



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 03:59 AM UTC

PDB ID : 7FJW / pdb_00007fjw
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P03H12 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 : 1.63 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

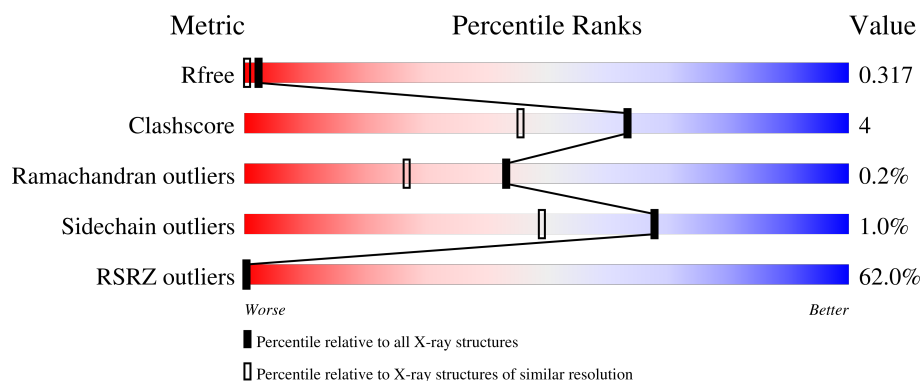
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.63 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	59% 83% 9% 8%
2	B	308	59% 87% 10% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9213 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	0	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	22	17	0

There are 20 discrepancies between the modelled and reference sequences:

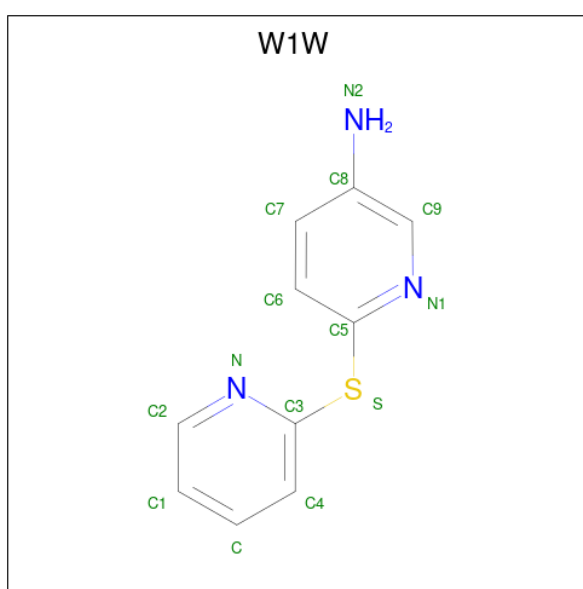
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN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

Continued on next page...

Continued from previous page...

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 6-[(pyridin-2-yl)sulfanyl]pyridin-3-amine (CCD ID: W1W) (formula: C₁₀H₉N₃S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	S	0	0
			14	10	3	1		

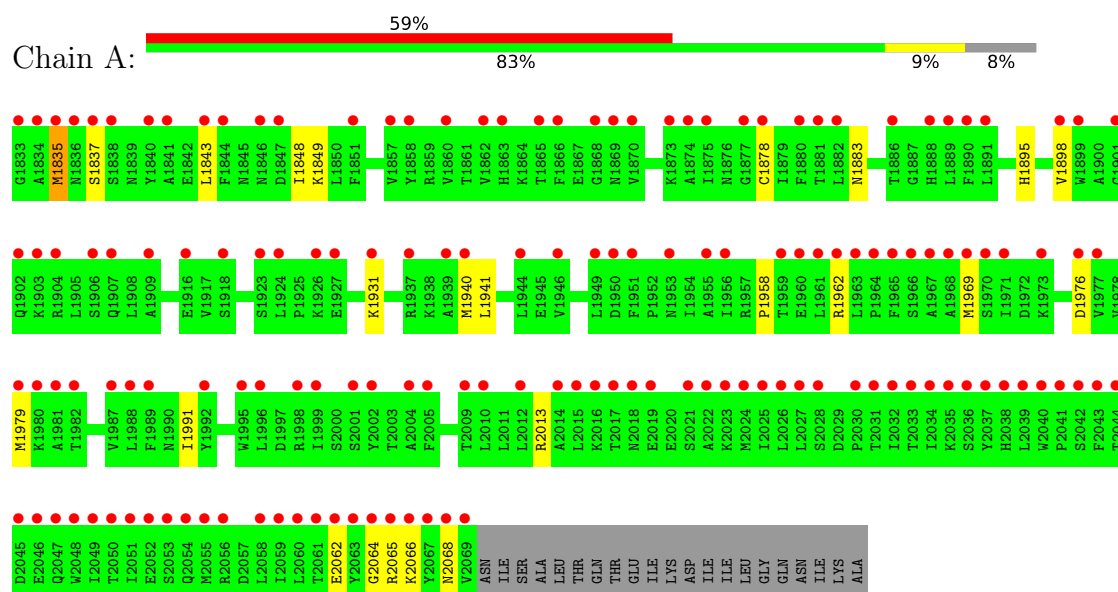
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	48	Total	O	0	0
			48	48		
4	B	39	Total	O	0	0
			39	39		

