



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 11:00 AM EDT

PDB ID : 7FKB / pdb_00007fkb
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P04C07 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 : 1.68 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

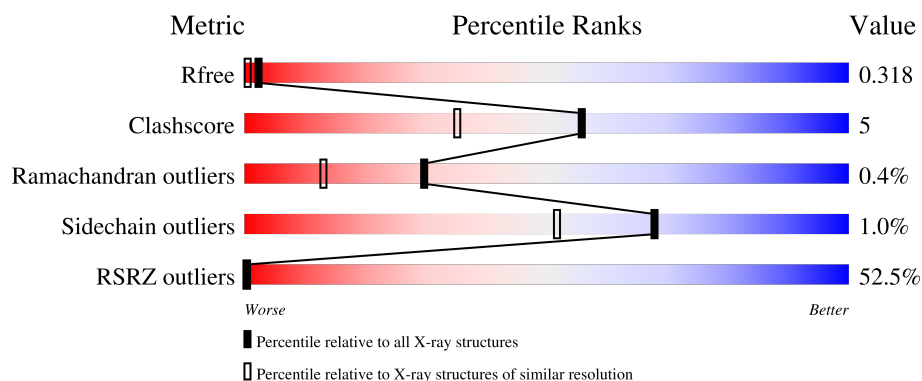
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	51% 81%10%8%
2	B	308	49% 85%12%..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9219 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	11	17	0

There are 20 discrepancies between the modelled and reference sequences:

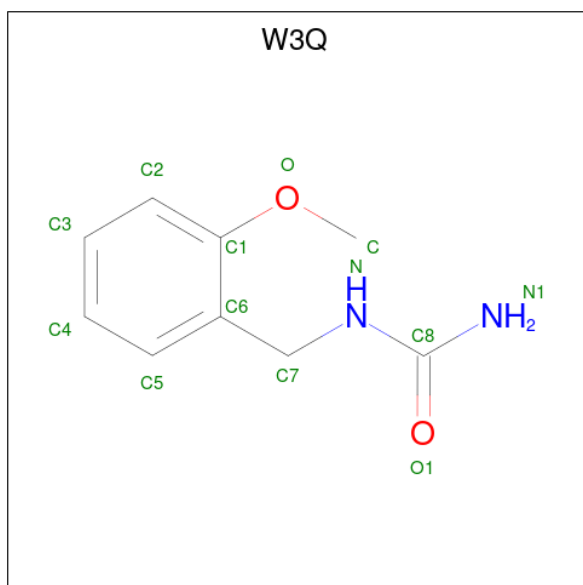
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN	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 N-[(2-methoxyphenyl)methyl]urea (CCD ID: W3Q) (formula: $C_9H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			13	9	2	2		

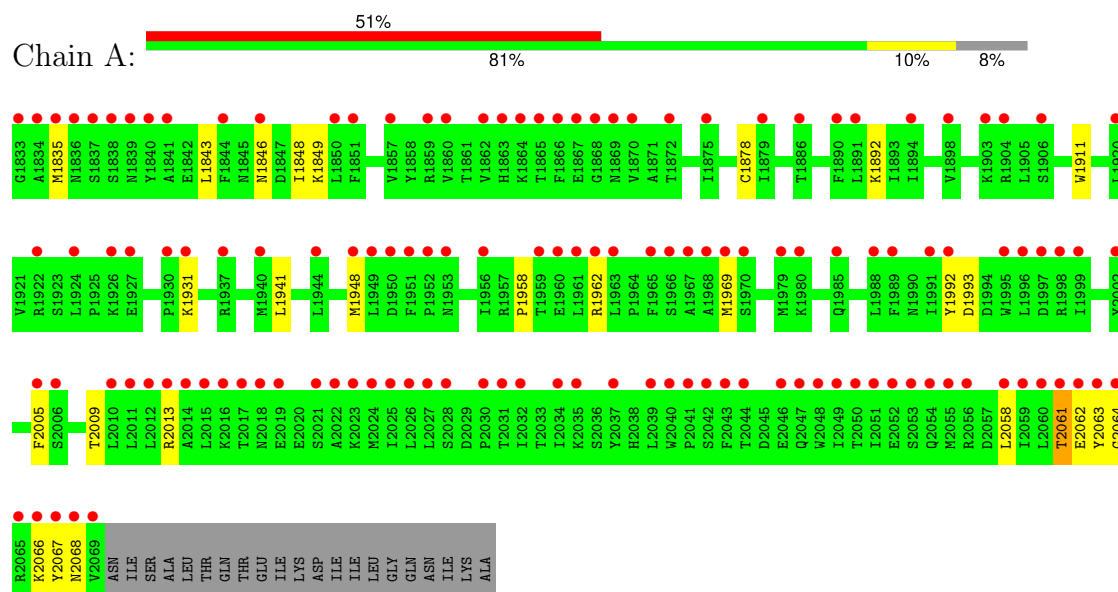
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total	O	0	0
			50	50		
4	B	44	Total	O	0	0
			44	44		

