



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:02 AM UTC

PDB ID : 7FN4 / pdb_00007fn4
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P06G11 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 : 1.72 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

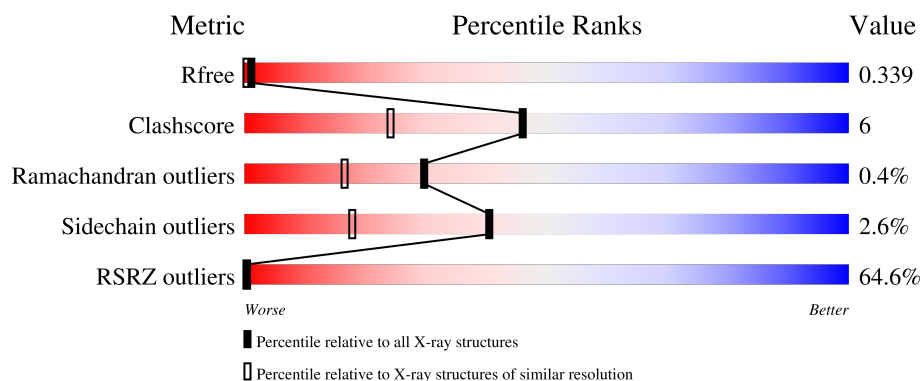
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	60% 76% 13% • 8%
2	B	308	63% 83% 14% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9188 atoms, of which 4516 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	5027	1649	2456	419	483	20	22	16	0

There are 20 discrepancies between the modelled and reference sequences:

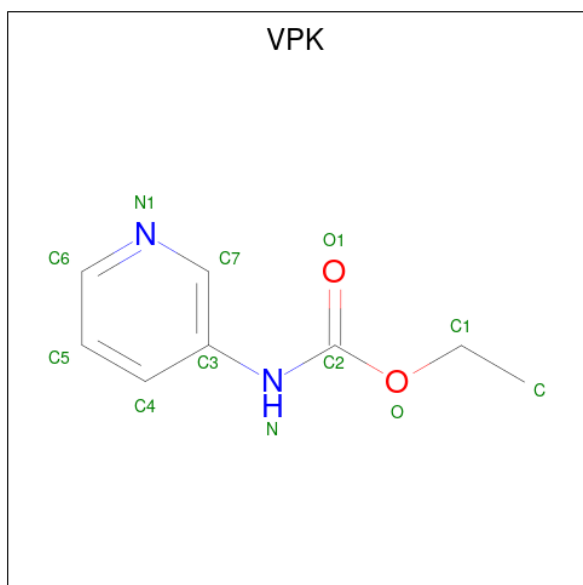
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN	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 ethyl pyridin-3-ylcarbamate (CCD ID: VPK) (formula: $C_8H_{10}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	8	2	2		
3	B	1	Total	C	N	O	0	0
			12	8	2	2		

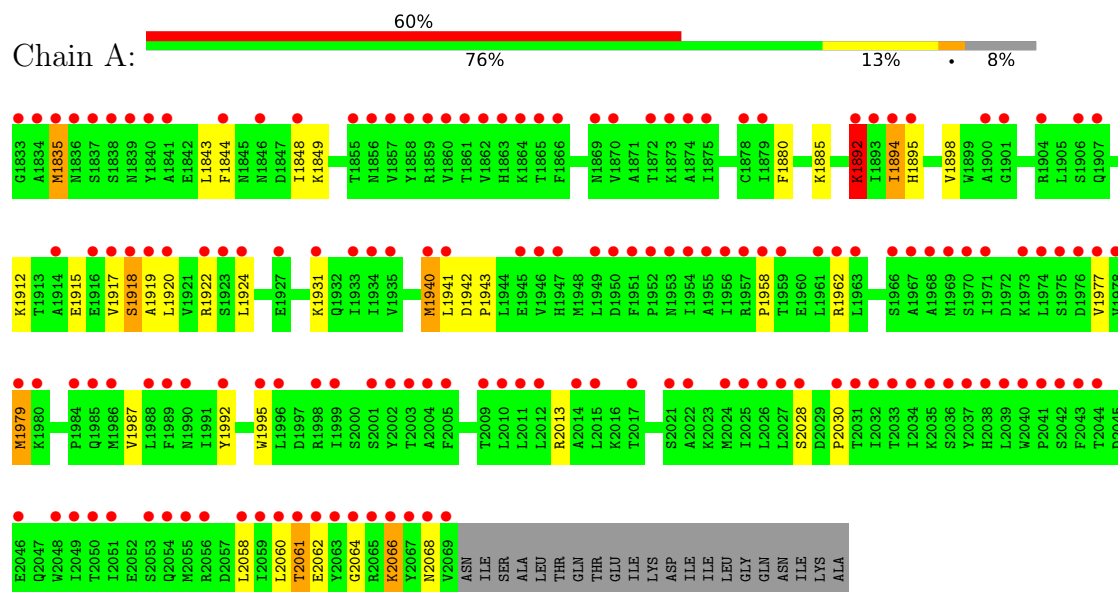
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		
4	B	40	Total	O	0	0
			40	40		

