



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:13 AM UTC

PDB ID : 7FPB / pdb_00007fpb
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P09C03 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 : 2.02 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

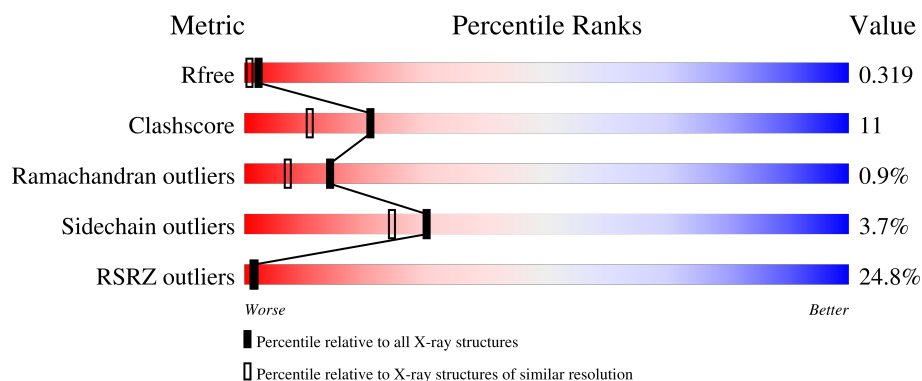
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	29% 66% 22% 8%
2	B	308	19% 76% 19% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9189 atoms, of which 4524 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pre-mRNA-splicing factor 8.

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

There are 20 discrepancies between the modelled and reference sequences:

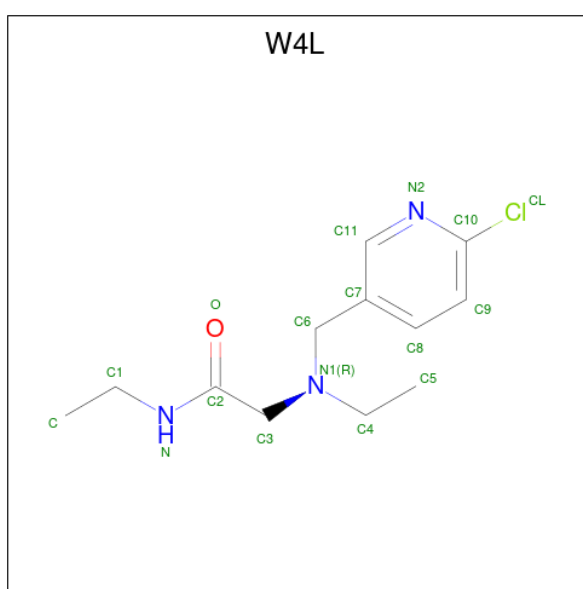
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN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

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

- Molecule 3 is N 2 -[(6-chloropyridin-3-yl)methyl]-N,N 2 -diethylglycinamide (CCD ID: W4L) (formula: C₁₂H₁₈ClN₃O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			17	12	1	3	1		

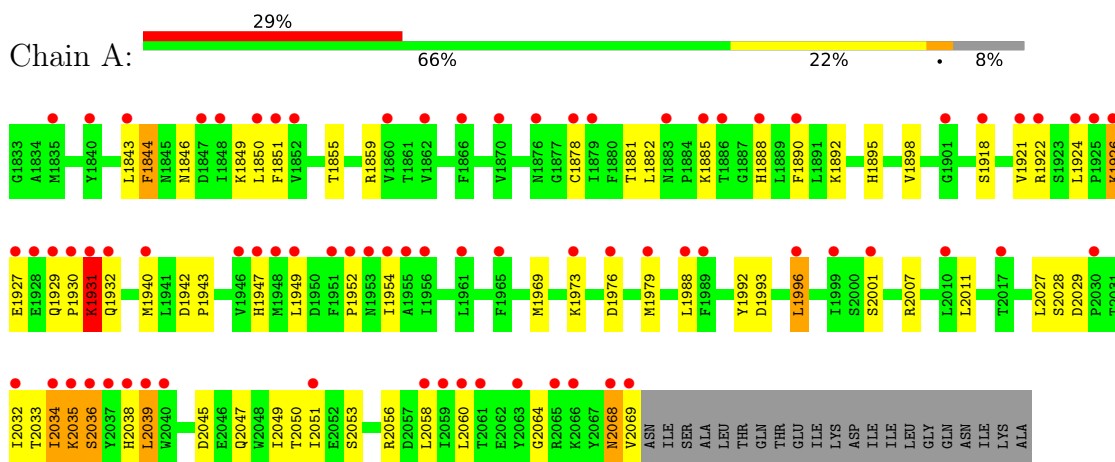
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	B	34	Total	O	0	0
			34	34		

