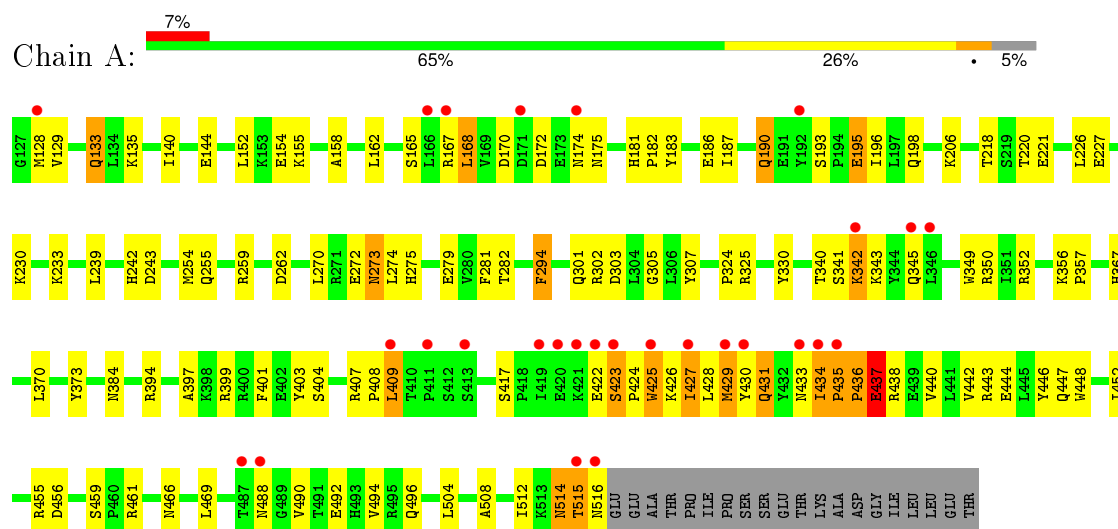
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	110.68Å 110.68Å 79.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.22 – 2.25 95.85 – 2.25	Depositor EDS
% Data completeness (in resolution range)	97.3 (36.22-2.25) 97.4 (95.85-2.25)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.15 (at 2.25Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.279 0.223 , 0.281	Depositor DCC
R_{free} test set	2646 reflections (10.03%)	DCC
Wilson B-factor (Å²)	43.5	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.30 , 52.4	EDS
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 27100 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3470	wwPDB-VP
Average B, all atoms (Å²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:
MN

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	0.37	0/3296	0.60	1/4479 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	172	ASP	N-CA-C	-5.06	97.34	111.00

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	116	0
2	A	2	0	0	0	0
3	A	252	0	0	8	0
All	All	3470	0	3205	116	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 18.