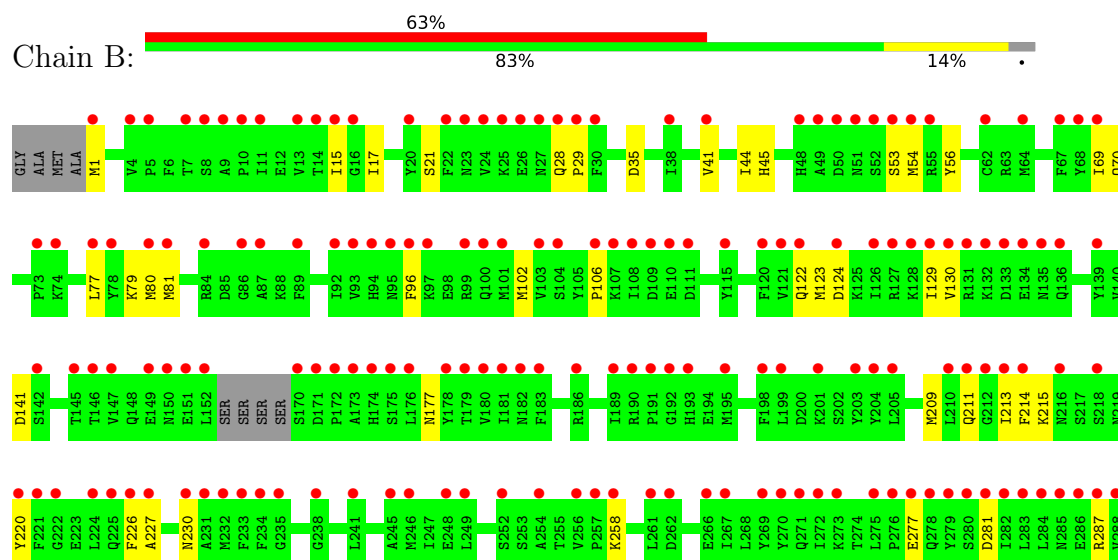
3 Residue-property plots

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



K289	K290	C291	C292	L293	Y294	S295	S296	F297	Q298	K299	N300	S301	L302	H303	N304	T305	E306	K307	I308	M309	E310	N311	K312	Y313	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	89.20Å 81.63Å 93.27Å 90.00° 108.28° 90.00°	Depositor
Resolution (Å)	44.28 – 1.72 44.28 – 1.72	Depositor EDS
% Data completeness (in resolution range)	97.5 (44.28-1.72) 97.9 (44.28-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.72Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.292 , 0.330 0.304 , 0.339	Depositor DCC
R_{free} test set	2101 reflections (3.18%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 56.0	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	0.93	EDS
Total number of atoms	9188	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.79% 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: VPK

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	0.88	6/2149 (0.3%)	1.06	14/2911 (0.5%)
2	B	0.75	2/2730 (0.1%)	0.97	4/3687 (0.1%)
All	All	0.81	8/4879 (0.2%)	1.01	18/6598 (0.3%)

