



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2025 – 01:06 PM EDT

PDB ID : 5SU2 / pdb_00005su2
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P03D10 from the F2X-Universal Library
Authors : Barthel, T.; Wollenhaupt, J.; Lima, G.M.A.; Wahl, M.C.; Weiss, M.S.
Deposited on : 2022-08-26
Resolution : 1.85 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

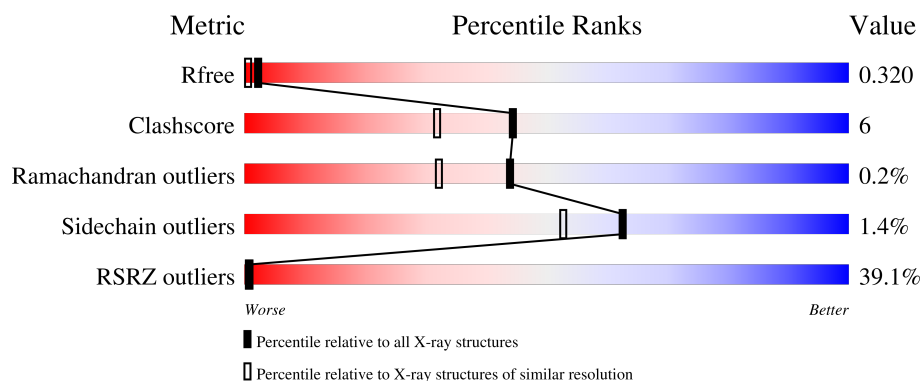
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	164625	3097 (1.86-1.86)
Clashscore	180529	3359 (1.86-1.86)
Ramachandran outliers	177936	3335 (1.86-1.86)
Sidechain outliers	177891	3335 (1.86-1.86)
RSRZ outliers	164620	3097 (1.86-1.86)

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	258	
2	B	308	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9188 atoms, of which 4524 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 Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	237	4068	1287	2060	336	373	12	18	21	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1833	GLY	-	expression tag	UNP P33334
A	1834	ALA	-	expression tag	UNP P33334
A	1835	MET	-	expression tag	UNP P33334

- Molecule 2 is a protein called A1 cistron-splicing factor AAR2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	300	5044	1654	2464	421	485	20	0	17	0

There are 20 discrepancies between the modelled and reference sequences:

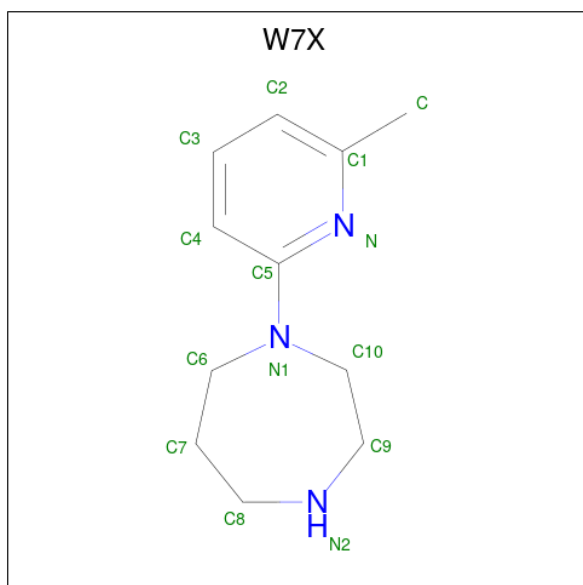
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357
B	?	-	ALA	deletion	UNP P32357
B	?	-	GLY	deletion	UNP P32357
B	?	-	SER	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	MET	deletion	UNP P32357
B	?	-	GLU	deletion	UNP P32357
B	?	-	ALA	deletion	UNP P32357
B	?	-	LYS	deletion	UNP P32357
B	?	-	ASN	deletion	UNP P32357
B	?	-	GLU	deletion	UNP P32357
B	170	SER	ASP	conflict	UNP P32357