All (116) 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:426:LYS:HE2	1:A:443:ARG:HG3	1.32	1.11
1:A:167:ARG:HG3	1:A:168:LEU:H	1.13	1.07
1:A:422:GLU:HB3	1:A:466:ASN:HD21	1.19	1.00
1:A:427:ILE:HG23	1:A:434:ILE:HD12	1.50	0.94
1:A:133:GLN:H	1:A:133:GLN:HE21	1.17	0.93
1:A:301:GLN:NE2	1:A:401:PHE:H	1.67	0.92
1:A:422:GLU:CB	1:A:466:ASN:HD21	1.90	0.84
1:A:422:GLU:HB3	1:A:466:ASN:ND2	1.93	0.83
1:A:167:ARG:HG3	1:A:168:LEU:N	1.95	0.80
1:A:183:TYR:HD1	1:A:186:GLU:HG3	1.49	0.78
1:A:294:PHE:HB2	1:A:399:ARG:NH1	2.00	0.76
1:A:181:HIS:HD2	1:A:183:TYR:H	1.35	0.75
1:A:301:GLN:HE22	1:A:401:PHE:H	1.34	0.75
1:A:167:ARG:O	1:A:168:LEU:HB2	1.88	0.72
1:A:431:GLN:C	1:A:433:ASN:H	1.92	0.71
1:A:429:MET:C	1:A:431:GLN:H	1.96	0.67
1:A:167:ARG:CG	1:A:168:LEU:H	1.97	0.66
1:A:193:SER:O	1:A:196:ILE:HG22	1.95	0.66
1:A:302:ARG:HG2	1:A:303:ASP:OD1	1.95	0.66
1:A:301:GLN:HE21	1:A:401:PHE:HB3	1.62	0.65
1:A:273:ASN:H	1:A:273:ASN:HD22	1.45	0.65
1:A:438:ARG:O	1:A:442:VAL:HG23	1.99	0.63
1:A:423:SER:HB3	1:A:428:LEU:HB3	1.82	0.61
1:A:428:LEU:HD12	1:A:434:ILE:HD13	1.83	0.61
1:A:341:SER:HB3	3:A:1192:HOH:O	2.02	0.60
1:A:133:GLN:HG2	1:A:140:ILE:CD1	2.32	0.59
1:A:436:PRO:HB2	3:A:1080:HOH:O	2.02	0.58
1:A:195:GLU:HA	1:A:198:GLN:NE2	2.19	0.58
1:A:273:ASN:N	1:A:273:ASN:HD22	2.01	0.57
1:A:183:TYR:CD1	1:A:186:GLU:HG3	2.35	0.57
1:A:220:THR:HG23	3:A:1071:HOH:O	2.04	0.57
1:A:302:ARG:NH1	1:A:303:ASP:OD1	2.38	0.57
1:A:133:GLN:NE2	1:A:133:GLN:H	1.97	0.57
1:A:488:ASN:HB3	3:A:1073:HOH:O	2.04	0.56
1:A:426:LYS:HE2	1:A:443:ARG:CG	2.21	0.56
1:A:342:LYS:HA	1:A:345:GLN:OE1	2.06	0.56
1:A:162:LEU:HD12	1:A:165:SER:HB2	1.87	0.55
1:A:508:ALA:O	1:A:512:ILE:HG12	2.06	0.55
1:A:431:GLN:C	1:A:433:ASN:N	2.61	0.54
1:A:324:PRO:HG2	1:A:330:TYR:OH	2.07	0.54
1:A:340:THR:HG22	1:A:341:SER:N	2.23	0.54
1:A:273:ASN:N	1:A:273:ASN:ND2	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:GLU:HB2	1:A:512:ILE:HD12	1.89	0.53
1:A:428:LEU:O	1:A:428:LEU:HD12	2.09	0.52
1:A:301:GLN:NE2	1:A:401:PHE:N	2.46	0.52
1:A:440:VAL:O	1:A:444:GLU:HG3	2.10	0.52
1:A:270:LEU:O	1:A:274:LEU:HG	2.09	0.52
1:A:190:GLN:HA	1:A:190:GLN:HE21	1.76	0.51
1:A:504:LEU:C	1:A:504:LEU:HD23	2.31	0.51
1:A:436:PRO:HA	3:A:1102:HOH:O	2.10	0.51
1:A:218:THR:OG1	1:A:221:GLU:HG3	2.11	0.51
1:A:349:TRP:O	1:A:352:ARG:NH2	2.43	0.51
1:A:425:TRP:NE1	1:A:426:LYS:HG3	2.26	0.50
1:A:429:MET:C	1:A:431:GLN:N	2.64	0.50
1:A:305:GLY:HA2	3:A:1047:HOH:O	2.10	0.50
1:A:422:GLU:CG	1:A:466:ASN:HD21	2.24	0.50
1:A:242:HIS:CD2	1:A:350:ARG:HD3	2.47	0.50
1:A:133:GLN:N	1:A:133:GLN:HE21	1.98	0.50
1:A:183:TYR:CZ	1:A:282:THR:HG21	2.47	0.50
1:A:175:ASN:ND2	1:A:408:PRO:HB3	2.27	0.49
1:A:404:SER:HA	1:A:417:SER:HB2	1.95	0.49
1:A:302:ARG:HH11	1:A:302:ARG:HG2	1.77	0.49
1:A:325:ARG:HB2	1:A:330:TYR:CG	2.47	0.49
1:A:455:ARG:NH1	1:A:456:ASP:OD1	2.46	0.49
1:A:424:PRO:O	1:A:425:TRP:C	2.52	0.48
1:A:302:ARG:HD3	1:A:401:PHE:CZ	2.48	0.47
1:A:195:GLU:HA	1:A:198:GLN:HE21	1.79	0.47
1:A:433:ASN:O	1:A:435:PRO:HD3	2.14	0.47
1:A:140:ILE:HD13	3:A:1055:HOH:O	2.14	0.47
1:A:186:GLU:CD	1:A:186:GLU:H	2.18	0.47
1:A:174:ASN:HA	1:A:409:LEU:HD12	1.96	0.47
1:A:262:ASP:OD2	1:A:367:HIS:HD2	1.98	0.47
1:A:181:HIS:CD2	1:A:183:TYR:H	2.22	0.47
1:A:427:ILE:HD13	1:A:442:VAL:HG21	1.97	0.46
1:A:442:VAL:O	1:A:446:TYR:HD2	1.99	0.46
1:A:422:GLU:OE2	1:A:461:ARG:HB3	2.16	0.46
1:A:431:GLN:HA	1:A:434:ILE:HG12	1.98	0.46
1:A:341:SER:C	1:A:343:LYS:H	2.19	0.46
1:A:226:LEU:O	1:A:230:LYS:HG3	2.16	0.46
1:A:167:ARG:HH11	1:A:167:ARG:HG2	1.81	0.46
1:A:356:LYS:N	1:A:357:PRO:HD2	2.31	0.46
1:A:187:ILE:O	1:A:394:ARG:HD2	2.16	0.45
1:A:430:TYR:O	1:A:431:GLN:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:LYS:O	1:A:343:LYS:HG2	2.16	0.45
1:A:243:ASP:O	1:A:459:SER:HB3	2.17	0.45
1:A:425:TRP:O	1:A:426:LYS:HB2	2.16	0.45
1:A:514:ASN:O	1:A:516:ASN:N	2.50	0.45
1:A:206:LYS:HG2	1:A:259:ARG:O	2.17	0.45
1:A:181:HIS:HE1	1:A:397:ALA:O	2.00	0.44
1:A:428:LEU:O	1:A:434:ILE:HD11	2.18	0.44
1:A:514:ASN:O	1:A:515:THR:C	2.56	0.44
1:A:448:TRP:O	1:A:452:ILE:HG12	2.17	0.44
1:A:469:LEU:C	1:A:469:LEU:HD23	2.38	0.44
1:A:370:LEU:O	1:A:373:TYR:HB3	2.18	0.43
1:A:272:GLU:CD	1:A:272:GLU:H	2.21	0.43
1:A:281:PHE:HB3	1:A:307:TYR:O	2.19	0.42
1:A:428:LEU:CD1	1:A:434:ILE:HD13	2.48	0.42
1:A:144:GLU:CD	1:A:403:TYR:HB3	2.40	0.42
1:A:434:ILE:HG12	1:A:434:ILE:H	1.58	0.42
1:A:155:LYS:HG3	1:A:183:TYR:CZ	2.54	0.42
1:A:152:LEU:HD11	1:A:154:GLU:O	2.20	0.42
1:A:133:GLN:HG2	1:A:140:ILE:HD12	1.99	0.42
1:A:239:LEU:HD23	1:A:254:MET:HG3	2.02	0.41
1:A:275:HIS:HD2	3:A:1173:HOH:O	2.02	0.41
1:A:155:LYS:O	1:A:158:ALA:HB2	2.20	0.41
1:A:230:LYS:HD3	1:A:279:GLU:OE2	2.20	0.41
1:A:443:ARG:HD3	1:A:447:GLN:CD	2.40	0.41
1:A:404:SER:O	1:A:407:ARG:HG2	2.20	0.41
1:A:492:GLU:O	1:A:496:GLN:HG3	2.20	0.41
1:A:490:VAL:HG13	1:A:494:VAL:HB	2.03	0.41
1:A:424:PRO:O	1:A:426:LYS:O	2.38	0.41
1:A:262:ASP:OD2	1:A:367:HIS:CD2	2.74	0.41
1:A:190:GLN:HE21	1:A:190:GLN:CA	2.33	0.40
1:A:135:LYS:HE3	1:A:135:LYS:HB2	1.97	0.40
1:A:428:LEU:HD12	1:A:434:ILE:CD1	2.49	0.40
1:A:181:HIS:HA	1:A:182:PRO:HD3	1.83	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%)	346 (89%)	29 (8%)	13 (3%)	5	2