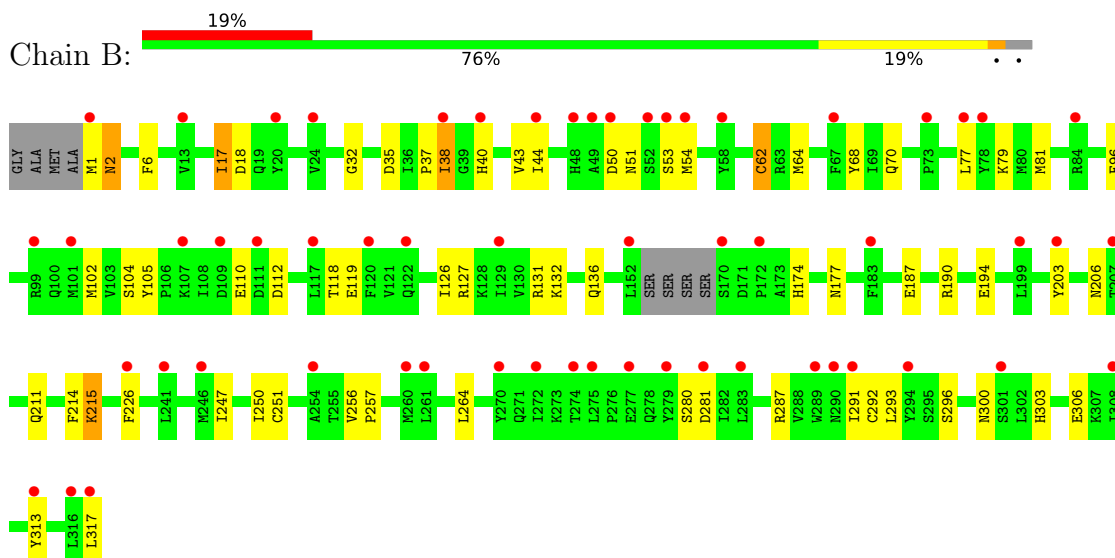
3 Residue-property plots

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	89.20Å 81.73Å 92.84Å 90.00° 108.32° 90.00°	Depositor
Resolution (Å)	29.40 – 2.02 29.40 – 2.02	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.40-2.02) 99.4 (29.40-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.03Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.237 , 0.289 0.267 , 0.319	Depositor DCC
R_{free} test set	2000 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9189	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 5.33% 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: W4L