- Molecule 3 is 1-(6-methylpyridin-2-yl)-1,4-diazepane (CCD ID: W7X) (formula: $C_{11}H_{17}N_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	N	0	0
			14	11	3		

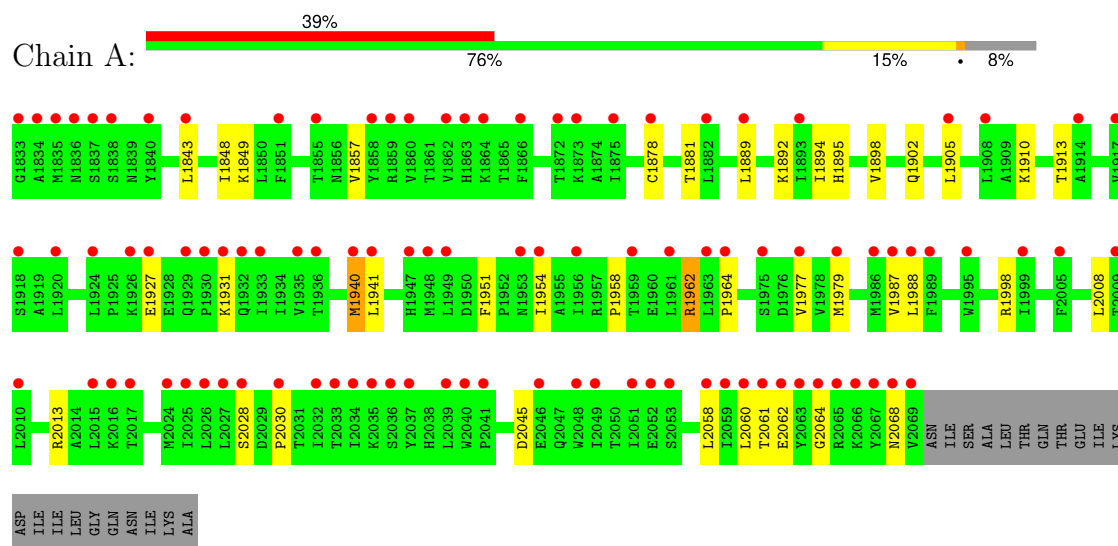
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		
4	B	32	Total	O	0	0
			32	32		

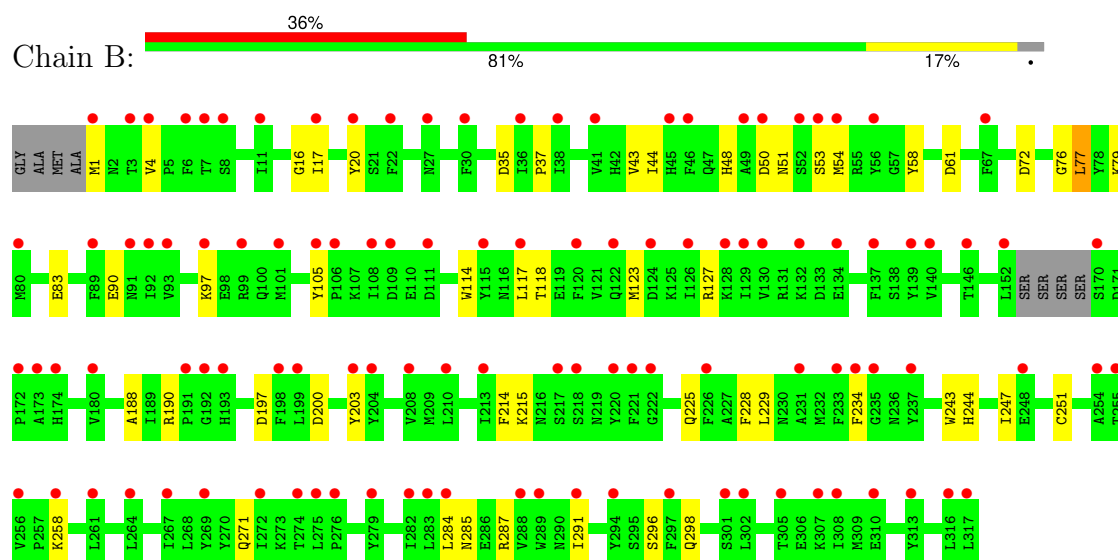
3 Residue-property plots [i](#)