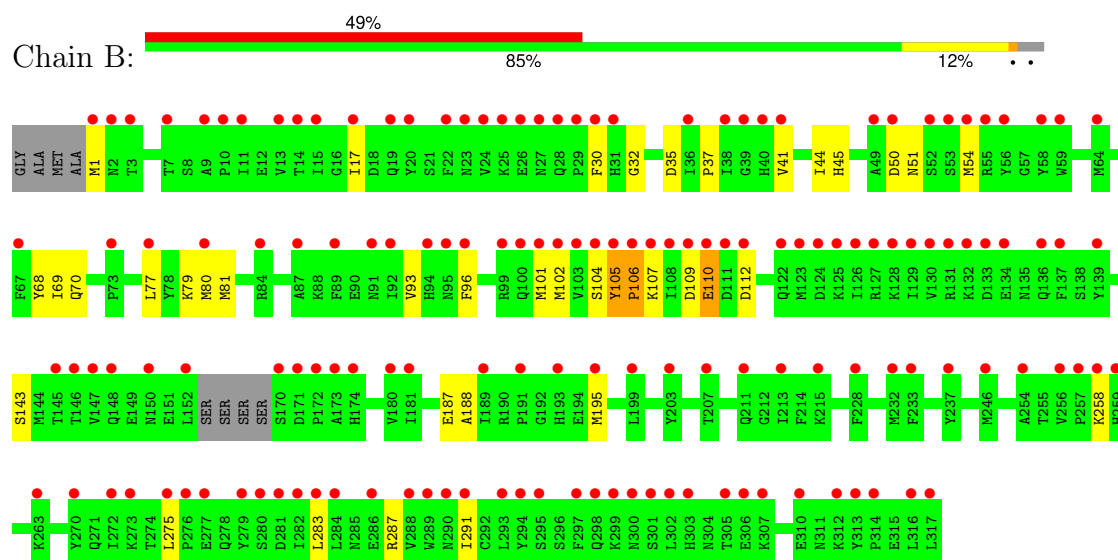
3 Residue-property plots

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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.74Å 81.59Å 93.35Å 90.00° 108.18° 90.00°	Depositor
Resolution (Å)	42.16 – 1.68 42.16 – 1.68	Depositor EDS
% Data completeness (in resolution range)	98.9 (42.16-1.68) 99.0 (42.16-1.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.94 (at 1.68Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.275 , 0.317 0.282 , 0.318	Depositor DCC
R_{free} test set	2091 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 45.1	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	0.94	EDS
Total number of atoms	9219	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: W3Q