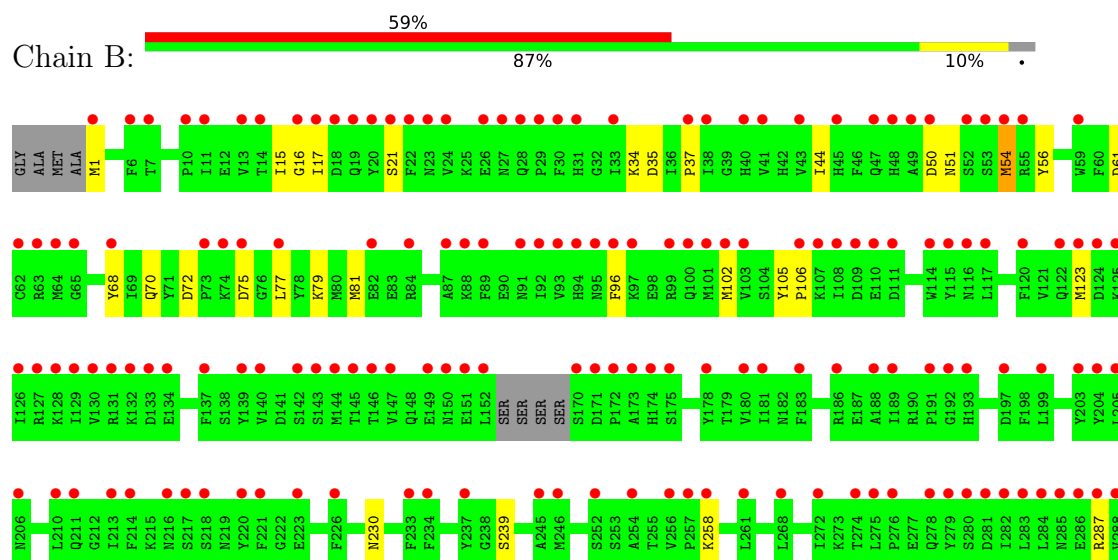
3 Residue-property plots

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: Pre-mRNA-splicing factor 8



• Molecule 2: A1 cistron-splicing factor AAR2



W289
N290
I291
C292
L293
Y294
S295
S296
F297
Q298
K299
N300
S301
L302
H303
N304
T305
E306
K307
I308
N311
K312
Y313
P314
E315
L316
L317

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.32Å 82.12Å 93.24Å 90.00° 108.31° 90.00°	Depositor
Resolution (Å)	44.78 – 1.63 44.78 – 1.63	Depositor EDS
% Data completeness (in resolution range)	97.8 (44.78-1.63) 98.0 (44.78-1.63)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 1.63Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.289 , 0.308 0.300 , 0.317	Depositor DCC
R_{free} test set	2096 reflections (2.68%)	wwPDB-VP
Wilson B-factor (Å ²)	44.9	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 60.1	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	0.93	EDS
Total number of atoms	9213	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% 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: W1W

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	0.83	2/2149 (0.1%)	0.84	3/2911 (0.1%)
2	B	0.70	0/2739	0.74	0/3699
All	All	0.76	2/4888 (0.0%)	0.79	3/6610 (0.0%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1883	ASN	C-N	14.50	1.52	1.34
1	A	1940	MET	SD-CE	-9.47	1.55	1.79

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1883	ASN	CA-C-N	8.65	128.30	119.56
1	A	1883	ASN	C-N-CA	8.65	128.30	119.56
1	A	1883	ASN	O-C-N	-6.65	115.85	121.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	54[A]	MET	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	2008	2060	1974	11	0
2	B	2580	2464	2398	24	0
3	A	14	0	0	0	0
4	A	48	0	0	2	0
4	B	39	0	0	3	0
All	All	4689	4524	4372	36	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 4.