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: Pre-mRNA-splicing factor 8



• Molecule 2: A1 cistron-splicing factor AAR2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	87.77Å 81.53Å 92.64Å 90.00° 107.93° 90.00°	Depositor
Resolution (Å)	44.07 – 1.85 44.07 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.8 (44.07-1.85) 97.9 (44.07-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 1.86Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.268 , 0.316 0.275 , 0.320	Depositor DCC
R_{free} test set	2097 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 80.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9188	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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: W7X

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	0.76	0/2149	0.86	2/2911 (0.1%)
2	B	0.83	3/2739 (0.1%)	0.91	5/3699 (0.1%)
All	All	0.80	3/4888 (0.1%)	0.89	7/6610 (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
2	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	20	TYR	CD2-CE2	5.75	1.48	1.39
2	B	225	GLN	CG-CD	5.41	1.63	1.51
2	B	234	PHE	CE1-CZ	5.12	1.47	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	117	LEU	CB-CG-CD1	-7.40	98.42	111.00
1	A	2008	LEU	CB-CG-CD1	-6.48	99.99	111.00
2	B	229	LEU	CB-CG-CD1	-6.14	100.56	111.00
2	B	284	LEU	CB-CG-CD2	6.08	121.33	111.00
2	B	200	ASP	CB-CG-OD1	5.57	123.31	118.30
2	B	197	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	1940	MET	CG-SD-CE	-5.00	92.19	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	97	LYS	Mainchain

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	2008	2060	1974	24	0
2	B	2580	2464	2398	30	0
3	B	14	0	0	0	0
4	A	30	0	0	3	0
4	B	32	0	0	1	0
All	All	4664	4524	4372	54	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 6.

