



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:59 PM UTC

PDB ID : 7FPD / pdb_00007fpd
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P09E01 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 : 1.61 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

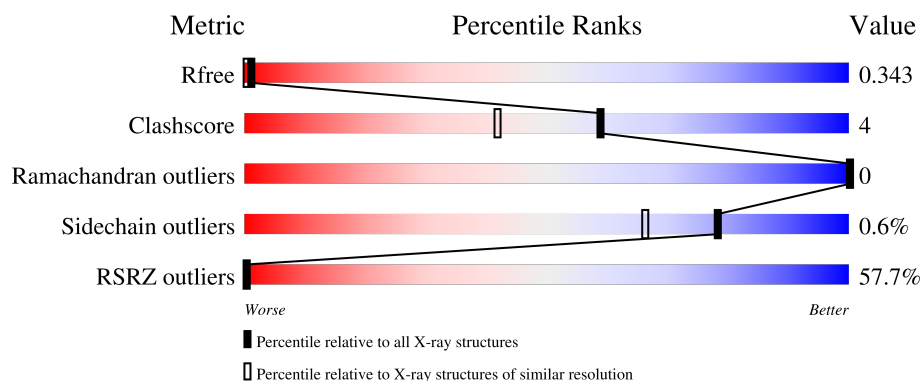
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.61 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	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (1.64-1.60)

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	58% 81% 11% 8%
2	B	308	52% 88% 9% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9225 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	33	17	0

There are 20 discrepancies between the modelled and reference sequences:

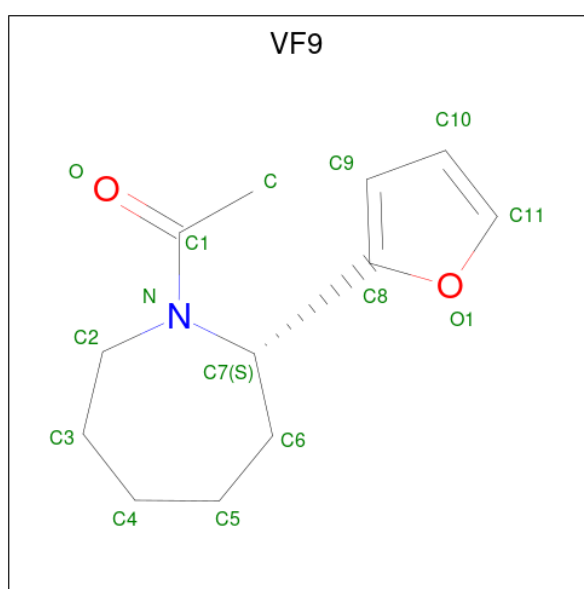
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN	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-[(2S)-2-(furan-2-yl)azepan-1-yl]ethan-1-one (CCD ID: VF9) (formula: C₁₂H₁₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	12	1	2		

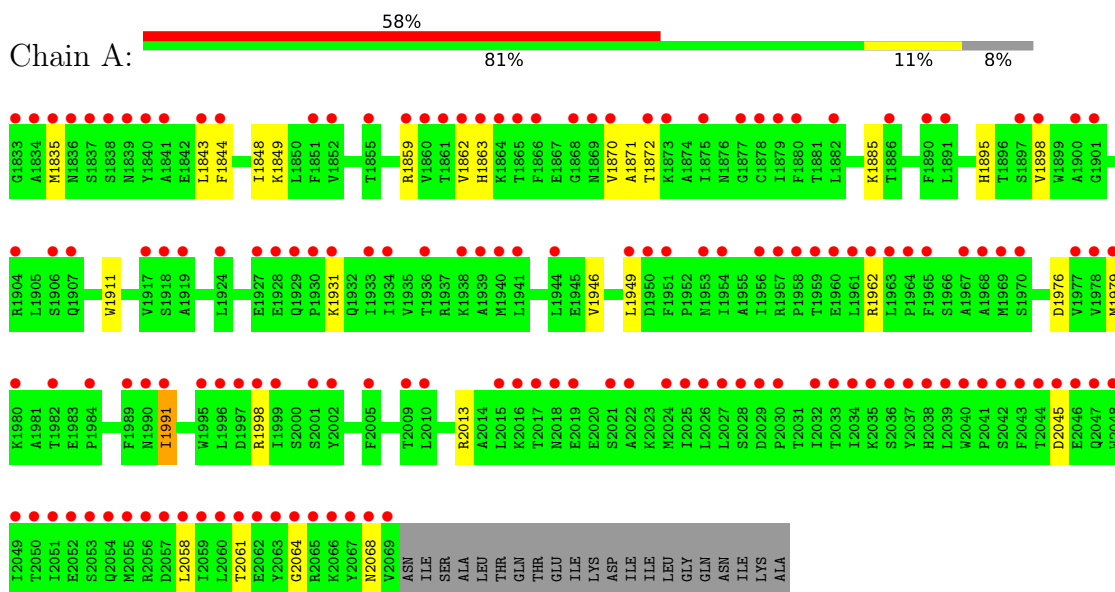
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total	O	0	0
			57	57		
4	B	41	Total	O	0	0
			41	41		