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
1	A	0	2
2	B	0	3
All	All	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1924	LEU	C-N	15.69	1.54	1.33
2	B	123[A]	MET	N-CA	7.06	1.55	1.46
2	B	123[B]	MET	N-CA	7.06	1.55	1.46
1	A	1919[A]	ALA	N-CA	6.31	1.54	1.46
1	A	1919[B]	ALA	N-CA	6.31	1.54	1.46
1	A	1918[A]	SER	C-N	6.08	1.42	1.33
1	A	1918[B]	SER	C-N	6.08	1.42	1.33
1	A	1915	GLU	C-O	-6.05	1.17	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1892	LYS	CB-CA-C	10.35	128.89	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1924	LEU	CA-C-N	8.69	128.76	119.89
1	A	1924	LEU	C-N-CA	8.69	128.76	119.89
1	A	1918[A]	SER	CA-C-N	-8.13	107.14	120.72
1	A	1918[A]	SER	C-N-CA	-8.13	107.14	120.72
1	A	1918[B]	SER	CA-C-N	-8.13	107.14	120.72
1	A	1918[B]	SER	C-N-CA	-8.13	107.14	120.72
2	B	227	ALA	N-CA-C	-6.30	104.03	111.03
1	A	1880	PHE	CA-C-O	-6.26	114.08	120.84
2	B	214	PHE	CA-C-N	6.26	133.50	121.54
2	B	214	PHE	C-N-CA	6.26	133.50	121.54
2	B	122	GLN	CA-C-O	-5.82	114.07	120.36
1	A	1922	ARG	CA-C-N	5.21	127.69	120.29
1	A	1922	ARG	C-N-CA	5.21	127.69	120.29
1	A	1940	MET	CA-C-N	-5.21	113.66	120.44
1	A	1940	MET	C-N-CA	-5.21	113.66	120.44
1	A	1880	PHE	CA-C-N	5.09	130.18	123.05
1	A	1880	PHE	C-N-CA	5.09	130.18	123.05

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1918[A]	SER	Mainchain
1	A	1918[B]	SER	Mainchain
2	B	177[A]	ASN	Mainchain
2	B	177[B]	ASN	Mainchain
2	B	211[A]	GLN	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	30	0
2	B	2571	2456	2390	23	0
3	A	12	0	0	3	0
3	B	12	0	0	0	0
4	A	29	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	40	0	0	2	0
All	All	4672	4516	4364	53	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 (53) 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:1962:ARG:O	1:A:2013:ARG:NH1	2.11	0.83
1:A:1894:ILE:CD1	3:A:2101:VPK:C	2.57	0.83
2:B:1:MET:N	4:B:501:HOH:O	2.23	0.71
2:B:70:GLN:HB3	2:B:81:MET:HE2	1.75	0.68
1:A:1898[A]:VAL:HG11	4:A:2202:HOH:O	1.97	0.63
1:A:2061:THR:O	1:A:2064:GLY:N	2.33	0.60
1:A:1898[B]:VAL:CG2	4:A:2202:HOH:O	2.50	0.59
1:A:1898[A]:VAL:CG1	4:A:2202:HOH:O	2.50	0.58
1:A:2064:GLY:O	1:A:2068:ASN:N	2.35	0.55
1:A:1898[B]:VAL:HG23	4:A:2202:HOH:O	2.06	0.55
1:A:1979[A]:MET:HE1	4:A:2214:HOH:O	2.06	0.54
1:A:1894:ILE:HD13	3:A:2101:VPK:C	2.36	0.54
1:A:1977:VAL:HG21	1:A:1987:VAL:HG21	1.90	0.54
2:B:277:GLU:CD	2:B:277:GLU:H	2.15	0.54
2:B:287:ARG:O	2:B:291:ILE:HD13	2.07	0.54
2:B:96:PHE:HB2	2:B:102:MET:HE3	1.90	0.54
2:B:258:LYS:HD2	2:B:258:LYS:H	1.74	0.53
2:B:1:MET:HB3	2:B:35:ASP:HA	1.91	0.52
1:A:1894:ILE:HD12	3:A:2101:VPK:C	2.40	0.51
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	1.92	0.51
2:B:17:ILE:HD13	2:B:44[B]:ILE:CG1	2.40	0.51
2:B:44[A]:ILE:O	2:B:44[A]:ILE:HG23	2.11	0.50
1:A:2060:LEU:HB2	4:A:2229:HOH:O	2.10	0.50
1:A:1844:PHE:O	1:A:1885:LYS:NZ	2.40	0.50
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.60	0.50
1:A:1892:LYS:NZ	1:A:1892:LYS:HB3	2.28	0.48
1:A:1920:LEU:O	1:A:1920:LEU:HD12	2.13	0.48
2:B:209:MET:HA	2:B:213:ILE:HD12	1.96	0.48
2:B:17:ILE:HD13	2:B:44[B]:ILE:HG12	1.95	0.48
2:B:96:PHE:CB	2:B:102:MET:HE3	2.44	0.47
2:B:77:LEU:HD21	2:B:79:LYS:HE3	1.97	0.47
2:B:28:GLN:HG3	2:B:29:PRO:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:ASP:OD1	2:B:141:ASP:C	2.59	0.46
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.41	0.46
1:A:1894:ILE:O	1:A:1894:ILE:HG22	2.15	0.45
2:B:41[A]:VAL:HG12	4:B:527:HOH:O	2.15	0.45
1:A:1898[B]:VAL:HG21	4:A:2202:HOH:O	2.16	0.44
2:B:220:TYR:C	2:B:220:TYR:CD1	2.96	0.44
1:A:1962:ARG:HD3	1:A:1962:ARG:H	1.84	0.43
1:A:2062:GLU:O	1:A:2066:LYS:HB2	2.19	0.42
2:B:28:GLN:CG	2:B:29:PRO:HD2	2.49	0.42
2:B:53:SER:O	2:B:54[A]:MET:HB3	2.19	0.42
1:A:2028:SER:O	1:A:2030:PRO:HD3	2.19	0.42
2:B:226:PHE:CZ	2:B:230[A]:ASN:ND2	2.77	0.41
1:A:1992:TYR:O	1:A:1995:TRP:CG	2.73	0.41
1:A:1835:MET:HE3	1:A:1835:MET:HB3	1.96	0.41
2:B:56:TYR:CZ	2:B:77:LEU:HB2	2.56	0.41
2:B:15:ILE:O	2:B:21:SER:HA	2.20	0.41
2:B:69:ILE:HD13	2:B:80:MET:HA	2.01	0.41
1:A:1895:HIS:N	4:A:2202:HOH:O	2.53	0.40
1:A:1940:MET:O	1:A:1941:LEU:C	2.63	0.40
1:A:1941:LEU:HD11	1:A:1958:PRO:HB3	2.03	0.40
1:A:1942:ASP:HB2	1:A:1943:PRO:HD3	2.03	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%)	249 (96%)	8 (3%)	1 (0%)	30	16
2	B	314/308 (102%)	301 (96%)	12 (4%)	1 (0%)	36	24
All	All	572/566 (101%)	550 (96%)	20 (4%)	2 (0%)	30	24