All (36) 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:96:PHE:HB2	2:B:102:MET:HE3	1.65	0.77
2:B:70:GLN:HB3	2:B:81:MET:HE2	1.67	0.77
2:B:77:LEU:HD21	2:B:79:LYS:HE3	1.69	0.74
1:A:2064:GLY:O	1:A:2068:ASN:N	2.30	0.64
2:B:96:PHE:CB	2:B:102:MET:HE3	2.28	0.64
2:B:287:ARG:O	2:B:291:ILE:HD13	1.98	0.63
2:B:1:MET:N	4:B:401:HOH:O	2.34	0.60
2:B:50:ASP:OD1	2:B:51:ASN:N	2.32	0.60
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.49	0.58
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	1.88	0.55
2:B:258:LYS:HD2	2:B:258:LYS:H	1.72	0.54
2:B:230[B]:ASN:ND2	2:B:239:SER:OG	2.40	0.54
2:B:68:TYR:CE2	2:B:81:MET:HE3	2.44	0.53
2:B:17:ILE:HD13	2:B:44[B]:ILE:CG1	2.40	0.52
1:A:1895:HIS:O	1:A:1898[A]:VAL:HG22	2.10	0.52
1:A:1979[B]:MET:HA	1:A:1979[B]:MET:HE2	1.91	0.52
2:B:70:GLN:HB3	2:B:81:MET:CE	2.38	0.52
2:B:37:PRO:HD3	2:B:105:TYR:CD1	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54[A]:MET:HE2	4:B:439:HOH:O	2.14	0.47
2:B:70:GLN:OE1	2:B:81:MET:HE1	2.16	0.46
1:A:1962:ARG:O	1:A:2013:ARG:NH1	2.49	0.46
1:A:1835:MET:HE3	1:A:1835:MET:HB3	1.87	0.45
1:A:2062:GLU:OE2	1:A:2065:ARG:NH1	2.50	0.45
2:B:72:ASP:OD2	2:B:79:LYS:NZ	2.46	0.44
1:A:1941:LEU:HD11	1:A:1958:PRO:HB3	2.00	0.43
1:A:1878:CYS:SG	1:A:1969:MET:HE3	2.59	0.42
2:B:1:MET:HB3	2:B:35:ASP:HA	2.03	0.41
1:A:1976:ASP:HB3	4:A:2203:HOH:O	2.20	0.41
2:B:15:ILE:O	2:B:21:SER:HA	2.19	0.41
2:B:34:LYS:NZ	4:B:403:HOH:O	2.53	0.41
2:B:75:ASP:OD2	2:B:79:LYS:NZ	2.40	0.41
2:B:56:TYR:CZ	2:B:77:LEU:HB2	2.56	0.40
2:B:1:MET:HE3	2:B:35:ASP:O	2.22	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	258/258 (100%)	254 (98%)	4 (2%)	0	100	100
2	B	315/308 (102%)	300 (95%)	14 (4%)	1 (0%)	36	20
All	All	573/566 (101%)	554 (97%)	18 (3%)	1 (0%)	43	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	106	PRO

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	237/233 (102%)	233 (98%)	4 (2%)	53	27
2	B	294/284 (104%)	292 (99%)	2 (1%)	76	62
All	All	531/517 (103%)	525 (99%)	6 (1%)	68	44

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1835	MET
1	A	1837	SER
1	A	1991	ILE
1	A	2066	LYS
2	B	123[A]	MET
2	B	123[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1907	GLN
1	A	2038	HIS
2	B	2	ASN
2	B	47	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 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	W1W	A	2101	-	15,15,15	2.53	5 (33%)	19,19,19	0.99	0

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	W1W	A	2101	-	-	1/4/4/4	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2101	W1W	C3-S	-6.96	1.68	1.77
3	A	2101	W1W	C5-S	4.29	1.82	1.77
3	A	2101	W1W	C7-C8	-2.95	1.33	1.40
3	A	2101	W1W	C3-N	-2.08	1.29	1.34
3	A	2101	W1W	C6-C7	-2.04	1.35	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2101	W1W	C6-C5-S-C3

There are no ring outliers.