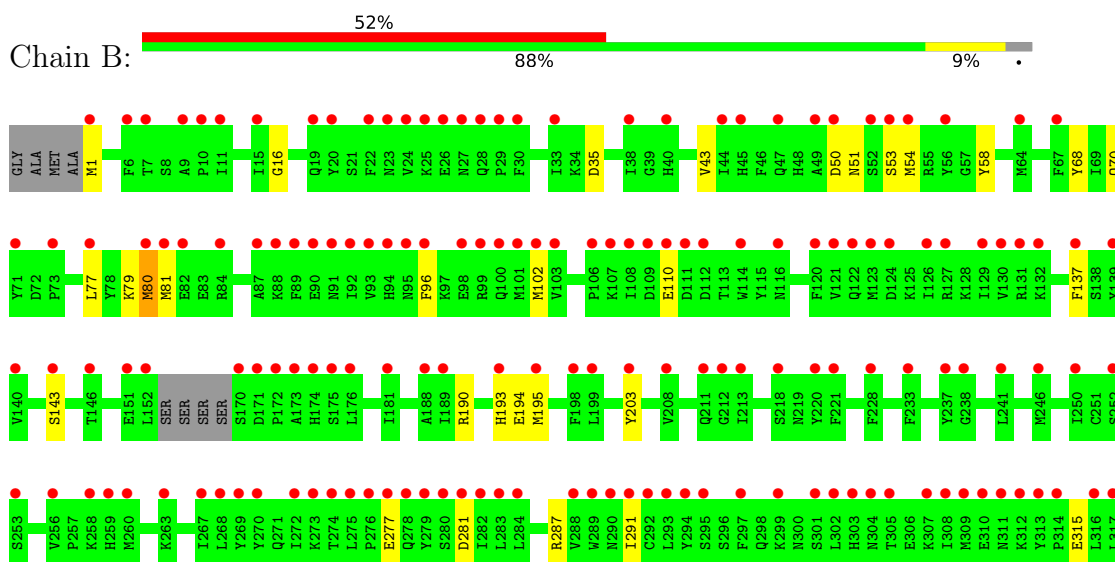
3 Residue-property plots

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	88.55Å 81.77Å 93.21Å 90.00° 108.27° 90.00°	Depositor
Resolution (Å)	42.04 – 1.61 42.04 – 1.61	Depositor EDS
% Data completeness (in resolution range)	99.1 (42.04-1.61) 99.3 (42.04-1.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.62Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.283 , 0.321 0.291 , 0.343	Depositor DCC
R_{free} test set	2100 reflections (2.61%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9225	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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: VF9

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	0.77	1/2149 (0.0%)	0.88	0/2911
2	B	0.64	1/2739 (0.0%)	0.79	0/3699
All	All	0.70	2/4888 (0.0%)	0.83	0/6610

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	80	MET	SD-CE	-7.71	1.60	1.79
1	A	1991	ILE	C-O	-5.45	1.17	1.24

