



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 10, 2023 – 08:12 PM JST

PDB ID : 7YIK
Title : The structure of archaeal nuclease RecJ2 from Methanocaldococcus jannaschii
Authors : Wang, W.W.; Liu, X.P.
Deposited on : 2022-07-16
Resolution : 2.19 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.34
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) : 2.34

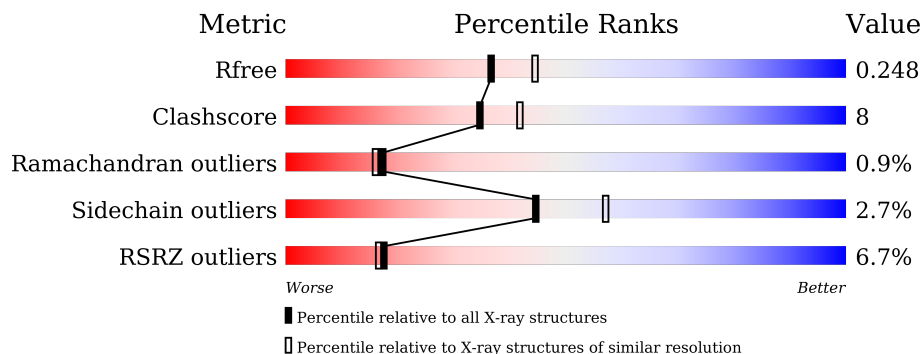
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	432	 8% 80% 17% ..
1	B	432	 6% 86% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7056 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 nuclease RecJ2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	429	3406	2200	571	621	14	0	0	0
1	B	431	3421	2209	575	623	14	0	0	0

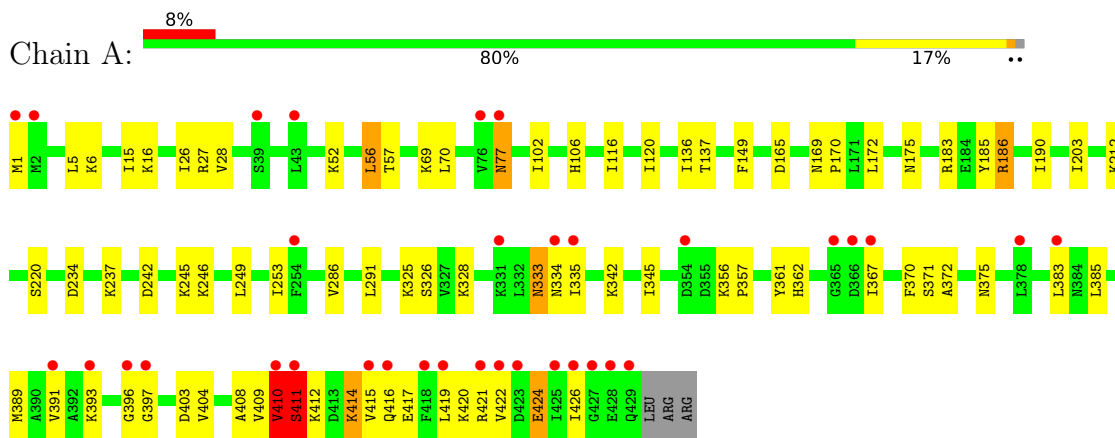
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	87	Total 87	O 87	0	0
2	B	142	Total 142	O 142	0	0