No monomer is involved in short contacts.

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, 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%)	3.05	151 (63%) 0 0	26, 79, 167, 356	12 (5%)
2	B	300/308 (97%)	2.71	182 (60%) 0 0	25, 80, 178, 283	9 (3%)
All	All	537/566 (94%)	2.86	333 (62%) 0 0	25, 79, 168, 356	21 (3%)

All (333) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1979[A]	MET	13.4
1	A	1961[A]	LEU	9.3
2	B	283	LEU	9.1
2	B	30	PHE	9.0
1	A	1898[A]	VAL	8.7
1	A	2051	ILE	8.2
1	A	2040	TRP	8.1
2	B	103	VAL	7.9
1	A	2069	VAL	7.8
1	A	2060	LEU	7.7
2	B	210	LEU	7.5
1	A	1834	ALA	7.3
1	A	1951	PHE	7.3
2	B	147	VAL	7.3
1	A	2048	TRP	7.2
1	A	2061	THR	7.2
2	B	284	LEU	7.1
1	A	2058	LEU	7.0
2	B	129	ILE	6.9
1	A	1862	VAL	6.8
2	B	275	LEU	6.8
2	B	316	LEU	6.8
1	A	1965	PHE	6.8
1	A	2059	ILE	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	11	ILE	6.7
1	A	1963	LEU	6.6
2	B	217	SER	6.6
1	A	1988	LEU	6.6
1	A	2017[A]	THR	6.5
1	A	2039	LEU	6.5
1	A	2037	TYR	6.5
1	A	1857	VAL	6.5
2	B	126	ILE	6.5
1	A	2015	LEU	6.4
1	A	2038	HIS	6.3
2	B	246	MET	6.3
1	A	1955	ALA	6.2
2	B	152	LEU	6.2
1	A	2063	TYR	6.1
2	B	20	TYR	6.1
2	B	193	HIS	6.1
1	A	1840	TYR	6.0
1	A	2055	MET	5.9
1	A	1860	VAL	5.9
2	B	203[A]	TYR	5.8
1	A	2067	TYR	5.8
2	B	130	VAL	5.7
2	B	124	ASP	5.6
2	B	108	ILE	5.6
2	B	29	PRO	5.6
2	B	14	THR	5.6
2	B	279	TYR	5.6
2	B	49	ALA	5.5
2	B	54[A]	MET	5.5
1	A	2068	ASN	5.4
1	A	1866	PHE	5.4
2	B	1	MET	5.4
2	B	206	ASN	5.4
1	A	2052	GLU	5.4
1	A	1835	MET	5.4
2	B	314	PRO	5.4
2	B	272	ILE	5.3
1	A	2064	GLY	5.3
1	A	1968	ALA	5.2
2	B	73	PRO	5.2
1	A	1927	GLU	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	170	SER	5.1
2	B	174	HIS	5.1
1	A	2026	LEU	5.0
1	A	2027	LEU	5.0
1	A	2035	LYS	4.9
2	B	192	GLY	4.9
2	B	111	ASP	4.9
2	B	101	MET	4.8
2	B	172	PRO	4.8
1	A	1833	GLY	4.8
1	A	2025	ILE	4.8
2	B	276	PRO	4.8
2	B	313	TYR	4.7
1	A	1931[A]	LYS	4.7
2	B	106	PRO	4.7
1	A	1863	HIS	4.7
1	A	1843	LEU	4.6
2	B	311	ASN	4.6
1	A	1880	PHE	4.6
1	A	1970	SER	4.6
2	B	21	SER	4.6
2	B	31	HIS	4.5
1	A	2010	LEU	4.5
2	B	43	VAL	4.5
1	A	1888	HIS	4.5
1	A	2034	ILE	4.5
1	A	2036	SER	4.4
2	B	40	HIS	4.4
2	B	19	GLN	4.4
2	B	92	ILE	4.4
1	A	1977	VAL	4.4
2	B	293	LEU	4.4
1	A	1966	SER	4.3
1	A	2024[A]	MET	4.3