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	17	0
2	B	2580	2464	2398	24	0
3	A	15	0	0	0	0
4	A	57	0	0	1	0
4	B	41	0	0	2	0
All	All	4701	4524	4372	40	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 (40) 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:1895:HIS:O	1:A:1898[A]:VAL:HG22	1.85	0.77
1:A:1976:ASP:HB3	4:A:2204:HOH:O	1.87	0.74
2:B:80:MET:SD	2:B:137:PHE:CG	2.80	0.74
2:B:96:PHE:HB2	2:B:102:MET:HE3	1.73	0.69
1:A:1862:VAL:HG22	1:A:1872:THR:HG22	1.75	0.68
1:A:1962:ARG:O	1:A:2013:ARG:NH1	2.29	0.66
2:B:80:MET:SD	2:B:137:PHE:CD2	2.89	0.66
1:A:2064:GLY:O	1:A:2068:ASN:N	2.25	0.64
1:A:2061:THR:O	1:A:2064:GLY:N	2.32	0.63
2:B:287:ARG:O	2:B:291:ILE:HD13	2.02	0.59
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.53	0.57
2:B:1:MET:HB3	2:B:35:ASP:HA	1.87	0.56
2:B:70:GLN:HB3	2:B:81:MET:HE2	1.87	0.56
2:B:77:LEU:HD21	2:B:79:LYS:HE3	1.89	0.55
2:B:1:MET:N	4:B:401:HOH:O	2.40	0.54
2:B:68:TYR:CE2	2:B:81:MET:HE3	2.44	0.53
1:A:1911:TRP:CD2	2:B:195:MET:HB2	2.45	0.51
2:B:96:PHE:CB	2:B:102:MET:HE3	2.42	0.49
1:A:1946:VAL:O	1:A:1949:LEU:HG	2.14	0.48
2:B:50:ASP:OD1	2:B:51:ASN:N	2.48	0.47
2:B:53:SER:HB2	4:B:433:HOH:O	2.15	0.46
1:A:1998:ARG:NH1	1:A:2045:ASP:OD2	2.45	0.45
2:B:1:MET:HE3	2:B:35:ASP:O	2.17	0.44
2:B:190:ARG:HG3	2:B:203[B]:TYR:CE2	2.52	0.44
1:A:1859:ARG:HH12	1:A:1979[A]:MET:CE	2.30	0.44
2:B:43:VAL:O	2:B:43:VAL:HG13	2.18	0.43
1:A:1844:PHE:O	1:A:1885:LYS:NZ	2.26	0.43
1:A:1863:HIS:CE1	1:A:1871:ALA:HB3	2.53	0.43
2:B:190:ARG:HG3	2:B:203[B]:TYR:CZ	2.53	0.43
2:B:110:GLU:O	2:B:110:GLU:HG2	2.20	0.42
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	2.02	0.42
2:B:277:GLU:CD	2:B:277:GLU:H	2.28	0.42
2:B:54[B]:MET:HE1	2:B:143:SER:HB3	2.02	0.41
2:B:193:HIS:O	2:B:194:GLU:C	2.63	0.41
1:A:1862:VAL:HG13	1:A:1870:VAL:CG1	2.49	0.41
2:B:43:VAL:HA	2:B:58:TYR:O	2.20	0.41
2:B:80:MET:CG	2:B:81:MET:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.45	0.41

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%)	252 (98%)	6 (2%)	0	100	100
2	B	315/308 (102%)	303 (96%)	12 (4%)	0	100	100
All	All	573/566 (101%)	555 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

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%)	236 (100%)	1 (0%)	84	75
2	B	294/284 (104%)	292 (99%)	2 (1%)	76	62
All	All	531/517 (103%)	528 (99%)	3 (1%)	78	66

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1991	Ile
2	B	281	ASP
2	B	315	GLU

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	1863	HIS
2	B	40	HIS
2	B	135	ASN
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	VF9	A	2101	-	15,16,16	2.09	5 (33%)	16,21,21	1.39	3 (18%)