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2061	THR
2	B	215	LYS

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%)	228 (96%)	9 (4%)	29	8
2	B	293/284 (103%)	286 (98%)	7 (2%)	43	20
All	All	530/517 (102%)	514 (97%)	16 (3%)	40	12

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1835	MET
1	A	1892	LYS
1	A	1894	ILE
1	A	1912	LYS
1	A	1917	VAL
1	A	1979[A]	MET
1	A	1979[B]	MET
1	A	1979[C]	MET
1	A	2066	LYS
2	B	45[A]	HIS
2	B	45[B]	HIS
2	B	106	PRO
2	B	124	ASP
2	B	129	ILE
2	B	130	VAL
2	B	281	ASP

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	1895	HIS
1	A	2038	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](#)

2 ligands are 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	VPK	A	2101	-	12,12,12	1.09	1 (8%)	14,14,14	1.23	1 (7%)
3	VPK	B	401	-	12,12,12	1.77	2 (16%)	14,14,14	1.50	2 (14%)

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	VPK	A	2101	-	-	0/7/7/7	0/1/1/1
3	VPK	B	401	-	-	2/7/7/7	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	VPK	C4-C3	-3.99	1.32	1.39
3	B	401	VPK	O-C1	-2.91	1.37	1.46
3	A	2101	VPK	C5-C4	-2.52	1.34	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	VPK	C3-N-C2	-3.69	120.56	126.39
3	B	401	VPK	O-C1-C	-3.39	96.23	108.40
3	A	2101	VPK	O1-C2-N	2.38	131.17	126.12

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	VPK	C7-C3-N-C2
3	B	401	VPK	C4-C3-N-C2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2101	VPK	3	0

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%)	2.99	154 (64%) 0 0	26, 84, 159, 241	12 (5%)
2	B	300/308 (97%)	2.85	193 (64%) 0 0	25, 84, 158, 287	8 (2%)
All	All	537/566 (94%)	2.91	347 (64%) 0 0	25, 84, 159, 287	20 (3%)