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	0.94	9/2149 (0.4%)	1.20	17/2911 (0.6%)
2	B	0.70	0/2739	0.87	0/3699
All	All	0.81	9/4888 (0.2%)	1.03	17/6610 (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	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1918[A]	SER	C-N	10.24	1.47	1.33
1	A	1918[B]	SER	C-N	10.24	1.47	1.33
1	A	1932[A]	GLN	N-CA	8.50	1.56	1.46
1	A	1932[B]	GLN	N-CA	8.50	1.56	1.46
1	A	1931[A]	LYS	C-N	6.91	1.42	1.33
1	A	1931[B]	LYS	C-N	6.91	1.42	1.33
1	A	1926	LYS	C-O	-6.59	1.16	1.24
1	A	1992	TYR	C-O	-5.32	1.16	1.24
1	A	2007	ARG	CZ-NH2	5.10	1.40	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1888	HIS	CB-CA-C	7.97	122.33	109.90
1	A	1992	TYR	CA-C-O	-7.58	110.69	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1931[A]	LYS	CA-C-N	-7.42	108.88	121.94
1	A	1931[A]	LYS	C-N-CA	-7.42	108.88	121.94
1	A	1931[B]	LYS	CA-C-N	-7.42	108.88	121.94
1	A	1931[B]	LYS	C-N-CA	-7.42	108.88	121.94
1	A	2034	ILE	N-CA-C	-7.24	96.05	106.55
1	A	1949	LEU	N-CA-C	-7.22	103.13	112.23
1	A	1954	ILE	CA-C-N	7.19	131.01	120.95
1	A	1954	ILE	C-N-CA	7.19	131.01	120.95
1	A	1952	PRO	N-CA-C	6.13	125.10	112.47
1	A	2038	HIS	CB-CA-C	-5.77	98.99	109.38
1	A	1952	PRO	CB-CA-C	-5.68	102.19	111.56
1	A	2035	LYS	CB-CA-C	5.57	119.79	109.54
1	A	1890	PHE	CA-CB-CG	-5.21	108.59	113.80
1	A	1851	PHE	CB-CA-C	-5.21	101.16	109.75
1	A	1844	PHE	CA-CB-CG	-5.01	108.79	113.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1930	PRO	Mainchain
1	A	1931[A]	LYS	Mainchain
1	A	1931[B]	LYS	Mainchain
1	A	2033	THR	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	54	2
2	B	2580	2464	2396	55	2
3	A	17	0	0	0	0
4	A	26	0	0	5	0
4	B	34	0	0	3	0
All	All	4665	4524	4370	101	2

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 11.