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	VF9	A	2101	-	-	1/4/20/20	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	VF9	C2-N	-5.05	1.39	1.47
3	A	2101	VF9	O1-C8	-3.88	1.29	1.36
3	A	2101	VF9	O1-C11	-2.81	1.28	1.37
3	A	2101	VF9	C9-C8	-2.22	1.27	1.34
3	A	2101	VF9	C10-C11	-2.01	1.25	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2101	VF9	C11-O1-C8	2.37	110.37	106.13
3	A	2101	VF9	C3-C2-N	-2.36	109.34	113.10
3	A	2101	VF9	C5-C6-C7	2.08	116.86	113.89

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2101	VF9	C-C1-N-C7

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%)	3.07	150 (63%) 0 0	22, 72, 152, 211	12 (5%)
2	B	300/308 (97%)	2.43	160 (53%) 0 0	23, 73, 139, 260	9 (3%)
All	All	537/566 (94%)	2.71	310 (57%) 0 0	22, 73, 145, 260	21 (3%)

All (310) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2039	LEU	12.2
1	A	2040	TRP	12.0
1	A	2037	TYR	11.8
1	A	1979[A]	MET	10.7
1	A	2048	TRP	10.0
2	B	152	LEU	9.3
1	A	2042	SER	8.6
1	A	2069	VAL	8.5
2	B	54[A]	MET	8.4
1	A	1931[A]	LYS	8.3
1	A	2034	ILE	8.2
1	A	2051	ILE	7.6
1	A	2060	LEU	7.5
2	B	283	LEU	7.5
1	A	2063	TYR	7.3
1	A	2041	PRO	7.2
2	B	275	LEU	7.1
2	B	316	LEU	7.1
1	A	2038	HIS	7.0
2	B	103	VAL	6.8
1	A	2036	SER	6.8
1	A	2017[A]	THR	6.7
2	B	106	PRO	6.3
1	A	2059	ILE	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	1852	VAL	6.2
1	A	1862	VAL	6.2
1	A	1927	GLU	6.1
2	B	289	TRP	6.1
2	B	126	ILE	6.1
1	A	2022	ALA	6.0
1	A	2065	ARG	5.9
2	B	101	MET	5.8
1	A	1964	PRO	5.8
2	B	279	TYR	5.8
1	A	2067	TYR	5.8
1	A	1880	PHE	5.8
2	B	203[A]	TYR	5.7
2	B	317	LEU	5.7
2	B	246	MET	5.7
2	B	22	PHE	5.5
1	A	1996	LEU	5.5
1	A	1840	TYR	5.5
1	A	2043	PHE	5.4
1	A	1860	VAL	5.4
2	B	174	HIS	5.4
1	A	1963	LEU	5.4
2	B	313	TYR	5.4
1	A	1834	ALA	5.3
1	A	1989	PHE	5.3
2	B	6	PHE	5.3
1	A	2068	ASN	5.3
2	B	281	ASP	5.2
2	B	80	MET	5.2
1	A	1866	PHE	5.2
1	A	2064	GLY	5.2
1	A	2058	LEU	5.1
1	A	2033	THR	5.1
2	B	294	TYR	5.0
2	B	1	MET	5.0
1	A	1872	THR	5.0
1	A	2035	LYS	5.0
2	B	30	PHE	5.0
1	A	2032	ILE	4.9
1	A	2052	GLU	4.9
1	A	1833	GLY	4.9
2	B	92	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
2	B	137	PHE	4.8
1	A	2026	LEU	4.8
1	A	1835	MET	4.8
1	A	2061	THR	4.8
2	B	111	ASP	4.7
2	B	276	PRO	4.7
1	A	1997	ASP	4.6