All (347) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2040	TRP	13.8
1	A	2039	LEU	13.6
2	B	246	MET	10.7
1	A	1878	CYS	10.6
1	A	1967	ALA	9.0
1	A	1996	LEU	8.9
2	B	261	LEU	8.9
2	B	80	MET	8.5
2	B	203[A]	TYR	8.3
1	A	2069	VAL	8.1
1	A	2060	LEU	8.0
1	A	1834	ALA	7.8
1	A	2009	THR	7.2
2	B	214	PHE	7.2
2	B	308	ILE	7.2
1	A	1970	SER	7.2
2	B	245	ALA	7.0
1	A	2043	PHE	6.9
1	A	2059	ILE	6.9
1	A	1969	MET	6.8
2	B	204[A]	TYR	6.6
1	A	2001[A]	SER	6.6
2	B	316	LEU	6.5
1	A	1995	TRP	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	1963	LEU	6.5
1	A	2037	TYR	6.5
1	A	1979[A]	MET	6.4
1	A	2017[A]	THR	6.3
1	A	1835	MET	6.2
2	B	152	LEU	6.2
2	B	272	ILE	6.2
2	B	297	PHE	6.2
1	A	2051	ILE	6.1
2	B	130	VAL	6.1
2	B	41[A]	VAL	5.9
1	A	1966	SER	5.9
1	A	2004	ALA	5.9
1	A	2058	LEU	5.9
1	A	1974	LEU	5.8
2	B	101	MET	5.8
2	B	210	LEU	5.7
1	A	1955	ALA	5.7
2	B	10	PRO	5.7
2	B	129	ILE	5.7
1	A	1892	LYS	5.7
1	A	1961[A]	LEU	5.7
1	A	2026	LEU	5.7
2	B	269	TYR	5.6
1	A	1968	ALA	5.5
2	B	8	SER	5.5
1	A	1875	ILE	5.5
2	B	49	ALA	5.4
2	B	126	ILE	5.3
2	B	199	LEU	5.3
1	A	2063	TYR	5.3
1	A	2034	ILE	5.3
2	B	89	PHE	5.3
1	A	1840	TYR	5.3
2	B	22	PHE	5.2
2	B	305	THR	5.2
2	B	146	THR	5.2
2	B	317	LEU	5.1
2	B	73	PRO	5.1
2	B	222	GLY	5.1
1	A	1860	VAL	5.1
2	B	220	TYR	5.1