All (101) 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:1947:HIS:CE1	2:B:194:GLU:HB2	1.73	1.22
1:A:1947:HIS:CE1	2:B:194:GLU:CB	2.24	1.21
1:A:1885:LYS:HD2	1:A:2001[A]:SER:OG	1.47	1.14
1:A:1885:LYS:CE	1:A:2001[A]:SER:OG	2.05	1.05
1:A:1885:LYS:CD	1:A:2001[A]:SER:OG	2.04	1.04
1:A:1947:HIS:HE1	2:B:194:GLU:HB2	1.18	0.95
1:A:1993:ASP:O	4:A:2202:HOH:O	1.92	0.87
1:A:1885:LYS:HD2	1:A:2001[B]:SER:CB	2.04	0.87
1:A:1885:LYS:HD2	1:A:2001[A]:SER:CB	2.05	0.87
1:A:1947:HIS:CE1	2:B:194:GLU:CG	2.64	0.80
2:B:70:GLN:HB3	2:B:81:MET:HE2	1.65	0.79
2:B:287:ARG:O	2:B:291:ILE:HD13	1.82	0.79
1:A:1885:LYS:HE3	1:A:2001[A]:SER:OG	1.81	0.79
1:A:2039:LEU:HD23	1:A:2039:LEU:N	2.01	0.76
1:A:2027:LEU:CD2	1:A:2034:ILE:HD11	2.15	0.75
1:A:1885:LYS:HD2	1:A:2001[B]:SER:HB3	1.66	0.75
1:A:1947:HIS:CE1	2:B:194:GLU:HB3	2.23	0.74
2:B:1:MET:N	4:B:401:HOH:O	2.23	0.72
2:B:96:PHE:HB2	2:B:102:MET:HE3	1.76	0.68
2:B:1:MET:HE3	2:B:35:ASP:HB3	1.76	0.67
2:B:131:ARG:NH2	2:B:177[B]:ASN:OD1	2.28	0.66
1:A:2064:GLY:O	1:A:2068:ASN:N	2.30	0.65
1:A:1843:LEU:HD23	1:A:1849:LYS:HD2	1.78	0.65
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.25	0.62
1:A:2039:LEU:HD23	1:A:2039:LEU:H	1.63	0.62
2:B:96:PHE:CB	2:B:102:MET:HE3	2.28	0.62
1:A:1947:HIS:ND1	2:B:194:GLU:HG2	2.17	0.59
1:A:1996:LEU:HD23	1:A:1996:LEU:N	2.17	0.59
1:A:1940:MET:C	1:A:1943:PRO:HD2	2.29	0.58
1:A:1973:LYS:NZ	4:A:2203:HOH:O	2.16	0.58
1:A:2045:ASP:O	1:A:2049:ILE:HG12	2.03	0.58
2:B:1:MET:N	2:B:38:ILE:HD11	2.19	0.58
1:A:2027:LEU:HD21	1:A:2034:ILE:HD11	1.85	0.58
1:A:1931[B]:LYS:HE2	1:A:1931[B]:LYS:HA	1.85	0.57
1:A:2069:VAL:HG12	1:A:2069:VAL:O	2.03	0.57
2:B:68:TYR:CE2	2:B:81:MET:HE3	2.40	0.56
2:B:64[A]:MET:HE2	2:B:136:GLN:OE1	2.07	0.55
2:B:206:ASN:O	2:B:211[A]:GLN:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ASN:OD1	2:B:62:CYS:HB3	2.07	0.55
2:B:300:ASN:O	2:B:303:HIS:NE2	2.40	0.55
1:A:1885:LYS:NZ	1:A:2001[A]:SER:OG	2.40	0.53
1:A:1895:HIS:O	1:A:1898[A]:VAL:HG22	2.09	0.52
2:B:50:ASP:OD1	2:B:51:ASN:N	2.42	0.52
1:A:1976:ASP:HB3	4:A:2211:HOH:O	2.08	0.51
1:A:1885:LYS:CD	1:A:2001[B]:SER:OG	2.58	0.51
2:B:77:LEU:HD21	2:B:79:LYS:HE3	1.94	0.49
2:B:44[A]:ILE:O	2:B:44[A]:ILE:HG23	2.12	0.49
2:B:43:VAL:HG13	2:B:43:VAL:O	2.12	0.49
1:A:1855[A]:THR:HG22	1:A:1855[A]:THR:O	2.12	0.49
1:A:1996:LEU:N	1:A:1996:LEU:CD2	2.76	0.49
2:B:251:CYS:O	2:B:296:SER:HB2	2.13	0.49
1:A:1885:LYS:HD2	1:A:2001[B]:SER:OG	2.06	0.48
2:B:126:ILE:HG12	2:B:226:PHE:CE1	2.48	0.48
2:B:104:SER:O	2:B:105:TYR:C	2.54	0.48
2:B:214:PHE:O	2:B:215:LYS:HB2	2.12	0.48
2:B:126:ILE:HG12	2:B:226:PHE:CZ	2.48	0.47
1:A:1947:HIS:CE1	2:B:194:GLU:HG2	2.45	0.47
1:A:2027:LEU:HD22	1:A:2034:ILE:HD11	1.92	0.47
1:A:1947:HIS:ND1	2:B:194:GLU:CG	2.76	0.47
2:B:17:ILE:HD12	2:B:44[B]:ILE:HG13	1.95	0.47
2:B:190:ARG:HG3	2:B:203[B]:TYR:CZ	2.50	0.47
1:A:2053[A]:SER:OG	1:A:2056[A]:ARG:NH2	2.48	0.47
2:B:6:PHE:CD1	2:B:32:GLY:HA2	2.50	0.47
1:A:2034:ILE:HG22	4:A:2203:HOH:O	2.15	0.46
1:A:1969:MET:HA	1:A:1969:MET:HE2	1.98	0.46
2:B:1:MET:H2	2:B:38:ILE:HD11	1.80	0.45
1:A:1878:CYS:HA	1:A:1892:LYS:O	2.17	0.45
1:A:1942:ASP:N	1:A:1943:PRO:CD	2.79	0.45
2:B:70:GLN:HB3	2:B:81:MET:CE	2.42	0.45
2:B:110:GLU:O	2:B:110:GLU:HG2	2.17	0.45
1:A:1885:LYS:HE3	1:A:2001[A]:SER:HG	1.82	0.45
2:B:281:ASP:OD1	2:B:281:ASP:N	2.48	0.45
2:B:1:MET:HB3	2:B:35:ASP:HA	1.99	0.44
2:B:247:ILE:HG22	2:B:292:CYS:SG	2.58	0.44
2:B:187:GLU:H	2:B:187:GLU:CD	2.26	0.44
2:B:37:PRO:HD3	2:B:105:TYR:CD1	2.53	0.44
1:A:1844:PHE:CD2	1:A:1844:PHE:N	2.86	0.43
1:A:2028:SER:OG	1:A:2029:ASP:N	2.51	0.43
1:A:1859:ARG:HH12	1:A:1979[A]:MET:CE	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:LEU:HD22	2:B:306:GLU:HB2	2.01	0.43
2:B:17:ILE:O	2:B:18:ASP:C	2.60	0.43
1:A:2047:GLN:O	1:A:2051:ILE:HG12	2.19	0.42
2:B:40:HIS:CD2	4:B:421:HOH:O	2.71	0.42
2:B:256:VAL:O	2:B:257:PRO:C	2.60	0.42
2:B:190:ARG:HG3	2:B:203[B]:TYR:CE2	2.55	0.42
2:B:250:ILE:HG21	2:B:264:LEU:HD22	2.02	0.41
1:A:2011:LEU:HD23	1:A:2011:LEU:HA	1.80	0.41
1:A:2058:LEU:HD23	1:A:2058:LEU:O	2.20	0.41
2:B:118:THR:O	2:B:119:GLU:C	2.63	0.41
1:A:2036:SER:HA	4:A:2203:HOH:O	2.19	0.41
2:B:291:ILE:O	2:B:296:SER:HB3	2.21	0.41
1:A:1846:ASN:HD22	1:A:1846:ASN:HA	1.71	0.41
1:A:1922:ARG:O	1:A:1922:ARG:HG2	2.21	0.41
2:B:44[A]:ILE:O	2:B:44[A]:ILE:CG2	2.69	0.41
2:B:51:ASN:OD1	2:B:53:SER:HB2	2.21	0.41
2:B:300:ASN:HB2	4:B:405:HOH:O	2.20	0.41
2:B:280:SER:HB3	2:B:313:TYR:CZ	2.56	0.41
2:B:2:ASN:HD22	2:B:2:ASN:HA	1.76	0.40
1:A:1850:LEU:HD22	1:A:1881:THR:HG22	2.03	0.40