1	A	2002[A]	TYR	4.6
1	A	1954	ILE	4.6
1	A	1886	THR	4.5
2	B	213	ILE	4.5
2	B	282	ILE	4.5
1	A	2056[A]	ARG	4.5
1	A	1851	PHE	4.5
2	B	122[A]	GLN	4.5
1	A	1959	THR	4.5
1	A	2027	LEU	4.4
2	B	312	LYS	4.4
1	A	2053[A]	SER	4.4
1	A	2024[A]	MET	4.3
1	A	1936	THR	4.2
1	A	1995	TRP	4.2
2	B	303	HIS	4.2
2	B	291	ILE	4.2
1	A	2044	THR	4.2
2	B	237	TYR	4.2
1	A	1933	ILE	4.2
2	B	129	ILE	4.2
2	B	173	ALA	4.1
2	B	96	PHE	4.1
2	B	288	VAL	4.1
1	A	1836	ASN	4.1
1	A	1984	PRO	4.1
1	A	2016	LYS	4.1
1	A	1924	LEU	4.0
2	B	24	VAL	4.0
2	B	284	LEU	4.0
2	B	280	SER	4.0
2	B	172	PRO	3.9
2	B	84	ARG	3.9
1	A	2025	ILE	3.9
2	B	181	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	274	THR	3.8
2	B	45[A]	HIS	3.8
2	B	233	PHE	3.8
2	B	272	ILE	3.8
1	A	1855[A]	THR	3.8
1	A	1978	VAL	3.8
2	B	95	ASN	3.8
2	B	108	ILE	3.7
1	A	2015	LEU	3.7
2	B	193	HIS	3.7
2	B	228	PHE	3.7
1	A	1990	ASN	3.7
2	B	29	PRO	3.7
2	B	293	LEU	3.7
1	A	1965	PHE	3.7
1	A	1898[A]	VAL	3.7
1	A	1863	HIS	3.6
2	B	143	SER	3.6
2	B	170	SER	3.6
2	B	198	PHE	3.6
1	A	1870	VAL	3.6
1	A	1939	ALA	3.6
2	B	49	ALA	3.6
2	B	87	ALA	3.6
2	B	130	VAL	3.6
1	A	2028	SER	3.6
2	B	107	LYS	3.6
1	A	1958	PRO	3.6
1	A	1998	ARG	3.6
1	A	1868	GLY	3.6
1	A	2001[A]	SER	3.6
1	A	2047	GLN	3.6
1	A	1873	LYS	3.5
2	B	307	LYS	3.5
2	B	292	CYS	3.5
2	B	20	TYR	3.5
1	A	1882	LEU	3.5
1	A	2030	PRO	3.5
1	A	2066	LYS	3.4
2	B	151	GLU	3.4
1	A	1934	ILE	3.4
1	A	1878	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	23	ASN	3.4
1	A	2049	ILE	3.3
2	B	131	ARG	3.3
2	B	267	ILE	3.3
2	B	10	PRO	3.3
2	B	314	PRO	3.3
2	B	208	VAL	3.3
2	B	53	SER	3.3
2	B	121	VAL	3.3
1	A	2055	MET	3.2
1	A	1837	SER	3.2
2	B	308	ILE	3.2
2	B	268	LEU	3.2
1	A	1953	ASN	3.2
2	B	139	TYR	3.2
2	B	146	THR	3.2
1	A	1951	PHE	3.2
2	B	94	HIS	3.2
2	B	110	GLU	3.2
1	A	2009	THR	3.2
2	B	40	HIS	3.1
2	B	258	LYS	3.1
2	B	123[A]	MET	3.1
2	B	52	SER	3.1
2	B	220	TYR	3.0
1	A	1869	ASN	3.0
1	A	1875	ILE	3.0
2	B	199	LEU	3.0
2	B	305	THR	3.0
1	A	2010	LEU	3.0
2	B	253	SER	3.0
2	B	102	MET	3.0
2	B	91	ASN	3.0
1	A	1961[A]	LEU	3.0
2	B	44[A]	ILE	3.0
1	A	2005	PHE	3.0
1	A	2050	THR	2.9
1	A	1956	ILE	2.9
2	B	93	VAL	2.9
1	A	1839	ASN	2.9
1	A	1879	ILE	2.9
2	B	273	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1838	SER	2.9
2	B	259	HIS	2.9
2	B	26	GLU	2.8
2	B	109	ASP	2.8