2	B	107	LYS	4.3
1	A	2031	THR	4.3
2	B	173	ALA	4.3
2	B	150	ASN	4.3
1	A	2030	PRO	4.3
2	B	93	VAL	4.2
1	A	1923	SER	4.2
1	A	2065	ARG	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	26	GLU	4.2
2	B	306	GLU	4.2
2	B	24	VAL	4.2
2	B	91	ASN	4.2
1	A	2002[A]	TYR	4.2
1	A	1949	LEU	4.1
2	B	186	ARG	4.1
1	A	2049	ILE	4.1
2	B	146	THR	4.0
2	B	213	ILE	4.0
2	B	295	SER	4.0
2	B	145	THR	4.0
1	A	1891	LEU	4.0
2	B	287	ARG	3.9
2	B	50	ASP	3.9
2	B	233	PHE	3.9
2	B	292	CYS	3.9
2	B	41[A]	VAL	3.9
2	B	218	SER	3.9
1	A	1907	GLN	3.9
1	A	1886	THR	3.9
2	B	143	SER	3.8
2	B	131	ARG	3.8
2	B	285	ASN	3.8
2	B	27	ASN	3.8
1	A	1916	GLU	3.8
2	B	100	GLN	3.8
1	A	1906	SER	3.8
1	A	1971	ILE	3.7
2	B	252	SER	3.7
2	B	254	ALA	3.7
1	A	2066	LYS	3.7
1	A	1999	ILE	3.7
1	A	2005	PHE	3.7
2	B	171	ASP	3.7
2	B	301	SER	3.7
2	B	291	ILE	3.7
1	A	1980[A]	LYS	3.6
1	A	2043	PHE	3.6
1	A	1967	ALA	3.6
2	B	109	ASP	3.6
2	B	294	TYR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1889	LEU	3.6
2	B	297	PHE	3.6
1	A	1987	VAL	3.6
2	B	282	ILE	3.5
2	B	302	LEU	3.5
2	B	317	LEU	3.5
2	B	48	HIS	3.5
2	B	122[A]	GLN	3.5
1	A	1874	ALA	3.5
2	B	22	PHE	3.5
1	A	1924	LEU	3.5
2	B	216	ASN	3.5
1	A	1890	PHE	3.4
2	B	140	VAL	3.4
2	B	288	VAL	3.4
1	A	1926	LYS	3.4
2	B	120	PHE	3.4
2	B	205	LEU	3.4
2	B	257	PRO	3.4
1	A	1881	THR	3.3
1	A	2062	GLU	3.3
2	B	74	LYS	3.3
2	B	16	GLY	3.3
2	B	117	LEU	3.3
1	A	1870	VAL	3.3
2	B	281	ASP	3.3
1	A	1846	ASN	3.3
1	A	2028	SER	3.3
2	B	38	ILE	3.3
1	A	1877	GLY	3.2
2	B	189	ILE	3.2
2	B	94	HIS	3.2
2	B	96	PHE	3.2
2	B	23	ASN	3.2
1	A	1878	CYS	3.2
1	A	2016	LYS	3.2
1	A	2032	ILE	3.2
1	A	2021	SER	3.2
1	A	1844	PHE	3.2
1	A	2014	ALA	3.2
1	A	2022	ALA	3.2
1	A	2001[A]	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	204[A]	TYR	3.1
2	B	110	GLU	3.1
1	A	1944	LEU	3.1
1	A	2047	GLN	3.1
1	A	2054[A]	GLN	3.1
1	A	1865	THR	3.1
2	B	137	PHE	3.1
2	B	299	LYS	3.0
2	B	308	ILE	3.0
2	B	7	THR	3.0
2	B	151	GLU	3.0
2	B	175	SER	3.0
2	B	128	LYS	3.0
2	B	181	ILE	3.0
1	A	1950	ASP	3.0
1	A	2050	THR	3.0
2	B	52	SER	3.0
2	B	64[A]	MET	3.0
2	B	261	LEU	3.0
2	B	180	VAL	2.9
2	B	45[A]	HIS	2.9
2	B	10	PRO	2.9
1	A	1989	PHE	2.9
1	A	2056[A]	ARG	2.9
2	B	127	ARG	2.9
2	B	115	TYR	2.9
2	B	220	TYR	2.9
2	B	139	TYR	2.9
2	B	237	TYR	2.9
