



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2IX1 / pdb_00002ix1
Title : RNase II D209N mutant
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Deposited on : 2006-07-05
Resolution : 2.74 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

<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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

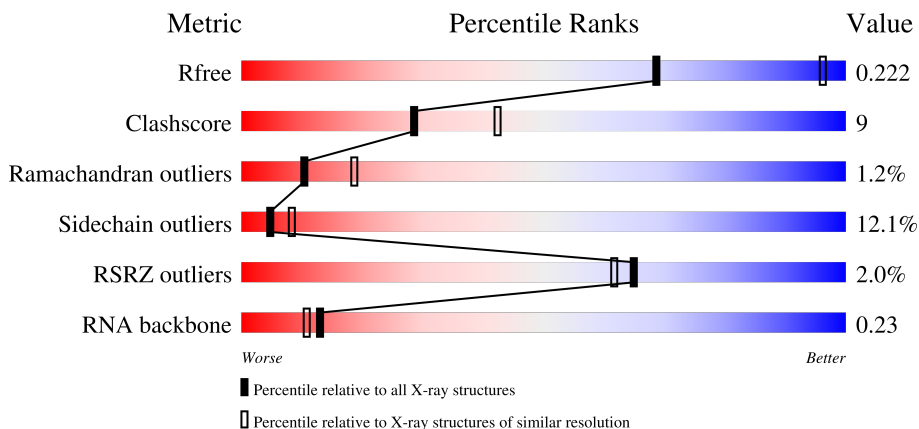
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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}	180053	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)
RNA backbone	3983	1136 (2.98-2.50)

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	664	2% 72% 21% • •
2	B	13	23% 23% 15% 54% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5439 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 EXORIBONUCLEASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	643	Total	C	N	O	S	0	3	0
			5103	3222	909	950	22			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	209	ASN	ASP	engineered mutation	UNP P30850

- Molecule 2 is a RNA chain called 5'-D(*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	P	0	0	0
			287	130	65	79	13			

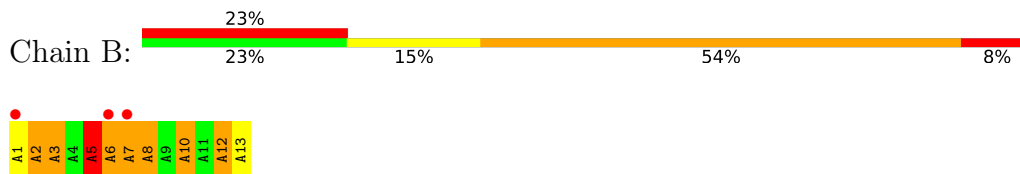
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	45	Total	O	0	0
			45	45		
4	B	3	Total	O	0	0
			3	3		

● Molecule 1: EXORIBONUCLEASE 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	86.32Å 86.32Å 279.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.30 – 2.74 29.30 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.30-2.74) 99.8 (29.30-2.74)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.225 0.177 , 0.222	Depositor DCC
R_{free} test set	1547 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	66.5	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.057 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5439	wwPDB-VP
Average B, all atoms (Å ²)	54.0	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

5.1 Standard geometry

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	0.68	3/5224 (0.1%)	0.93	8/7073 (0.1%)
2	B	0.68	0/325	1.34	3/503 (0.6%)
All	All	0.68	3/5549 (0.1%)	0.96	11/7576 (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	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MET	CG-SD	9.19	2.03	1.80
1	A	1	MET	N-CA	6.60	1.58	1.46
1	A	1	MET	CA-CB	6.02	1.65	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	10	A	O4'-C4'-C3'	-8.34	95.66	104.00
1	A	248	ARG	N-CA-C	-6.56	99.21	109.25
1	A	501	LYS	N-CA-C	6.31	118.98	108.13
1	A	296	ASP	N-CA-C	6.28	119.10	111.82
1	A	5	ASP	N-CA-C	6.06	123.20	109.81
1	A	248	ARG	CA-C-N	-5.78	113.01	122.54
1	A	248	ARG	C-N-CA	-5.78	113.01	122.54
1	A	174	ALA	CA-C-N	5.61	125.62	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	ALA	C-N-CA	5.61	125.62	119.90
2	B	5	A	O4'-C1'-N9	5.51	116.47	108.20
2	B	12	A	C4'-C3'-C2'	-5.03	97.57	102.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	4	ALA	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	5103	0	5082	91	0
2	B	287	0	144	11	0
3	A	1	0	0	0	0
4	A	45	0	0	2	0
4	B	3	0	0	0	0
All	All	5439	0	5226	93	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 9.