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	423	SER
1	A	431	GLN
1	A	515	THR
1	A	168	LEU
1	A	170	ASP
1	A	342	LYS
1	A	409	LEU
1	A	437	GLU
1	A	436	PRO
1	A	129	VAL
1	A	435	PRO
1	A	514	ASN
1	A	427	ILE

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	360/377 (96%)	346 (96%)	14 (4%)	39	48

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	MET
1	A	133	GLN
1	A	190	GLN
1	A	195	GLU
1	A	227	GLU
1	A	233	LYS
1	A	255	GLN
1	A	273	ASN
1	A	294	PHE
1	A	384	ASN
1	A	425	TRP
1	A	429	MET
1	A	434	ILE
1	A	437	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	142	ASN
1	A	146	HIS
1	A	181	HIS
1	A	190	GLN
1	A	198	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
1	A	467	GLN

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)

Of 2 ligands modelled in this entry, 2 are 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 (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(Å²)	Q<0.9
1	A	390/410 (95%)	0.26	28 (7%)	18	20	26, 49, 110, 133	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	425	TRP	7.5
1	A	429	MET	7.1
1	A	423	SER	6.9
1	A	128	MET	5.7
1	A	427	ILE	4.8
1	A	421	LYS	4.6
1	A	166	LEU	4.5
1	A	430	TYR	3.9
1	A	409	LEU	3.8
1	A	192	TYR	3.6
1	A	345	GLN	3.6
1	A	487	THR	3.5
1	A	167	ARG	3.4
1	A	435	PRO	3.1
1	A	516	ASN	3.0
1	A	422	GLU	2.6
1	A	174	ASN	2.6
1	A	433	ASN	2.5
1	A	171	ASP	2.5
1	A	411	PRO	2.5
1	A	434	ILE	2.5
1	A	419	ILE	2.3
1	A	346	LEU	2.3
1	A	515	THR	2.3
1	A	488	ASN	2.2
1	A	420	GLU	2.1
1	A	342	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	413	SER	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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors($Å^2$)	Q<0.9
2	MN	A	1001	1/1	1.00	0.13	-0.33	36,36,36,36	0
2	MN	A	1002	1/1	0.99	0.15	-	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.