All (54) 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)
2:B:1:MET:N	4:B:501:HOH:O	2.06	0.87
1:A:1962:ARG:O	1:A:2013:ARG:NH1	2.23	0.71
2:B:50:ASP:OD1	2:B:51:ASN:N	2.24	0.70
1:A:1927:GLU:OE1	4:A:2101:HOH:O	2.15	0.65
2:B:77:LEU:HD21	2:B:79:LYS:HE3	1.77	0.64
2:B:4:VAL:HG12	2:B:4:VAL:O	1.99	0.61
2:B:4:VAL:HG11	2:B:44[B]:ILE:CD1	2.33	0.59
1:A:1998:ARG:NH1	1:A:2045:ASP:OD2	2.32	0.59
2:B:53:SER:O	2:B:54[A]:MET:HB3	2.03	0.59
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	1.83	0.59
2:B:243:TRP:O	2:B:247:ILE:HG13	2.05	0.57
1:A:2064:GLY:O	1:A:2068:ASN:N	2.37	0.57
2:B:37:PRO:HD3	2:B:105:TYR:CD1	2.40	0.57
2:B:190:ARG:HG3	2:B:203[B]:TYR:CZ	2.42	0.55
2:B:4:VAL:HG11	2:B:44[B]:ILE:HD13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:GLU:HA	2:B:83:GLU:OE1	2.08	0.53
1:A:1894:ILE:HA	4:A:2107:HOH:O	2.09	0.52
2:B:228:PHE:CD2	2:B:271:GLN:HG2	2.44	0.52
2:B:1:MET:HB3	2:B:35:ASP:HA	1.92	0.52
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.57	0.51
2:B:43:VAL:HG13	2:B:43:VAL:O	2.09	0.51
1:A:1902:GLN:HB2	1:A:1905:LEU:HD21	1.93	0.50
1:A:1962:ARG:HD3	1:A:1962:ARG:H	1.77	0.49
1:A:1895:HIS:O	1:A:1898[A]:VAL:HG22	2.12	0.49
2:B:258:LYS:HD2	2:B:258:LYS:H	1.79	0.48
1:A:1977:VAL:HG21	1:A:1987:VAL:HG21	1.97	0.47
1:A:1881:THR:O	1:A:1889:LEU:HD12	2.15	0.47
1:A:1951:PHE:HB3	1:A:1954:ILE:HD12	1.97	0.46
2:B:251:CYS:O	2:B:296:SER:HB2	2.16	0.46
1:A:2061:THR:O	1:A:2064:GLY:N	2.49	0.46
1:A:1913:THR:HB	1:A:1940:MET:HE1	1.97	0.45
2:B:72:ASP:O	2:B:76:GLY:N	2.47	0.45
2:B:287:ARG:O	2:B:291:ILE:HD13	2.17	0.45
2:B:17:ILE:HD13	2:B:44[B]:ILE:CG1	2.48	0.44
2:B:298:GLN:HA	2:B:298:GLN:OE1	2.18	0.43
2:B:43:VAL:HA	2:B:58:TYR:O	2.19	0.43
2:B:244:HIS:CD2	2:B:285:ASN:HB3	2.54	0.43
1:A:1941:LEU:HD11	1:A:1958:PRO:HB3	2.01	0.43
1:A:1902:GLN:HB2	1:A:1905:LEU:CD2	2.49	0.42
2:B:44[A]:ILE:O	2:B:44[A]:ILE:HG23	2.19	0.42
1:A:2028:SER:O	1:A:2030:PRO:HD3	2.20	0.41
2:B:214:PHE:O	2:B:215:LYS:HB2	2.20	0.41
2:B:48:HIS:N	2:B:48:HIS:CD2	2.87	0.41
1:A:1910:LYS:NZ	4:A:2105:HOH:O	2.52	0.41
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.41	0.41
1:A:1857:VAL:HG21	1:A:1913:THR:OG1	2.21	0.41
1:A:1910:LYS:HG2	1:A:1940:MET:SD	2.60	0.41
2:B:114:TRP:CE2	2:B:118:THR:HG21	2.56	0.41
1:A:1878:CYS:HA	1:A:1892:LYS:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	258/258 (100%)	247 (96%)	10 (4%)	1 (0%)	30	18
2	B	315/308 (102%)	302 (96%)	13 (4%)	0	100	100
All	All	573/566 (101%)	549 (96%)	23 (4%)	1 (0%)	44	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1964	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	237/233 (102%)	231 (98%)	6 (2%)	42	28
2	B	294/284 (104%)	290 (99%)	4 (1%)	62	53
All	All	531/517 (103%)	521 (98%)	10 (2%)	62	39

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1962	ARG
1	A	1979[A]	MET
1	A	1979[B]	MET
1	A	1979[C]	MET
1	A	1988	LEU

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Mol	Chain	Res	Type
1	A	2060	LEU
2	B	77	LEU
2	B	90	GLU
2	B	123[A]	MET
2	B	123[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	W7X	B	401	-	14,15,15	2.38	7 (50%)	14,19,19	1.68	4 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	W7X	B	401	-	-	0/4/13/13	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	W7X	C4-C5	-3.91	1.29	1.39
3	B	401	W7X	C9-N2	3.63	1.54	1.47
3	B	401	W7X	C2-C1	-3.27	1.31	1.39
3	B	401	W7X	C3-C4	-3.15	1.33	1.38
3	B	401	W7X	C8-N2	2.91	1.53	1.47
3	B	401	W7X	C1-N	-2.60	1.30	1.34
3	B	401	W7X	C3-C2	-2.08	1.35	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	W7X	C2-C3-C4	3.51	124.76	120.24
3	B	401	W7X	C6-C7-C8	-2.64	107.70	113.91
3	B	401	W7X	C3-C4-C5	-2.47	114.22	117.61
3	B	401	W7X	N-C5-N1	-2.14	113.85	116.56