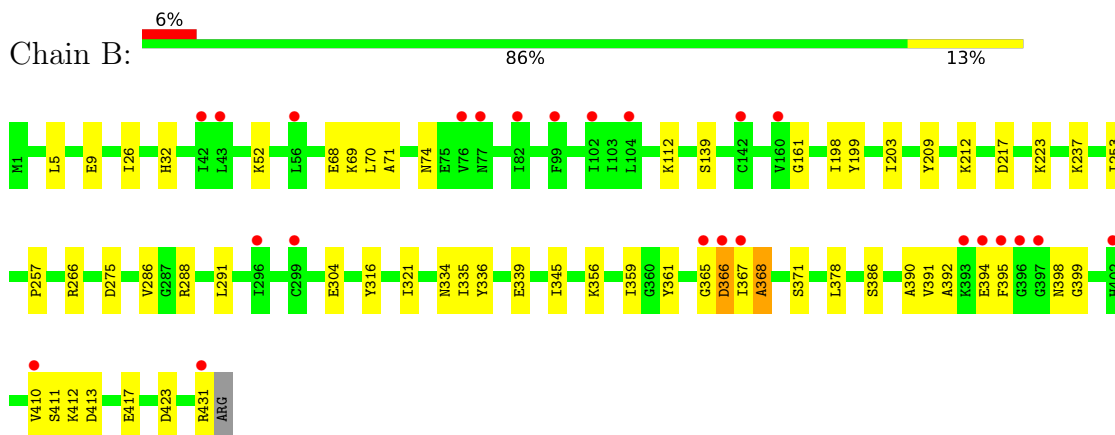
3 Residue-property plots

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: nuclease RecJ2



- Molecule 1: nuclease RecJ2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.52Å 177.82Å 66.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.64 – 2.19 29.64 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.64-2.19) 96.9 (29.64-2.19)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.195 , 0.250 0.198 , 0.248	Depositor DCC
R_{free} test set	2000 reflections (3.82%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtrriage
Anisotropy	0.352	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7056	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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	0.40	0/3465	0.55	0/4662
1	B	0.48	0/3480	0.57	0/4683
All	All	0.44	0/6945	0.56	0/9345