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	0.69	0/2149	0.72	0/2911
2	B	0.91	2/2739 (0.1%)	0.92	8/3699 (0.2%)
All	All	0.82	2/4888 (0.0%)	0.84	8/6610 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	106	PRO	N-CA	29.23	1.69	1.47
2	B	30	PHE	C-O	-5.30	1.18	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	106	PRO	CA-C-O	-12.94	111.73	121.31
2	B	105	TYR	CA-C-N	9.96	135.36	121.91
2	B	105	TYR	C-N-CA	9.96	135.36	121.91
2	B	32	GLY	N-CA-C	6.99	119.67	111.63
2	B	106	PRO	CA-N-CD	-6.74	102.56	112.00
2	B	109	ASP	CB-CA-C	6.62	121.92	110.01
2	B	106	PRO	N-CA-C	-6.16	102.86	113.70
2	B	30	PHE	CA-CB-CG	-5.63	108.17	113.80

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	2008	2060	1974	18	1
2	B	2580	2464	2398	26	1
3	B	13	0	0	0	0
4	A	50	0	0	0	0
4	B	44	0	0	2	0
All	All	4695	4524	4372	43	1

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 5.

All (43) 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:106:PRO:N	2:B:106:PRO:CA	1.69	1.47
2:B:17:ILE:HD13	2:B:44[B]:ILE:HG12	1.55	0.88
2:B:37:PRO:HD3	2:B:105:TYR:CD1	2.13	0.84
2:B:70:GLN:HB3	2:B:81:MET:HE2	1.61	0.81
2:B:77:LEU:HD21	2:B:79:LYS:HE3	1.66	0.78
2:B:17:ILE:HD13	2:B:44[B]:ILE:CG1	2.17	0.75
2:B:1:MET:N	4:B:501:HOH:O	2.20	0.73
1:A:1962:ARG:O	1:A:2013:ARG:NH1	2.24	0.70
2:B:106:PRO:N	2:B:106:PRO:C	2.51	0.68
2:B:37:PRO:CD	2:B:105:TYR:CE1	2.79	0.66
2:B:68:TYR:CE2	2:B:81:MET:HE3	2.32	0.65
2:B:37:PRO:CD	2:B:105:TYR:CD1	2.80	0.64
2:B:258:LYS:HD2	2:B:258:LYS:H	1.63	0.62
1:A:1878:CYS:SG	1:A:1969:MET:HE3	2.40	0.61
1:A:2061:THR:O	1:A:2064:GLY:N	2.33	0.60
2:B:96:PHE:HB2	2:B:102:MET:HE2	1.86	0.58
2:B:1:MET:HB3	2:B:35:ASP:HA	1.85	0.58
1:A:2064:GLY:O	1:A:2068:ASN:N	2.38	0.55
1:A:1911:TRP:CD1	2:B:195:MET:HE3	2.40	0.55
1:A:1941:LEU:HD11	1:A:1958:PRO:HB3	1.90	0.54
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	1.90	0.54
2:B:287:ARG:O	2:B:291:ILE:HD13	2.10	0.52
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.56	0.52
2:B:110:GLU:O	2:B:110:GLU:HG3	2.10	0.52
2:B:37:PRO:HD2	2:B:105:TYR:CE1	2.45	0.51
2:B:54[B]:MET:HE1	2:B:143:SER:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.37	0.49
2:B:41[A]:VAL:HG12	4:B:526:HOH:O	2.13	0.48
2:B:93:VAL:HG13	2:B:102:MET:HE1	1.96	0.47
1:A:1962:ARG:HD3	1:A:1962:ARG:H	1.81	0.45
2:B:275:LEU:CD2	2:B:283:LEU:HD13	2.47	0.45
2:B:69:ILE:HD13	2:B:80:MET:HA	1.99	0.44
1:A:2005:PHE:O	1:A:2009:THR:HG23	2.18	0.43
1:A:1878:CYS:HA	1:A:1892:LYS:O	2.18	0.43
2:B:50:ASP:OD1	2:B:51:ASN:N	2.52	0.43
1:A:1948:MET:HE3	1:A:1948:MET:HB3	1.94	0.42
2:B:187:GLU:H	2:B:187:GLU:CD	2.28	0.42
1:A:2061:THR:O	1:A:2063:TYR:N	2.53	0.41
1:A:1992:TYR:O	1:A:1993:ASP:C	2.62	0.41
1:A:2063:TYR:C	1:A:2063:TYR:CD1	2.98	0.41
1:A:2066:LYS:HD2	1:A:2067:TYR:CE1	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1846:ASN:OD1	2:B:112:ASP:OD1[4_555]	2.14	0.06