All (2) 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:110:GLU:O[4_555]	1.92	0.28
1:A:1846:ASN:H	2:B:112:ASP:OD2[4_555]	1.42	0.18

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%)	245 (95%)	12 (5%)	1 (0%)	30	22
2	B	315/308 (102%)	298 (95%)	12 (4%)	5 (2%)	7	2
All	All	573/566 (101%)	543 (95%)	24 (4%)	6 (1%)	14	5

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2068	ASN
2	B	62	CYS
2	B	54[A]	MET
2	B	54[B]	MET
2	B	132	LYS
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%)	224 (94%)	13 (6%)	19	12
2	B	294/284 (104%)	289 (98%)	5 (2%)	53	53
All	All	531/517 (103%)	513 (97%)	18 (3%)	30	28

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1882	LEU
1	A	1921	VAL
1	A	1924	LEU
1	A	1926	LYS
1	A	1927	GLU
1	A	1929	GLN
1	A	1988	LEU
1	A	1996	LEU
1	A	2032	ILE
1	A	2035	LYS

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Mol	Chain	Res	Type
1	A	2036	SER
1	A	2039	LEU
1	A	2060	LEU
2	B	2	ASN
2	B	17	ILE
2	B	38	ILE
2	B	174	HIS
2	B	317	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1846	ASN
1	A	1907	GLN
2	B	31	HIS
2	B	47	GLN
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	W4L	A	2101	-	17,17,17	1.85	2 (11%)	21,21,21	1.58	2 (9%)

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	W4L	A	2101	-	-	5/13/13/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2101	W4L	C6-N1	5.02	1.57	1.47
3	A	2101	W4L	C10-CL	-4.27	1.65	1.74

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2101	W4L	C7-C6-N1	-5.26	102.39	113.15
3	A	2101	W4L	C2-C3-N1	-3.33	105.66	113.41

There are no chirality outliers.