All (93) 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:1:MET:SD	1:A:1:MET:CG	2.03	1.46
1:A:297:ASN:HD22	1:A:297:ASN:H	1.18	0.88
1:A:620:VAL:O	1:A:621:THR:HB	1.76	0.85
1:A:126:ASP:HB3	1:A:153:PHE:HD1	1.48	0.78
1:A:179:ALA:HB2	1:A:266:LEU:HD22	1.65	0.78
1:A:129:VAL:HG13	1:A:149[A]:GLN:HB3	1.65	0.77
1:A:191:ASP:OD1	1:A:193:THR:HB	1.85	0.76
1:A:382:ARG:NH2	2:B:10:A:N7	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ARG:NH1	1:A:540:MET:HE1	2.01	0.75
1:A:598:ARG:H	1:A:598:ARG:HE	1.34	0.73
1:A:536:ARG:HG3	2:B:7:A:N1	2.04	0.72
1:A:102:ASP:HB3	2:B:5:A:H61	1.54	0.72
1:A:19:THR:HG22	1:A:20:PRO:HD2	1.77	0.67
1:A:598:ARG:H	1:A:598:ARG:NE	1.93	0.66
1:A:297:ASN:HD22	1:A:297:ASN:N	1.93	0.65
1:A:487:LEU:HB3	1:A:489:LEU:HD22	1.80	0.64
1:A:265:GLU:O	1:A:269:ASP:HB3	1.97	0.63
1:A:291:ASP:OD1	1:A:293:THR:HG23	1.98	0.62
1:A:568:ILE:HD11	1:A:571:ILE:HD11	1.79	0.62
1:A:19:THR:HG22	1:A:20:PRO:CD	2.30	0.62
1:A:428:ALA:HA	1:A:438:VAL:HG13	1.82	0.62
1:A:5:ASP:O	1:A:6:PRO:C	2.44	0.61
1:A:129:VAL:HG13	1:A:149[B]:GLN:HB3	1.84	0.60
1:A:208:MET:N	1:A:208:MET:HE3	2.16	0.60
1:A:205:THR:HG22	1:A:208:MET:HE2	1.85	0.59
1:A:293:THR:HG22	1:A:350:TRP:CD1	2.39	0.58
1:A:245:ALA:O	1:A:248:ARG:O	2.23	0.57
1:A:1:MET:CG	1:A:1:MET:CE	2.84	0.56
1:A:57:GLY:C	1:A:82:PHE:HB2	2.30	0.56
1:A:293:THR:HG22	1:A:350:TRP:NE1	2.21	0.55
1:A:293:THR:HG22	1:A:350:TRP:HE1	1.73	0.54
1:A:612:ILE:O	1:A:612:ILE:HG13	2.07	0.54
1:A:536:ARG:NH1	1:A:540:MET:CE	2.70	0.54
1:A:598:ARG:HE	1:A:598:ARG:N	2.04	0.54
1:A:297:ASN:H	1:A:297:ASN:ND2	1.95	0.52
1:A:264:ARG:HD3	1:A:268:ASP:OD2	2.10	0.52
1:A:208:MET:HE3	1:A:208:MET:H	1.75	0.50
1:A:115:ALA:HB3	1:A:118:LEU:HD13	1.94	0.50
1:A:601:LEU:HD23	1:A:612:ILE:HG22	1.92	0.50
1:A:1:MET:SD	1:A:1:MET:CB	2.96	0.49
1:A:503:GLY:HA2	1:A:531:MET:HE1	1.95	0.48
1:A:536:ARG:HH12	1:A:540:MET:HE1	1.74	0.48
1:A:201:ASP:O	1:A:312:VAL:HA	2.14	0.48
2:B:7:A:H2'	2:B:8:A:H5''	1.95	0.48
1:A:358:PHE:CZ	2:B:8:A:C6	3.02	0.48
1:A:130:ALA:HB2	1:A:147:LEU:HD23	1.96	0.47
1:A:536:ARG:HD3	4:A:2040:HOH:O	2.13	0.47