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Mol	Chain	Res	Type	RSRZ
2	B	30	PHE	5.1
2	B	106	PRO	5.1
2	B	256	VAL	5.1
2	B	172	PRO	5.0
1	A	1857	VAL	5.0
1	A	2061	THR	5.0
2	B	276	PRO	5.0
2	B	54[A]	MET	5.0
1	A	1917	VAL	5.0
2	B	198	PHE	5.0
2	B	279	TYR	5.0
1	A	2064	GLY	4.9
2	B	226	PHE	4.9
2	B	96	PHE	4.9
1	A	2038	HIS	4.9
2	B	211[A]	GLN	4.8
2	B	180	VAL	4.8
2	B	296	SER	4.8
1	A	1919[A]	ALA	4.7
1	A	2027	LEU	4.7
1	A	1992	TYR	4.6
2	B	24	VAL	4.6
2	B	302	LEU	4.6
2	B	29	PRO	4.6
2	B	170	SER	4.6
2	B	145	THR	4.6
2	B	303	HIS	4.6
1	A	2022	ALA	4.6
2	B	134	GLU	4.5
2	B	313	TYR	4.5
2	B	283	LEU	4.5
1	A	1999	ILE	4.5
1	A	2067	TYR	4.5
2	B	111	ASP	4.5
2	B	174	HIS	4.5
2	B	16	GLY	4.5
1	A	2012	LEU	4.5
2	B	235	GLY	4.4
2	B	183	PHE	4.4
2	B	23	ASN	4.4
2	B	173	ALA	4.4
1	A	2010	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	92	ILE	4.4
2	B	128	LYS	4.4
2	B	227	ALA	4.4
2	B	93	VAL	4.3
2	B	291	ILE	4.2
2	B	234	PHE	4.2
1	A	2041	PRO	4.2
2	B	1	MET	4.2
2	B	205	LEU	4.2
1	A	2065	ARG	4.1
2	B	115	TYR	4.1
1	A	1978	VAL	4.1
1	A	1900	ALA	4.1
2	B	67	PHE	4.1
1	A	2036	SER	4.0
2	B	252	SER	4.0
1	A	2068	ASN	4.0
1	A	2025	ILE	3.9
1	A	1872	THR	3.9
2	B	97	LYS	3.9
1	A	1988	LEU	3.9
2	B	275	LEU	3.9
2	B	289	TRP	3.9
1	A	1954	ILE	3.9
1	A	2032	ILE	3.9
1	A	2050	THR	3.9
2	B	249	LEU	3.9
2	B	294	TYR	3.8
1	A	1866	PHE	3.8
1	A	2021	SER	3.8
1	A	1879	ILE	3.8
1	A	1941	LEU	3.8
2	B	191	PRO	3.8
1	A	1971	ILE	3.8
2	B	52	SER	3.8
2	B	107	LYS	3.7
2	B	212[A]	GLY	3.7
1	A	1858	TYR	3.7
1	A	1894	ILE	3.7
2	B	189	ILE	3.7
1	A	2028	SER	3.7
1	A	1931[A]	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	190	ARG	3.7
2	B	62	CYS	3.7
2	B	304	ASN	3.7
1	A	1862	VAL	3.7
1	A	2015	LEU	3.7
2	B	192	GLY	3.7
1	A	1975	SER	3.7
2	B	7	THR	3.6
2	B	103	VAL	3.6
2	B	149	GLU	3.6
1	A	1985	GLN	3.6
2	B	241	LEU	3.6
2	B	201	LYS	3.5
2	B	267	ILE	3.5
2	B	232	MET	3.5
2	B	195	MET	3.5
2	B	262	ASP	3.5
2	B	224	LEU	3.5
1	A	2003	THR	3.5
2	B	307	LYS	3.5
2	B	81	MET	3.4
1	A	1920	LEU	3.4
1	A	1855[A]	THR	3.4
2	B	257	PRO	3.4
1	A	1838	SER	3.4
1	A	1986	MET	3.4
2	B	301	SER	3.4
1	A	2024[A]	MET	3.4
2	B	312	LYS	3.3
2	B	282	ILE	3.3
1	A	1922	ARG	3.3
1	A	1833	GLY	3.3
2	B	95	ASN	3.3
2	B	100	GLN	3.3
2	B	221	PHE	3.3
1	A	1933	ILE	3.2
2	B	25	LYS	3.2
1	A	2030	PRO	3.2
2	B	293	LEU	3.2
1	A	2053[A]	SER	3.2
2	B	273	LYS	3.1
2	B	287	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	2002[A]	TYR	3.1
2	B	69	ILE	3.1
1	A	1949	LEU	3.1
1	A	2014	ALA	3.1
2	B	64[A]	MET	3.1
1	A	1864	LYS	3.1
1	A	1906	SER	3.1
2	B	38	ILE	3.1
2	B	216	ASN	3.1
2	B	193	HIS	3.0
2	B	28	GLN	3.0
1	A	2011	LEU	3.0
2	B	295	SER	3.0
2	B	233	PHE	3.0
1	A	1924	LEU	3.0
1	A	2031	THR	3.0
2	B	108	ILE	3.0
2	B	309	MET	3.0
1	A	1870	VAL	2.9
2	B	142	SER	2.9