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, 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	237/258 (91%)	2.03	100 (42%) 1 0	30, 78, 144, 237	12 (5%)
2	B	300/308 (97%)	1.80	110 (36%) 1 1	23, 77, 130, 223	9 (3%)
All	All	537/566 (94%)	1.90	210 (39%) 1 1	23, 78, 142, 237	21 (3%)

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1979[A]	MET	7.7
2	B	54[A]	MET	7.1
1	A	1940	MET	7.0
1	A	1878	CYS	6.9
1	A	2039	LEU	6.5
1	A	2040	TRP	6.5
1	A	2069	VAL	5.9
2	B	256	VAL	5.9
1	A	2059	ILE	5.5
1	A	2060	LEU	5.4
2	B	152	LEU	5.4
1	A	2063	TYR	5.2
2	B	6	PHE	5.2
1	A	1963	LEU	5.1
1	A	2034	ILE	5.1
1	A	2068	ASN	5.0
1	A	1866	PHE	4.9
1	A	1840	TYR	4.8
2	B	203[A]	TYR	4.6
2	B	316	LEU	4.6
2	B	129	ILE	4.6
1	A	1927	GLU	4.4
2	B	283	LEU	4.2
1	A	1948	MET	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	2036	SER	4.1
1	A	2048	TRP	4.0
2	B	288	VAL	4.0
2	B	172	PRO	4.0
1	A	1956	ILE	4.0
1	A	1855[A]	THR	3.9
1	A	2065	ARG	3.9
2	B	80	MET	3.9
1	A	1964	PRO	3.9
2	B	170	SER	3.9
2	B	4	VAL	3.9
2	B	67	PHE	3.9
1	A	2005	PHE	3.8
1	A	1875	ILE	3.8
1	A	2064	GLY	3.8
2	B	120	PHE	3.8
1	A	2033	THR	3.8
2	B	255	THR	3.7
1	A	2032	ILE	3.7
1	A	1872	THR	3.7
1	A	2061	THR	3.7
2	B	130	VAL	3.6
1	A	2027	LEU	3.5
1	A	1893	ILE	3.5
2	B	92	ILE	3.5
1	A	1905	LEU	3.5
1	A	1988	LEU	3.5
2	B	279	TYR	3.5
1	A	2051	ILE	3.5
2	B	275	LEU	3.5
1	A	1929	GLN	3.4
2	B	1	MET	3.4
2	B	117	LEU	3.4
2	B	173	ALA	3.4
2	B	89	PHE	3.4
1	A	1859	ARG	3.4
1	A	1920	LEU	3.4
2	B	254	ALA	3.3
1	A	1975	SER	3.3
2	B	122[A]	GLN	3.3
2	B	20	TYR	3.3
2	B	284	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	2009	THR	3.3
1	A	2035	LYS	3.2
2	B	101	MET	3.2
2	B	289	TRP	3.2
1	A	1833	GLY	3.2
2	B	272	ILE	3.2
1	A	1918[A]	SER	3.2
1	A	1986	MET	3.2
2	B	174	HIS	3.2
1	A	1933	ILE	3.1
2	B	11	ILE	3.1
2	B	106	PRO	3.1
2	B	317	LEU	3.1
1	A	1931[A]	LYS	3.1
1	A	2053[A]	SER	3.1
2	B	282	ILE	3.1
2	B	234	PHE	3.1
1	A	2058	LEU	3.1
2	B	313	TYR	3.1
2	B	52	SER	3.1
2	B	235	GLY	3.0
2	B	218	SER	3.0
2	B	41[A]	VAL	3.0
1	A	2066	LYS	3.0
1	A	1836	ASN	3.0
1	A	2041	PRO	3.0
1	A	2017[A]	THR	3.0
2	B	124	ASP	3.0
2	B	276	PRO	2.9
2	B	261	LEU	2.9
1	A	1860	VAL	2.9
2	B	49	ALA	2.9
1	A	2010	LEU	2.9
1	A	2026	LEU	2.9
1	A	1924	LEU	2.9
2	B	294	TYR	2.9