All (5) torsion outliers are listed below:

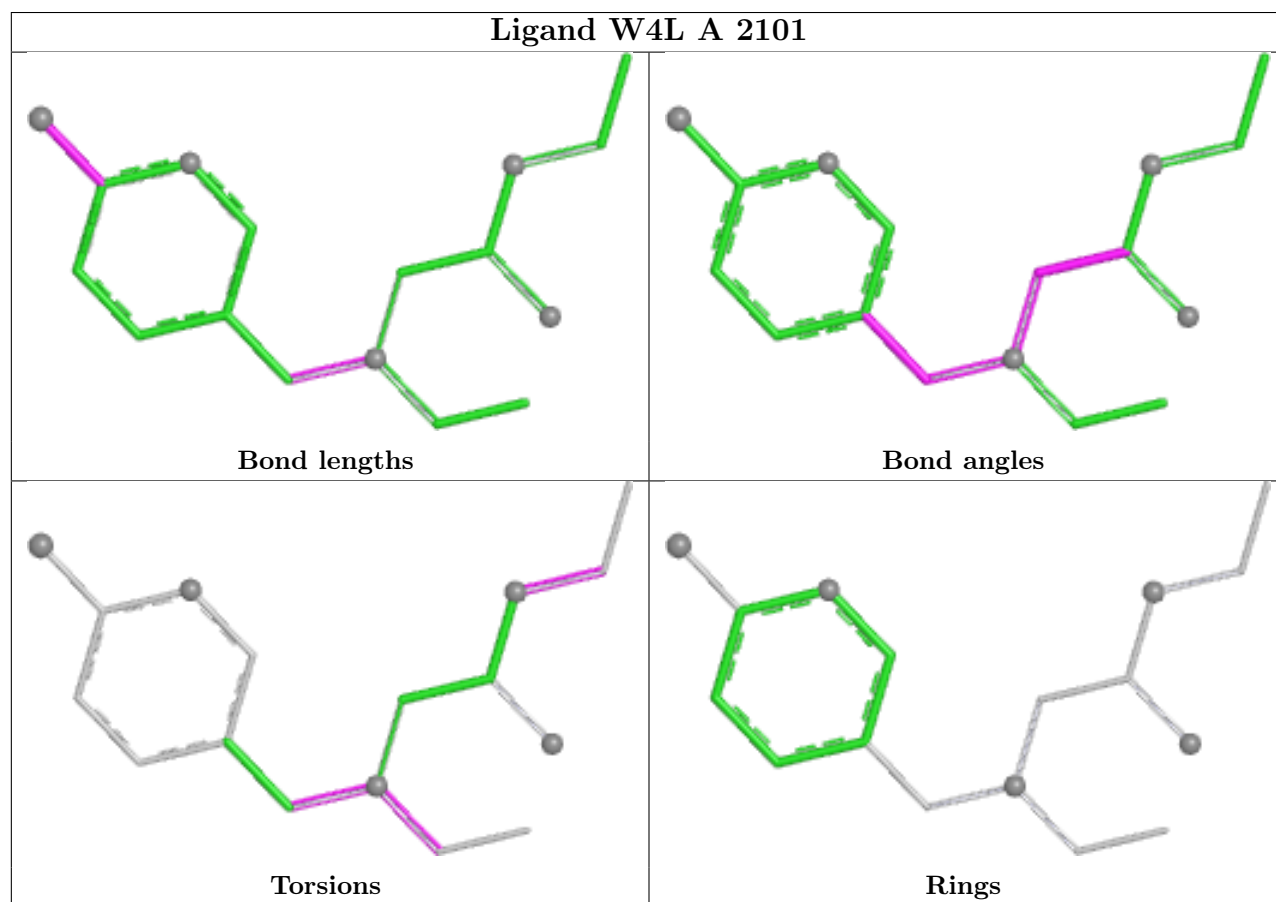
Mol	Chain	Res	Type	Atoms
3	A	2101	W4L	C-C1-N-C2
3	A	2101	W4L	C5-C4-N1-C6
3	A	2101	W4L	C5-C4-N1-C3
3	A	2101	W4L	C7-C6-N1-C4
3	A	2101	W4L	C7-C6-N1-C3

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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%)	1.78	75 (31%) 1 1	26, 78, 123, 185	12 (5%)
2	B	300/308 (97%)	1.29	58 (19%) 3 3	25, 77, 127, 168	9 (3%)
All	All	537/566 (94%)	1.51	133 (24%) 2 1	25, 78, 127, 185	21 (3%)