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%)	249 (96%)	7 (3%)	2 (1%)	16	4
2	B	315/308 (102%)	300 (95%)	15 (5%)	0	100	100
All	All	573/566 (101%)	549 (96%)	22 (4%)	2 (0%)	30	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2061	THR
1	A	2062	GLU

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%)	237 (100%)	0	100	100
2	B	294/284 (104%)	288 (98%)	6 (2%)	48	23
All	All	531/517 (103%)	525 (99%)	6 (1%)	68	47

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

Mol	Chain	Res	Type
2	B	45[A]	HIS
2	B	45[B]	HIS
2	B	101	MET
2	B	104	SER
2	B	107	LYS
2	B	110	GLU

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

Mol	Chain	Res	Type
2	B	47	GLN
2	B	135	ASN
2	B	174	HIS
2	B	259	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 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	W3Q	B	401	-	13,13,13	1.34	2 (15%)	16,16,16	1.03	1 (6%)

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	W3Q	B	401	-	-	0/7/7/7	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	W3Q	C8-N	2.64	1.38	1.34
3	B	401	W3Q	O1-C8	-2.44	1.20	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	W3Q	C-O-C1	-2.57	113.74	117.51

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

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%)	2.81	132 (55%) 0 0	22, 61, 140, 186	12 (5%)
2	B	300/308 (97%)	2.47	150 (50%) 0 0	20, 61, 128, 178	9 (3%)
All	All	537/566 (94%)	2.62	282 (52%) 0 0	20, 61, 135, 186	21 (3%)