1	A	1954	ILE	2.8
1	A	1862	VAL	2.8
2	B	180	VAL	2.8
2	B	199	LEU	2.8
1	A	1995	TRP	2.8
1	A	1858	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	2067	TYR	2.8
2	B	231	ALA	2.8
2	B	220	TYR	2.7
2	B	53	SER	2.7
2	B	146	THR	2.7
2	B	126	ILE	2.7
1	A	1889	LEU	2.7
2	B	210	LEU	2.7
2	B	233	PHE	2.7
2	B	307	LYS	2.7
1	A	2037	TYR	2.7
2	B	140	VAL	2.7
2	B	274	THR	2.7
1	A	2049	ILE	2.7
2	B	139	TYR	2.6
2	B	192	GLY	2.6
2	B	109	ASP	2.6
1	A	2016	LYS	2.6
2	B	36	ILE	2.6
1	A	1961[A]	LEU	2.6
2	B	198	PHE	2.6
1	A	1999	ILE	2.6
2	B	17	ILE	2.6
2	B	3	THR	2.6
2	B	248	GLU	2.6
1	A	1873	LYS	2.5
2	B	46	PHE	2.5
1	A	1932[A]	GLN	2.5
2	B	111	ASP	2.5
1	A	1851	PHE	2.5
2	B	308	ILE	2.5
1	A	1949	LEU	2.5
2	B	30	PHE	2.5
2	B	221	PHE	2.5
2	B	213	ILE	2.5
2	B	7	THR	2.5
1	A	1917	VAL	2.5
1	A	1989	PHE	2.5
1	A	1930	PRO	2.4
2	B	222	GLY	2.4
1	A	1864	LYS	2.4
2	B	132	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	204[A]	TYR	2.4
2	B	310	GLU	2.4
2	B	258	LYS	2.4
2	B	217	SER	2.4
2	B	50	ASP	2.4
2	B	226	PHE	2.4
2	B	269	TYR	2.4
1	A	1953	ASN	2.4
2	B	264	LEU	2.4
1	A	2030	PRO	2.4
2	B	297	PHE	2.4
1	A	1936	THR	2.4
2	B	38	ILE	2.3
2	B	91	ASN	2.3
1	A	2024[A]	MET	2.3
2	B	97	LYS	2.3
2	B	301	SER	2.3
1	A	1947	HIS	2.3
1	A	1926	LYS	2.3
1	A	1863	HIS	2.3
2	B	137	PHE	2.3
1	A	1843	LEU	2.3
2	B	105	TYR	2.3
2	B	237	TYR	2.3
2	B	191	PRO	2.2
1	A	1959	THR	2.2
2	B	208	VAL	2.2
1	A	1914	ALA	2.2
1	A	1987	VAL	2.2
2	B	56	TYR	2.2
1	A	2028	SER	2.2
2	B	8	SER	2.2
1	A	1977	VAL	2.2
1	A	1835	MET	2.2
1	A	1908	LEU	2.2
1	A	1941	LEU	2.2
1	A	2046	GLU	2.1
2	B	134	GLU	2.1
1	A	1834	ALA	2.1
1	A	1882	LEU	2.1
2	B	302	LEU	2.1
2	B	108	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	115	TYR	2.1
2	B	291	ILE	2.1
2	B	45[A]	HIS	2.1
2	B	193	HIS	2.1
2	B	267	ILE	2.1
2	B	305	THR	2.1
1	A	2052	GLU	2.1
1	A	2015	LEU	2.1
1	A	2062	GLU	2.1
2	B	93	VAL	2.0
2	B	22	PHE	2.0
2	B	128	LYS	2.0
1	A	1837	SER	2.0
1	A	1838	SER	2.0
1	A	2025	ILE	2.0
2	B	27	ASN	2.0
2	B	99	ARG	2.0
1	A	1935	VAL	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, 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(\AA^2)	Q<0.9
3	W7X	B	401	14/14	0.71	0.20	20,20,20,20	14

6.5 Other polymers [i](#)

There are no such residues in this entry.