2	B	127	ARG	2.8
2	B	120	PHE	2.8
2	B	295	SER	2.8
1	A	1843	LEU	2.8
1	A	2029	ASP	2.8
2	B	124	ASP	2.8
2	B	99	ARG	2.8
1	A	1960[A]	GLU	2.8
2	B	50	ASP	2.8
1	A	1962	ARG	2.7
1	A	2046	GLU	2.7
2	B	256	VAL	2.7
1	A	1991	ILE	2.7
2	B	38	ILE	2.7
1	A	1861	THR	2.7
2	B	7	THR	2.7
2	B	310	GLU	2.7
2	B	241	LEU	2.7
2	B	90	GLU	2.7
2	B	116	ASN	2.7
2	B	260	MET	2.7
1	A	2057[A]	ASP	2.7
2	B	112	ASP	2.7
1	A	2062	GLU	2.6
2	B	175	SER	2.6
2	B	297	PHE	2.6
2	B	309	MET	2.6
2	B	189	ILE	2.6
2	B	28	GLN	2.6
1	A	1859	ARG	2.6
2	B	302	LEU	2.6
2	B	15	ILE	2.6
1	A	1897	SER	2.6
1	A	1970	SER	2.6
1	A	1865	THR	2.6
1	A	1967	ALA	2.6
1	A	1901	GLY	2.5
1	A	2054[A]	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	100	GLN	2.5
1	A	1890	PHE	2.5
1	A	1941	LEU	2.5
2	B	88	LYS	2.5
1	A	2018[A]	ASN	2.5
1	A	2019	GLU	2.5
2	B	27	ASN	2.5
2	B	82	GLU	2.5
1	A	1907	GLN	2.5
1	A	1968	ALA	2.5
2	B	11	ILE	2.5
1	A	1940	MET	2.5
2	B	290	ASN	2.5
1	A	1929	GLN	2.5
2	B	278	GLN	2.5
2	B	221	PHE	2.5
1	A	1928	GLU	2.5
2	B	77	LEU	2.4
2	B	263	LYS	2.4
2	B	98	GLU	2.4
1	A	1917	VAL	2.4
1	A	1877	GLY	2.4
1	A	1891	LEU	2.4
1	A	1949	LEU	2.4
2	B	73	PRO	2.4
2	B	176	LEU	2.4
2	B	252	SER	2.4
2	B	33	ILE	2.4
1	A	1864	LYS	2.4
1	A	1957	ARG	2.4
1	A	1844	PHE	2.4
2	B	277	GLU	2.4
2	B	195	MET	2.4
1	A	1900	ALA	2.3
1	A	1919[A]	ALA	2.3
1	A	1969	MET	2.3
1	A	1999	ILE	2.3
1	A	1938	LYS	2.3
2	B	132	LYS	2.3
1	A	1841	ALA	2.3
2	B	270	TYR	2.3
2	B	311	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1906	SER	2.3
2	B	25	LYS	2.3
2	B	89	PHE	2.3
1	A	1977	VAL	2.3
2	B	9	ALA	2.2
2	B	304	ASN	2.2
2	B	212[A]	GLY	2.2
1	A	1904	ARG	2.2
2	B	188	ALA	2.2
2	B	301	SER	2.2
1	A	1930	PRO	2.2
2	B	299	LYS	2.2
2	B	218	SER	2.2
2	B	81	MET	2.2
2	B	56	TYR	2.2
2	B	269	TYR	2.2
2	B	47	GLN	2.1
2	B	19	GLN	2.1
1	A	2021	SER	2.1
1	A	2045	ASP	2.1
1	A	1982	THR	2.1
2	B	67	PHE	2.1
2	B	250	ILE	2.1
2	B	238	GLY	2.1
1	A	1950	ASP	2.1
2	B	211[A]	GLN	2.1
2	B	64[A]	MET	2.0
1	A	1918[A]	SER	2.0
2	B	140	VAL	2.0
1	A	1944	LEU	2.0
2	B	114	TRP	2.0
2	B	71	TYR	2.0
2	B	171	ASP	2.0
1	A	1980[A]	LYS	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 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	VF9	A	2101	15/15	0.75	0.16	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.