All (282) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2059	ILE	12.2
1	A	2060	LEU	10.8
2	B	29	PRO	10.5
2	B	49	ALA	8.9
1	A	2069	VAL	8.7
1	A	1965	PHE	8.7
1	A	1840	TYR	8.2
1	A	2015	LEU	8.1
1	A	2017[A]	THR	8.1
2	B	152	LEU	8.1
1	A	1930	PRO	8.0
1	A	1951	PHE	7.7
2	B	256	VAL	7.3
1	A	2063	TYR	6.8
1	A	2061	THR	6.8
1	A	2051	ILE	6.8
1	A	2048	TRP	6.8
2	B	24	VAL	6.8
1	A	2002[A]	TYR	6.8
1	A	1979[A]	MET	6.7
2	B	1	MET	6.6
2	B	106	PRO	6.6
2	B	283	LEU	6.6
2	B	316	LEU	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	2040	TRP	6.4
1	A	2014	ALA	6.3
2	B	275	LEU	6.2
1	A	2067	TYR	6.0
1	A	2016	LYS	6.0
1	A	1961[A]	LEU	6.0
1	A	2065	ARG	6.0
2	B	41[A]	VAL	5.9
2	B	291	ILE	5.9
2	B	279	TYR	5.9
1	A	2058	LEU	5.9
2	B	111	ASP	5.9
2	B	172	PRO	5.9
1	A	2025	ILE	5.8
2	B	101	MET	5.8
2	B	54[A]	MET	5.8
1	A	1999	ILE	5.7
2	B	22	PHE	5.7
1	A	2055	MET	5.7
2	B	170	SER	5.6
1	A	2022	ALA	5.6
1	A	1948	MET	5.6
1	A	2023	LYS	5.6
2	B	127	ARG	5.5
2	B	129	ILE	5.5
1	A	1835	MET	5.4
2	B	108	ILE	5.4
2	B	28	GLN	5.3
2	B	128	LYS	5.3
2	B	203[A]	TYR	5.3
1	A	2027	LEU	5.2
2	B	147	VAL	5.2
2	B	280	SER	5.2
2	B	92	ILE	5.1
2	B	132	LYS	5.1
1	A	1956	ILE	5.0
1	A	2050	THR	5.0
2	B	281	ASP	5.0
1	A	1834	ALA	5.0
1	A	1866	PHE	5.0
2	B	23	ASN	4.9
2	B	270	TYR	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	2026	LEU	4.8
1	A	2021	SER	4.8
2	B	313	TYR	4.8
2	B	282	ILE	4.8
2	B	294	TYR	4.8
2	B	13	VAL	4.8
2	B	174	HIS	4.7
1	A	2056[A]	ARG	4.6
2	B	130	VAL	4.6
2	B	299	LYS	4.6
1	A	2011	LEU	4.6
2	B	103	VAL	4.5
2	B	180	VAL	4.5
1	A	1940	MET	4.5
2	B	80	MET	4.5
2	B	104	SER	4.5
1	A	2066	LYS	4.5
2	B	38	ILE	4.5
1	A	2013	ARG	4.4
2	B	317	LEU	4.4
2	B	134	GLU	4.4
1	A	2018[A]	ASN	4.3
1	A	2064	GLY	4.3
2	B	290	ASN	4.3
1	A	2044	THR	4.3
2	B	50	ASP	4.3
2	B	96	PHE	4.3
1	A	1841	ALA	4.2
2	B	307	LYS	4.2
2	B	181	ILE	4.2
2	B	213	ILE	4.2
1	A	2068	ASN	4.2
2	B	27	ASN	4.2
1	A	2019	GLU	4.1
1	A	2039	LEU	4.1
1	A	1995	TRP	4.1
1	A	2046	GLU	4.1
2	B	20	TYR	4.1
1	A	2043	PHE	4.1
1	A	1870	VAL	4.1
1	A	1898[A]	VAL	4.1
1	A	1966	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	1864	LYS	4.1
1	A	1998	ARG	4.0
2	B	284	LEU	4.0
1	A	1931[A]	LYS	4.0
1	A	2032	ILE	4.0
2	B	52	SER	4.0
1	A	1862	VAL	4.0
2	B	312	LYS	3.9
1	A	1927	GLU	3.9
1	A	1952	PRO	3.9
2	B	107	LYS	3.9
1	A	2005	PHE	3.9
2	B	30	PHE	3.9
1	A	1860	VAL	3.8
1	A	2062	GLU	3.8
2	B	11	ILE	3.8
2	B	7	THR	3.8
2	B	124	ASP	3.8
2	B	39	GLY	3.7
2	B	305	THR	3.7
1	A	2049	ILE	3.7
1	A	1865	THR	3.7
1	A	2006	SER	3.7
1	A	1926	LYS	3.7
1	A	1886	THR	3.7
1	A	2054[A]	GLN	3.6
1	A	1869	ASN	3.6
2	B	95	ASN	3.6
2	B	136	GLN	3.6
1	A	1967	ALA	3.5
2	B	303	HIS	3.5
2	B	3	THR	3.5
2	B	276	PRO	3.5
1	A	1953	ASN	3.5
2	B	40	HIS	3.5
2	B	173	ALA	3.5
1	A	2035	LYS	3.5