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	3406	0	3512	84	0
1	B	3421	0	3525	31	0
2	A	87	0	0	2	0
2	B	142	0	0	3	0
All	All	7056	0	7037	115	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 (115) 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:334:ASN:HD21	1:A:426:ILE:HG12	1.22	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:GLY:HA3	1:A:410:VAL:CG2	1.88	1.02
1:A:397:GLY:CA	1:A:410:VAL:CG2	2.42	0.97
1:A:408:ALA:HB3	1:A:421:ARG:HH22	1.33	0.93
1:A:367:ILE:HD12	1:A:409:VAL:HG13	1.52	0.91
1:A:408:ALA:CB	1:A:421:ARG:HH22	1.85	0.89
1:A:410:VAL:HG12	1:A:411:SER:CB	2.12	0.80
1:A:367:ILE:HD12	1:A:409:VAL:CG1	2.12	0.79
1:A:410:VAL:CB	1:A:411:SER:HB3	2.13	0.78
1:A:27:ARG:HH12	1:A:57:THR:HG23	1.49	0.76
1:A:397:GLY:HA3	1:A:410:VAL:HG23	1.68	0.74
1:A:410:VAL:HB	1:A:411:SER:HB3	1.70	0.74
1:A:397:GLY:HA3	1:A:410:VAL:HG22	1.69	0.73
1:A:410:VAL:HG12	1:A:411:SER:HB2	1.69	0.72
1:B:334:ASN:ND2	1:B:423:ASP:O	2.23	0.70
1:A:397:GLY:CA	1:A:410:VAL:HG21	2.20	0.70
1:A:328:LYS:NZ	2:A:504:HOH:O	2.23	0.70
1:A:417:GLU:OE1	1:A:421:ARG:NH1	2.26	0.68
1:A:410:VAL:HG12	1:A:411:SER:HB3	1.76	0.68
1:B:335:ILE:HD12	1:B:359:ILE:HD12	1.76	0.66
1:A:409:VAL:HG12	1:A:410:VAL:N	2.11	0.66
1:A:69:LYS:O	1:A:70:LEU:HB2	1.95	0.66
1:A:408:ALA:CB	1:A:421:ARG:NH2	2.57	0.66
1:B:275:ASP:HB2	2:B:502:HOH:O	1.97	0.65
1:A:249:LEU:O	1:A:253:ILE:HG13	1.96	0.65
1:A:334:ASN:HB2	1:A:356:LYS:HD2	1.77	0.64
1:A:410:VAL:CG1	1:A:411:SER:HB3	2.27	0.64
1:A:334:ASN:ND2	1:A:426:ILE:HG12	2.04	0.64
1:B:266:ARG:NH2	2:B:502:HOH:O	2.23	0.63
1:A:385:LEU:O	1:A:389:MET:HG2	1.99	0.63
1:B:286:VAL:HG13	1:B:291:LEU:HB2	1.82	0.62
1:A:6:LYS:N	1:A:6:LYS:HD2	2.15	0.62
1:A:389:MET:HB3	1:A:421:ARG:HH21	1.64	0.62
1:A:286:VAL:HG13	1:A:291:LEU:HB2	1.81	0.61
1:A:212:LYS:O	1:A:212:LYS:HG3	2.01	0.61
1:A:397:GLY:CA	1:A:410:VAL:HG22	2.28	0.61
1:A:411:SER:O	1:A:412:LYS:HG3	2.02	0.59
1:B:367:ILE:O	1:B:410:VAL:O	2.20	0.59
1:B:69:LYS:O	1:B:71:ALA:N	2.33	0.58
1:A:1:MET:N	2:A:508:HOH:O	2.36	0.58
1:A:414:LYS:HG2	1:A:415:VAL:N	2.17	0.57
1:A:397:GLY:N	1:A:410:VAL:HG21	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ALA:HB2	1:A:421:ARG:NH2	2.20	0.56
1:B:5:LEU:O	1:B:9:GLU:HG2	2.05	0.56
1:B:304:GLU:OE2	2:B:501:HOH:O	2.18	0.55
1:A:391:VAL:HG11	1:A:424:GLU:OE2	2.07	0.55
1:B:253:ILE:HG13	1:B:257:PRO:HA	1.88	0.55
1:A:15:ILE:HG23	1:A:102:ILE:HD13	1.89	0.54
1:B:395:PHE:HE2	1:B:417:GLU:HB3	1.71	0.54
1:A:356:LYS:HD3	1:A:357:PRO:HD2	1.90	0.53
1:B:366:ASP:OD1	1:B:412:LYS:HD3	2.08	0.53
1:A:403:ASP:OD1	1:A:404:VAL:N	2.42	0.53
1:A:414:LYS:CG	1:A:415:VAL:N	2.71	0.53
1:A:136:ILE:HA	1:A:175:ASN:OD1	2.08	0.53
1:A:409:VAL:CG1	1:A:410:VAL:N	2.72	0.52
1:A:422:VAL:O	1:A:426:ILE:HG13	2.10	0.52
1:A:393:LYS:O	1:A:393:LYS:HG2	2.10	0.51
1:A:414:LYS:CD	1:A:415:VAL:H	2.23	0.51
1:A:396:GLY:C	1:A:410:VAL:HG21	2.31	0.51
1:A:203:ILE:HG12	1:A:237:LYS:O	2.10	0.51
1:A:416:GLN:O	1:A:419:LEU:HD23	2.10	0.51
1:B:413:ASP:OD1	1:B:413:ASP:N	2.43	0.51
1:B:345:ILE:HG22	1:B:371:SER:HB2	1.92	0.51
1:B:198:ILE:HD11	1:B:199:TYR:CZ	2.46	0.50
1:B:339:GLU:HA	1:B:361:TYR:O	2.12	0.50
1:A:397:GLY:HA2	1:A:410:VAL:CG2	2.41	0.49
1:A:372:ALA:CB	1:A:389:MET:HE2	2.42	0.49
1:B:411:SER:OG	1:B:413:ASP:OD1	2.14	0.49
1:B:139:SER:OG	1:B:161:GLY:HA3	2.13	0.48
1:A:409:VAL:HG12	1:A:410:VAL:H	1.78	0.48
1:A:16:LYS:HG3	1:A:149:PHE:CZ	2.47	0.48
1:A:367:ILE:HA	1:A:411:SER:HA	1.95	0.48
1:B:203:ILE:HG12	1:B:237:LYS:O	2.14	0.48
1:A:397:GLY:N	1:A:410:VAL:CG2	2.76	0.48
1:A:409:VAL:CG1	1:A:410:VAL:H	2.27	0.48
1:A:116:ILE:HB	1:A:120:ILE:HB	1.95	0.47
1:A:342:LYS:HG3	1:A:362:HIS:CE1	2.49	0.47
1:A:424:GLU:OE1	1:A:424:GLU:N	2.49	0.46
1:B:112:LYS:HB3	1:B:112:LYS:HE2	1.59	0.46
1:B:336:TYR:CE2	1:B:356:LYS:HB2	2.51	0.46
1:A:245:LYS:O	1:A:249:LEU:HG	2.16	0.46
1:A:333:ASN:HB2	1:A:422:VAL:CG2	2.45	0.46
1:A:333:ASN:HB2	1:A:422:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ALA:HB2	1:A:389:MET:HE2	1.97	0.45
1:B:390:ALA:C	1:B:392:ALA:H	2.19	0.45
1:B:398:ASN:OD1	1:B:399:GLY:N	2.50	0.45
1:A:334:ASN:O	1:A:356:LYS:HD2	2.17	0.44
1:B:69:LYS:O	1:B:70:LEU:HB2	2.17	0.44
1:A:183:ARG:HE	1:A:190:ILE:HD12	1.81	0.44
1:A:408:ALA:HB2	1:A:421:ARG:HH22	1.71	0.44
1:B:71:ALA:O	1:B:74:ASN:HB2	2.18	0.44
1:A:77:ASN:HD22	1:A:77:ASN:HA	1.62	0.44
1:A:345:ILE:HG22	1:A:371:SER:HB2	1.99	0.44
1:A:169:ASN:HA	1:A:170:PRO:HA	1.84	0.44
1:A:335:ILE:HG12	1:A:422:VAL:HB	1.98	0.44
1:A:389:MET:HE3	1:A:421:ARG:NH2	2.33	0.44
1:A:410:VAL:CA	1:A:411:SER:HB3	2.48	0.43
1:B:68:GLU:C	1:B:69:LYS:O	2.56	0.43
1:A:26:ILE:HD12	1:A:52:LYS:HB3	2.01	0.42
1:A:242:ASP:OD2	1:A:246:LYS:NZ	2.28	0.42
1:B:217:ASP:O	1:B:223:LYS:HD2	2.20	0.42
1:A:389:MET:SD	1:A:421:ARG:NE	2.91	0.42
1:A:106:HIS:CD2	1:A:137:THR:HA	2.55	0.42
1:A:185:TYR:C	1:A:186:ARG:HD3	2.40	0.42
1:B:288:ARG:HD3	1:B:316:TYR:CE1	2.54	0.42
1:A:170:PRO:HG2	1:A:172:LEU:HD11	2.01	0.42
1:B:26:ILE:HD12	1:B:52:LYS:HB3	2.02	0.41
1:B:209:TYR:HA	1:B:321:ILE:HG13	2.02	0.41
1:A:28:VAL:HB	1:A:56:LEU:HD12	2.02	0.41
1:B:368:ALA:HB3	1:B:410:VAL:O	2.21	0.41
1:A:234:ASP:HB3	1:A:237:LYS:HD2	2.03	0.41
1:A:414:LYS:HD2	1:A:415:VAL:H	1.86	0.41
1:A:361:TYR:HB3	1:A:370:PHE:CD2	2.56	0.40
1:A:333:ASN:N	1:A:333:ASN:HD22	2.19	0.40
1:A:27:ARG:HH22	1:A:57:THR:HG21	1.86	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	427/432 (99%)	404 (95%)	19 (4%)	4 (1%)	17	16
1	B	429/432 (99%)	410 (96%)	15 (4%)	4 (1%)	17	16
All	All	856/864 (99%)	814 (95%)	34 (4%)	8 (1%)	17	16