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2037	TYR	8.5
1	A	2034	ILE	7.1
1	A	1948	MET	7.0
1	A	1848	ILE	6.6
1	A	2038	HIS	6.4
1	A	2069	VAL	6.0
1	A	2039	LEU	5.9
1	A	1925	PRO	5.7
1	A	1888	HIS	5.5
1	A	2036	SER	5.3
1	A	1878	CYS	5.2
2	B	54[A]	MET	5.2
1	A	1924	LEU	5.0
1	A	1951	PHE	4.9
2	B	279	TYR	4.7
1	A	1890	PHE	4.4
1	A	1988	LEU	4.4
1	A	1930	PRO	4.4
2	B	50	ASP	4.3
1	A	1886	THR	4.2
1	A	1979[A]	MET	4.2
1	A	1885	LYS	4.2
2	B	152	LEU	4.0
1	A	1956	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	2040	TRP	3.9
2	B	254	ALA	3.9
1	A	1996	LEU	3.9
1	A	1929	GLN	3.8
1	A	1954	ILE	3.8
2	B	170	SER	3.8
1	A	2035	LYS	3.8
2	B	101	MET	3.7
1	A	1866	PHE	3.7
1	A	1928	GLU	3.6
2	B	73	PRO	3.6
1	A	2065	ARG	3.6
1	A	1955	ALA	3.6
1	A	1947	HIS	3.6
2	B	203[A]	TYR	3.5
2	B	77	LEU	3.5
1	A	1901	GLY	3.5
1	A	1847	ASP	3.5
1	A	2058	LEU	3.4
1	A	2068	ASN	3.4
2	B	291	ILE	3.3
1	A	1922	ARG	3.3
1	A	1835	MET	3.3
2	B	316	LEU	3.2
1	A	1976	ASP	3.2
2	B	84	ARG	3.0
1	A	2060	LEU	3.0
2	B	261	LEU	3.0
1	A	2032	ILE	3.0
1	A	2001[A]	SER	2.9
2	B	38	ILE	2.9
2	B	301	SER	2.9
1	A	1843	LEU	2.9
1	A	1940	MET	2.9
1	A	1952	PRO	2.9
1	A	1953	ASN	2.9
1	A	1961[A]	LEU	2.8
2	B	109	ASP	2.8
1	A	1926	LYS	2.8
1	A	1931[A]	LYS	2.8
1	A	1932[A]	GLN	2.8
2	B	78	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1876	ASN	2.7
1	A	1883	ASN	2.7
1	A	1927	GLU	2.7
1	A	2066	LYS	2.7
1	A	2030	PRO	2.7
2	B	1	MET	2.7
2	B	277	GLU	2.7
2	B	53	SER	2.7
2	B	49	ALA	2.6
2	B	241	LEU	2.6
2	B	122[A]	GLN	2.6
2	B	246	MET	2.6
2	B	20	TYR	2.6
2	B	260	MET	2.6
2	B	294	TYR	2.6
1	A	1850	LEU	2.6
2	B	290	ASN	2.5
2	B	281	ASP	2.5
1	A	1862	VAL	2.5
1	A	1921	VAL	2.5
2	B	24	VAL	2.5
2	B	275	LEU	2.5
2	B	111	ASP	2.5
1	A	1918[A]	SER	2.5
2	B	317	LEU	2.5
1	A	1989	PHE	2.5
1	A	2051	ILE	2.5
2	B	13	VAL	2.4
2	B	58	TYR	2.4
1	A	1949	LEU	2.4
1	A	2063	TYR	2.4
2	B	172	PRO	2.4
1	A	1965	PHE	2.4
1	A	2061	THR	2.4
1	A	1999	ILE	2.3
1	A	1946	VAL	2.3
2	B	207	THR	2.3
2	B	313	TYR	2.3
1	A	2010	LEU	2.3
2	B	289	TRP	2.3
1	A	2059	ILE	2.3
2	B	129	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1870	VAL	2.3
2	B	226	PHE	2.2
2	B	48	HIS	2.2
2	B	99	ARG	2.2
2	B	183	PHE	2.2
1	A	1852	VAL	2.2
2	B	117	LEU	2.2
2	B	199	LEU	2.2
1	A	1851	PHE	2.2
2	B	120	PHE	2.2
2	B	308	ILE	2.2
2	B	272	ILE	2.1
1	A	1860	VAL	2.1
2	B	283	LEU	2.1
1	A	1840	TYR	2.1
1	A	2017[A]	THR	2.1
1	A	1879	ILE	2.1
2	B	52	SER	2.1
1	A	1973	LYS	2.0
2	B	44[A]	ILE	2.0
2	B	67	PHE	2.0
2	B	40	HIS	2.0
2	B	107	LYS	2.0
2	B	274	THR	2.0
2	B	270	TYR	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 ⓘ