2	B	109	ASP	3.4
2	B	126	ILE	3.4
1	A	1963	LEU	3.4
1	A	2052	GLU	3.4
2	B	89	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	2053[A]	SER	3.3
1	A	1922	ARG	3.3
2	B	64[A]	MET	3.3
1	A	1989	PHE	3.3
2	B	10	PRO	3.3
1	A	1837	SER	3.3
2	B	272	ILE	3.3
1	A	1924	LEU	3.3
1	A	2012	LEU	3.3
2	B	254	ALA	3.3
2	B	257	PRO	3.2
1	A	1949	LEU	3.2
2	B	233	PHE	3.2
1	A	2047	GLN	3.2
2	B	14	THR	3.2
2	B	56	TYR	3.2
2	B	146	THR	3.2
1	A	1863	HIS	3.2
2	B	53	SER	3.2
2	B	26	GLU	3.2
2	B	306	GLU	3.2
1	A	1903	LYS	3.2
2	B	258	LYS	3.2
1	A	2010	LEU	3.1
1	A	1833	GLY	3.1
2	B	122[A]	GLN	3.1
2	B	211[A]	GLN	3.1
2	B	131	ARG	3.1
2	B	2	ASN	3.1
2	B	314	PRO	3.1
1	A	1960[A]	GLU	3.1
2	B	310	GLU	3.1
1	A	1857	VAL	3.0
2	B	94	HIS	3.0
2	B	273	LYS	3.0
2	B	286	GLU	3.0
1	A	2024[A]	MET	3.0
2	B	102	MET	3.0
2	B	195	MET	3.0
2	B	246	MET	3.0
1	A	1962	ARG	3.0
2	B	237	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	1997	ASP	3.0
1	A	1944	LEU	3.0
2	B	301	SER	2.9
2	B	277	GLU	2.9
1	A	1879	ILE	2.9
1	A	1894	ILE	2.9
1	A	1846	ASN	2.9
2	B	150	ASN	2.9
1	A	1838	SER	2.9
1	A	1970	SER	2.9
2	B	105	TYR	2.9
1	A	1868	GLY	2.9
2	B	171	ASP	2.9
1	A	1867	GLU	2.9
2	B	193	HIS	2.9
2	B	139	TYR	2.9
2	B	125	LYS	2.8
2	B	232	MET	2.8
2	B	9	ALA	2.8
2	B	288	VAL	2.8
1	A	1891	LEU	2.8
1	A	1991	ILE	2.8
2	B	300	ASN	2.8
2	B	298	GLN	2.8
1	A	1959	THR	2.8
2	B	137	PHE	2.7
2	B	87	ALA	2.7
1	A	1906	SER	2.7
2	B	36	ILE	2.7
1	A	2042	SER	2.6
2	B	110	GLU	2.6
1	A	2030	PRO	2.6
2	B	91	ASN	2.6
1	A	1937	ARG	2.5
2	B	55[A]	ARG	2.5
1	A	1836	ASN	2.5
2	B	84	ARG	2.5
1	A	2034	ILE	2.5
2	B	145	THR	2.5
2	B	99	ARG	2.5
2	B	25	LYS	2.5
1	A	2028	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	191	PRO	2.4
1	A	1985	GLN	2.4
2	B	259	HIS	2.4
2	B	293	LEU	2.4
2	B	297	PHE	2.4
2	B	112	ASP	2.4
2	B	123[A]	MET	2.4
1	A	2031	THR	2.3
1	A	1969	MET	2.3
1	A	1890	PHE	2.3
2	B	228	PHE	2.3
1	A	1992	TYR	2.3
1	A	1996	LEU	2.3
1	A	1980[A]	LYS	2.3
1	A	2037	TYR	2.3
2	B	289	TRP	2.2
2	B	73	PRO	2.2
2	B	133	ASP	2.2
1	A	1844	PHE	2.2
1	A	1851	PHE	2.2
1	A	2041	PRO	2.2
1	A	1859	ARG	2.2
1	A	1904	ARG	2.2
2	B	263	LYS	2.2
1	A	1920	LEU	2.2
2	B	302	LEU	2.2
1	A	1875	ILE	2.2
1	A	1850	LEU	2.2
2	B	148	GLN	2.1
2	B	59	TRP	2.1
2	B	199	LEU	2.1
2	B	215	LYS	2.1
2	B	58	TYR	2.1
1	A	1968	ALA	2.1
2	B	100	GLN	2.1
1	A	1872	THR	2.1
2	B	207	THR	2.1
2	B	67	PHE	2.1
2	B	15	ILE	2.1
2	B	17	ILE	2.1
1	A	1839	ASN	2.1
2	B	19	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1988	LEU	2.1
2	B	189	ILE	2.1
1	A	1950	ASP	2.0
2	B	77	LEU	2.0
2	B	295	SER	2.0
2	B	31	HIS	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(Å ²)	Q<0.9
3	W3Q	B	401	13/13	0.75	0.17	20,20,20,20	13

6.5 Other polymers [i](#)

There are no such residues in this entry.