1:A:568:ILE:HG12	1:A:620:VAL:HA	1.97	0.47
1:A:361:ARG:HB2	1:A:362:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:HD23	1:A:138:LYS:HE2	1.96	0.47
1:A:595:HIS:O	1:A:596:ALA:HB3	2.15	0.46
1:A:620:VAL:O	1:A:621:THR:CB	2.51	0.46
1:A:555:LYS:HD2	1:A:633:MET:HE3	1.98	0.46
1:A:224:LEU:HB2	1:A:343:ILE:HD13	1.98	0.46
1:A:632:ARG:NH2	2:B:2:A:C2	2.83	0.46
1:A:46:ILE:HA	1:A:47:PRO:HD2	1.85	0.45
1:A:506:ILE:HD12	1:A:531:MET:HE1	1.96	0.45
1:A:377:ILE:HD12	1:A:553:PHE:CD2	2.52	0.45
1:A:182:MET:HE3	1:A:233:ALA:HB1	1.99	0.45
1:A:397:ASN:OD1	1:A:494:THR:HA	2.16	0.45
1:A:483:PRO:HA	1:A:490:GLU:O	2.17	0.45
1:A:374:VAL:HG21	1:A:553:PHE:HB2	1.98	0.44
1:A:591:ALA:O	1:A:594:LEU:HB2	2.17	0.44
1:A:50:GLN:CD	1:A:74:GLU:HG3	2.43	0.44
1:A:428:ALA:HA	1:A:438:VAL:CG1	2.46	0.44
1:A:442:GLU:O	1:A:448:GLY:HA3	2.18	0.44
1:A:134:ARG:HB3	1:A:144:TYR:HB3	1.98	0.44
1:A:568:ILE:HA	1:A:578:VAL:HG12	1.99	0.44
1:A:23:GLU:OE1	1:A:59:ARG:NH2	2.50	0.43
1:A:297:ASN:N	1:A:297:ASN:ND2	2.61	0.43
1:A:552:ARG:HA	1:A:633:MET:HE1	2.00	0.43
1:A:75:PRO:HB2	1:A:137:LEU:HD21	2.00	0.43
1:A:465:ASP:O	1:A:468:ILE:HG13	2.18	0.43
1:A:540:MET:HE2	2:B:6:A:H5'	1.99	0.43
1:A:207:ASP:HB3	1:A:268:ASP:OD1	2.18	0.43
1:A:551:ALA:C	1:A:633:MET:HE1	2.44	0.43
1:A:207:ASP:OD2	2:B:13:A:O3'	2.34	0.42
1:A:634:GLU:H	1:A:634:GLU:HG3	1.56	0.42
1:A:103:HIS:CE1	1:A:105:LEU:HB2	2.55	0.42
1:A:256:GLY:O	1:A:257:PHE:HB3	2.20	0.42
1:A:430:LEU:O	1:A:433:THR:HG22	2.20	0.42
1:A:456:LEU:HD12	1:A:456:LEU:HA	1.93	0.42
1:A:256:GLY:HA3	1:A:368:LEU:HD12	2.02	0.41
1:A:263:PRO:HB2	1:A:266:LEU:HD23	2.03	0.41
1:A:274:ARG:HD3	4:A:2026:HOH:O	2.18	0.41
1:A:358:PHE:HZ	2:B:8:A:C6	2.39	0.41
1:A:566:ALA:HB1	1:A:578:VAL:HB	2.03	0.41
1:A:235:ILE:HG23	1:A:241:LEU:HB2	2.02	0.41
1:A:620:VAL:O	1:A:620:VAL:HG12	2.20	0.41
1:A:165:LEU:HD21	1:A:254:LEU:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ARG:NH1	2:B:2:A:H2	2.19	0.40
2:B:3:A:OP2	2:B:3:A:H8	2.04	0.40
1:A:63:VAL:HG23	1:A:65:HIS:NE2	2.36	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	644/664 (97%)	612 (95%)	24 (4%)	8 (1%)	10 19