2	B	131	ARG	2.9
2	B	14	THR	2.9
2	B	299	LYS	2.9
1	A	1973	LYS	2.9
2	B	48	HIS	2.9
1	A	1956	ILE	2.9
2	B	213	ILE	2.9
2	B	133	ASP	2.9
1	A	1856[A]	ASN	2.9
1	A	1935	VAL	2.9
2	B	136	GLN	2.9
1	A	1952	PRO	2.9
1	A	1958	PRO	2.8
2	B	53	SER	2.8
2	B	27	ASN	2.8
1	A	1869	ASN	2.8
2	B	109	ASP	2.8
2	B	87	ALA	2.8
1	A	1904	ARG	2.8
1	A	1918[A]	SER	2.8
1	A	2066	LYS	2.7
2	B	20	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	77	LEU	2.7
1	A	1950	ASP	2.7
2	B	181	ILE	2.7
2	B	99	ARG	2.7
2	B	284	LEU	2.7
1	A	1837	SER	2.7
2	B	280	SER	2.7
2	B	151	GLU	2.7
2	B	277	GLU	2.7
1	A	1836	ASN	2.7
1	A	2035	LYS	2.7
1	A	1874	ALA	2.7
2	B	50	ASP	2.7
1	A	1998	ARG	2.7
1	A	1923	SER	2.7
1	A	2048	TRP	2.7
2	B	124	ASP	2.7
1	A	1859	ARG	2.6
1	A	1959	THR	2.6
2	B	132	LYS	2.6
2	B	179	THR	2.6
2	B	178[A]	TYR	2.6
2	B	288	VAL	2.6
1	A	2049	ILE	2.6
2	B	186	ARG	2.6
1	A	1927	GLU	2.6
2	B	110	GLU	2.6
1	A	2042	SER	2.6
2	B	182	ASN	2.6
1	A	2005	PHE	2.6
1	A	1893	ILE	2.6
2	B	231	ALA	2.6
1	A	1951	PHE	2.6
1	A	1895	HIS	2.6
1	A	1946	VAL	2.6
2	B	270	TYR	2.6
2	B	11	ILE	2.6
2	B	74	LYS	2.6
2	B	278	GLN	2.5
2	B	218	SER	2.5
1	A	2056[A]	ARG	2.5
1	A	2062	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	127	ARG	2.5
2	B	306	GLU	2.5
2	B	171	ASP	2.5
1	A	1873	LYS	2.5
2	B	55[A]	ARG	2.5
2	B	254	ALA	2.5
2	B	286	GLU	2.5
1	A	1947	HIS	2.4
1	A	1989	PHE	2.4
2	B	78	TYR	2.4
2	B	4	VAL	2.4
1	A	2046	GLU	2.4
1	A	2055	MET	2.4
2	B	104	SER	2.4
2	B	225	GLN	2.4
1	A	1916	GLU	2.4
1	A	1945	GLU	2.4
1	A	1940	MET	2.4
1	A	1846	ASN	2.4
2	B	68	TYR	2.4
1	A	1977	VAL	2.4
1	A	1907	GLN	2.3
1	A	2054[A]	GLN	2.3
2	B	121	VAL	2.3
2	B	147	VAL	2.3
1	A	1839	ASN	2.3
1	A	1953	ASN	2.3
2	B	51	ASN	2.3
2	B	150	ASN	2.3
2	B	300	ASN	2.3
2	B	238	GLY	2.3
1	A	1984	PRO	2.3
2	B	5	PRO	2.3
2	B	94	HIS	2.3
1	A	1844	PHE	2.3
1	A	1990	ASN	2.3
2	B	281	ASP	2.3
2	B	86	GLY	2.3
1	A	1863	HIS	2.2
2	B	248	GLU	2.2
1	A	1934	ILE	2.2
2	B	122	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	285	ASN	2.2
2	B	175	SER	2.2
1	A	1914	ALA	2.2
1	A	1976	ASP	2.2
2	B	290	ASN	2.2
2	B	139	TYR	2.2
1	A	1848	ILE	2.2
2	B	26	GLU	2.1
2	B	84	ARG	2.1
1	A	1901	GLY	2.1
2	B	176	LEU	2.1
1	A	1861	THR	2.1
1	A	1865	THR	2.1
1	A	1841	ALA	2.1
1	A	1980[A]	LYS	2.1
2	B	311	ASN	2.1
2	B	9	ALA	2.1
2	B	266	GLU	2.1
1	A	1962	ARG	2.1
1	A	2033	THR	2.1
2	B	258	LYS	2.1
2	B	15	ILE	2.1
2	B	135	ASN	2.0
1	A	1957	ARG	2.0
1	A	2044	THR	2.0
2	B	230[A]	ASN	2.0
2	B	271	GLN	2.0
2	B	120	PHE	2.0
2	B	13	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 ⓘ

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	VPK	A	2101	12/12	0.66	0.16	20,20,20,20	12
3	VPK	B	401	12/12	0.80	0.13	20,20,20,20	12

6.5 Other polymers [i](#)

There are no such residues in this entry.