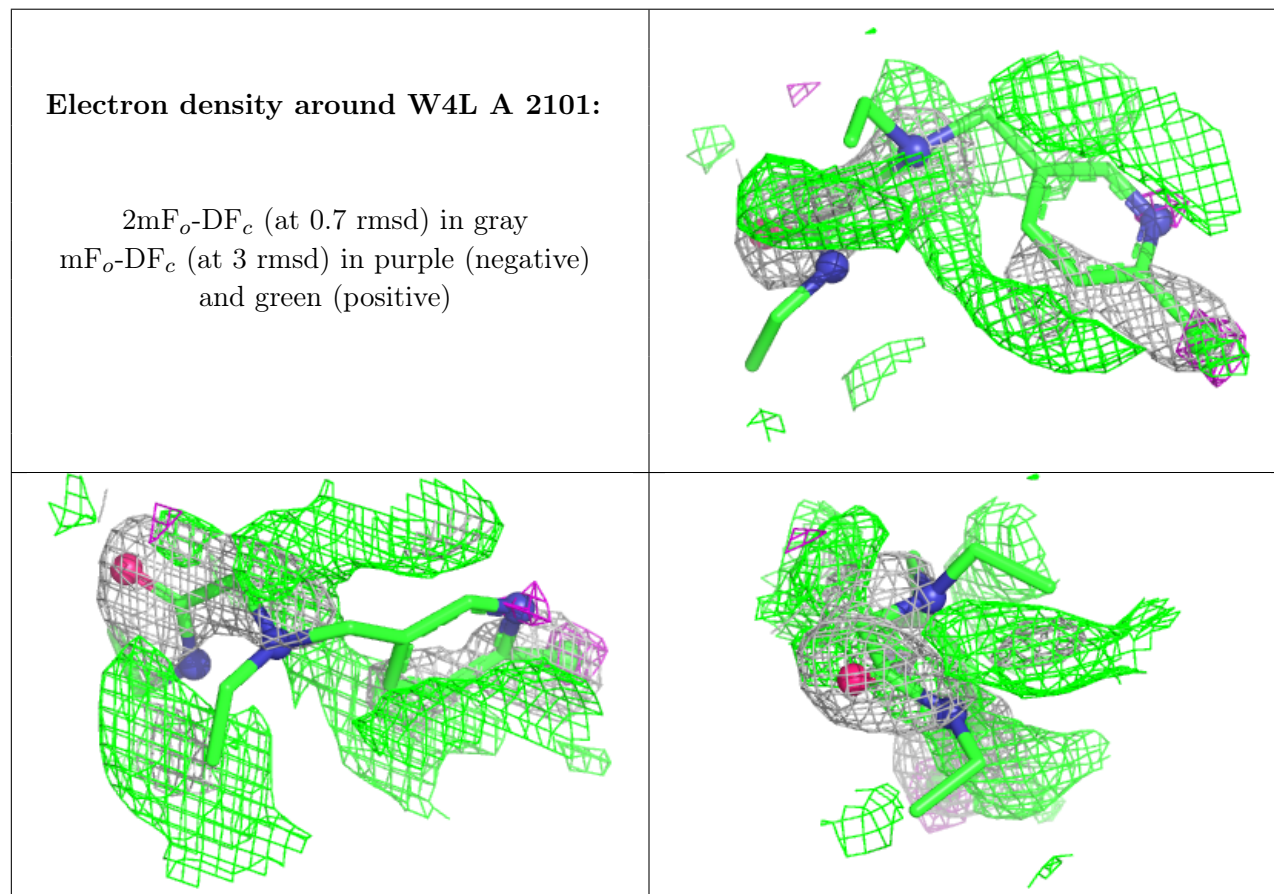
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	W4L	A	2101	17/17	0.59	0.33	20,20,20,20	17

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.