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	PRO
1	A	94	ASN
1	A	621	THR
1	A	330	SER
1	A	470	ARG
1	A	322	ASN
1	A	620	VAL
1	A	5	ASP

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	539/553 (98%)	474 (88%)	65 (12%)	5 8

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	19	THR
1	A	70	ARG
1	A	90	VAL
1	A	96	ARG
1	A	97	LEU
1	A	100	VAL
1	A	113	ARG
1	A	116	ARG
1	A	124	GLU
1	A	129	VAL
1	A	137	LEU
1	A	152	THR
1	A	159	VAL
1	A	167	ARG
1	A	172	LYS
1	A	182	MET
1	A	188	VAL
1	A	193	THR
1	A	202	SER
1	A	208	MET
1	A	240	LYS
1	A	277	GLU
1	A	288	LEU
1	A	295	GLU
1	A	297	ASN
1	A	312	VAL
1	A	323	THR
1	A	329	GLU
1	A	333	ILE
1	A	359	LYS
1	A	361	ARG
1	A	374	VAL
1	A	375	LEU
1	A	380	GLU
1	A	383	ARG
1	A	427	LEU
1	A	443	VAL

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Mol	Chain	Res	Type
1	A	446	LEU
1	A	456	LEU
1	A	467	ARG
1	A	470	ARG
1	A	473	SER
1	A	479	THR
1	A	489	LEU
1	A	521	THR
1	A	522	ARG
1	A	524	GLN
1	A	525	ASP
1	A	527	ILE
1	A	533	GLU
1	A	560	THR
1	A	562	THR
1	A	568	ILE
1	A	569	VAL
1	A	594	LEU
1	A	598	ARG
1	A	611	GLN
1	A	612	ILE
1	A	617	VAL
1	A	621	THR
1	A	631	VAL
1	A	632	ARG
1	A	634	GLU
1	A	637	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	ASN
1	A	354	HIS
1	A	423	ASN
1	A	434	HIS
1	A	459	GLN
1	A	524	GLN
1	A	538	ASN
1	A	607	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	13/13 (100%)	6 (46%)	4 (30%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	2	A
2	B	3	A
2	B	5	A
2	B	6	A
2	B	7	A
2	B	8	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	1	A
2	B	2	A
2	B	5	A
2	B	12	A

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 oligosaccharides 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 [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	643/664 (96%)	-0.23	10 (1%) 70 68	25, 51, 76, 93	3 (0%)
2	B	13/13 (100%)	0.42	3 (23%) 2 2	42, 105, 164, 178	0
All	All	656/677 (96%)	-0.21	13 (1%) 65 62	25, 51, 79, 178	3 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1	A	3.0
2	B	7	A	2.8
1	A	116	ARG	2.7
2	B	6	A	2.7
1	A	5	ASP	2.6
1	A	6	PRO	2.6
1	A	105	LEU	2.3
1	A	104	PRO	2.3
1	A	18	GLN	2.2
1	A	1	MET	2.2
1	A	620	VAL	2.1
1	A	371	LYS	2.1
1	A	2	LEU	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 oligosaccharides in this entry.

6.4 Ligands

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, 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	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	1644	1/1	0.98	0.06	51,51,51,51	0

6.5 Other polymers

There are no such residues in this entry.