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	410	VAL
1	B	365	GLY
1	A	383	LEU
1	A	411	SER
1	B	368	ALA
1	B	394	GLU
1	A	77	ASN
1	B	391	VAL

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	369/373 (99%)	355 (96%)	14 (4%)	33	42
1	B	370/373 (99%)	364 (98%)	6 (2%)	62	76
All	All	739/746 (99%)	719 (97%)	20 (3%)	44	57

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	56	LEU
1	A	165	ASP
1	A	186	ARG

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Mol	Chain	Res	Type
1	A	220	SER
1	A	325	LYS
1	A	326	SER
1	A	333	ASN
1	A	375	ASN
1	A	410	VAL
1	A	411	SER
1	A	414	LYS
1	A	420	LYS
1	A	424	GLU
1	B	32	HIS
1	B	212	LYS
1	B	366	ASP
1	B	378	LEU
1	B	386	SER
1	B	431	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	333	ASN
1	A	334	ASN
1	B	126	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](#)

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	429/432 (99%)	0.48	34 (7%) 12 11	27, 51, 82, 93	0
1	B	431/432 (99%)	0.30	24 (5%) 24 23	27, 41, 76, 92	0
All	All	860/864 (99%)	0.39	58 (6%) 17 16	27, 46, 80, 93	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	410	VAL	7.4
1	A	426	ILE	7.4
1	B	410	VAL	5.2
1	A	418	PHE	4.8
1	B	367	ILE	4.8
1	A	366	ASP	4.6
1	A	254	PHE	4.5
1	B	431	ARG	4.1
1	A	335	ILE	4.0
1	A	367	ILE	4.0
1	A	411	SER	3.8
1	B	397	GLY	3.8
1	A	397	GLY	3.7
1	B	104	LEU	3.3
1	A	334	ASN	3.3
1	B	366	ASP	3.2
1	B	393	LYS	3.2
1	A	77	ASN	3.2
1	A	427	GLY	3.1
1	B	42	ILE	3.1
1	A	383	LEU	3.0
1	B	76	VAL	2.9
1	B	43	LEU	2.9
1	B	142	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	419	LEU	2.8
1	B	396	GLY	2.8
1	A	365	GLY	2.8
1	A	2	MET	2.7
1	B	77	ASN	2.7
1	A	425	ILE	2.6
1	A	43	LEU	2.6
1	A	415	VAL	2.6
1	A	378	LEU	2.5
1	B	402	HIS	2.5
1	A	1	MET	2.5
1	A	428	GLU	2.5
1	A	421	ARG	2.5
1	A	416	GLN	2.5
1	A	354	ASP	2.4
1	A	393	LYS	2.4
1	A	396	GLY	2.4
1	A	391	VAL	2.4
1	A	331	LYS	2.4
1	A	39	SER	2.4
1	A	423	ASP	2.4
1	B	394	GLU	2.3
1	B	395	PHE	2.3
1	B	102	ILE	2.3
1	B	365	GLY	2.3
1	B	82	ILE	2.3
1	A	422	VAL	2.2
1	A	429	GLN	2.2
1	A	76	VAL	2.1
1	B	299	CYS	2.1
1	B	56	LEU	2.0
1	B	99	PHE	2.0
1	B	296	ILE	2.0
1	B	160	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.