1	A	2053[A]	SER	2.9
2	B	221	PHE	2.8
2	B	256	VAL	2.8
2	B	97	LYS	2.8
1	A	1858	TYR	2.8
1	A	2012	LEU	2.8
1	A	1982	THR	2.8
1	A	2044	THR	2.8
2	B	183	PHE	2.8
1	A	1939	ALA	2.8
2	B	191	PRO	2.8
1	A	1937	ARG	2.8
1	A	2042	SER	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	62	CYS	2.8
1	A	1969	MET	2.8
1	A	1901	GLY	2.8
2	B	280	SER	2.8
2	B	6	PHE	2.7
2	B	134	GLU	2.7
1	A	1962	ARG	2.7
1	A	1841	ALA	2.7
1	A	2023	LYS	2.7
2	B	89	PHE	2.7
1	A	2046	GLU	2.7
2	B	114	TRP	2.7
1	A	1981	ALA	2.7
1	A	1964	PRO	2.6
2	B	65[A]	GLY	2.6
2	B	13	VAL	2.6
2	B	28	GLN	2.6
2	B	87	ALA	2.6
2	B	95	ASN	2.6
2	B	214	PHE	2.6
2	B	286	GLU	2.6
2	B	68	TYR	2.6
1	A	1899[A]	TRP	2.6
1	A	2018[A]	ASN	2.5
2	B	37	PRO	2.5
2	B	18	ASP	2.5
1	A	1998	ARG	2.5
2	B	77	LEU	2.5
2	B	33	ILE	2.5
1	A	1904	ARG	2.5
2	B	59	TRP	2.5
2	B	234	PHE	2.5
1	A	1995	TRP	2.4
2	B	132	LYS	2.4
2	B	53	SER	2.4
2	B	223	GLU	2.4
2	B	274	THR	2.4
2	B	278	GLN	2.4
2	B	116	ASN	2.4
2	B	142	SER	2.4
2	B	289	TRP	2.4
1	A	1992	TYR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1875	ILE	2.4
2	B	123[A]	MET	2.4
2	B	304	ASN	2.3
1	A	1960[A]	GLU	2.3
1	A	1959	THR	2.3
2	B	55[A]	ARG	2.3
1	A	1902	GLN	2.3
1	A	2019	GLU	2.3
1	A	1869	ASN	2.3
2	B	99	ARG	2.3
1	A	1847	ASP	2.3
1	A	1976	ASP	2.3
2	B	75	ASP	2.3
1	A	1909	ALA	2.3
1	A	1873	LYS	2.3
1	A	1973	LYS	2.3
2	B	258	LYS	2.3
1	A	1940	MET	2.3
1	A	1836	ASN	2.2
1	A	1837	SER	2.2
2	B	197	ASP	2.2
2	B	47	GLN	2.2
2	B	82	GLU	2.2
2	B	149	GLU	2.2
2	B	84	ARG	2.2
1	A	1953	ASN	2.2
1	A	1882	LEU	2.2
2	B	102	MET	2.2
2	B	315	GLU	2.2
1	A	2041	PRO	2.2
1	A	1903	LYS	2.2
1	A	1918[A]	SER	2.2
1	A	2045	ASP	2.2
2	B	298	GLN	2.2
1	A	1851	PHE	2.2
2	B	290	ASN	2.2
1	A	1956	ILE	2.2
1	A	2033	THR	2.2
2	B	133	ASP	2.1
1	A	1946	VAL	2.1
2	B	188	ALA	2.1
2	B	88	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	211[A]	GLN	2.1
1	A	1838	SER	2.1
2	B	226	PHE	2.1
1	A	2004	ALA	2.1
2	B	245	ALA	2.1
1	A	2009	THR	2.1
2	B	17	ILE	2.1
1	A	1868	GLY	2.0
2	B	63	ARG	2.0
1	A	1996	LEU	2.0
2	B	199	LEU	2.0
2	B	268	LEU	2.0
2	B	144	MET	2.0
2	B	178[A]	TYR	2.0
2	B	125	LYS	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	W1W	A	2101	14/14	0.81	0.15	20,20,20,20	14

6.5 Other polymers [i](#)

There are no such residues in this entry.