



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:12 AM UTC

PDB ID : 7FOH / pdb_00007foh
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P08B05 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 : 1.69 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

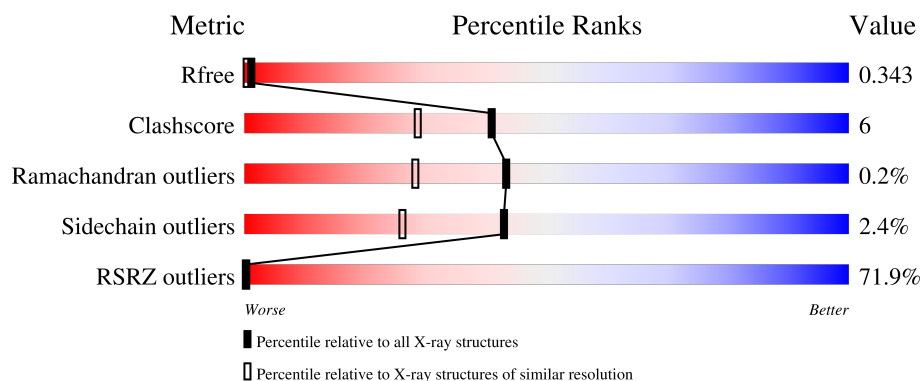
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	64% 81%10%8%
2	B	308	72% 76%19%...

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	W5U	B	401	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9200 atoms, of which 4524 are hydrogens and 0 are deuteriums.

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

There are 20 discrepancies between the modelled and reference sequences:

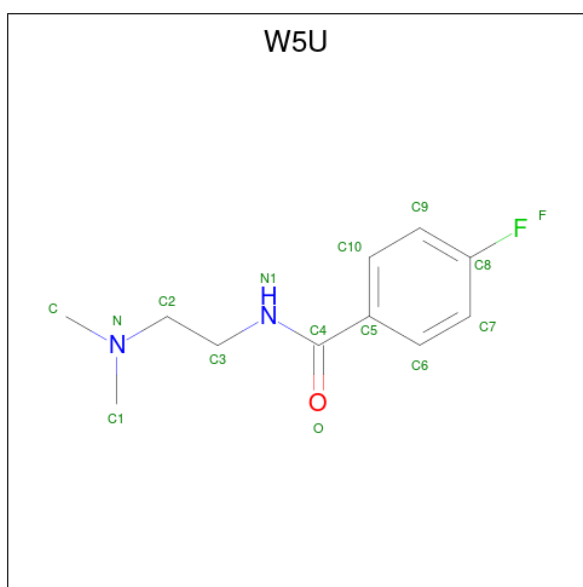
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is N-[2-(dimethylamino)ethyl]-4-fluorobenzamide (CCD ID: W5U) (formula: $C_{11}H_{15}FN_2O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	0	0
			15	11	1	2	1		
3	B	1	Total	C	F	N	O	0	0
			15	11	1	2	1		

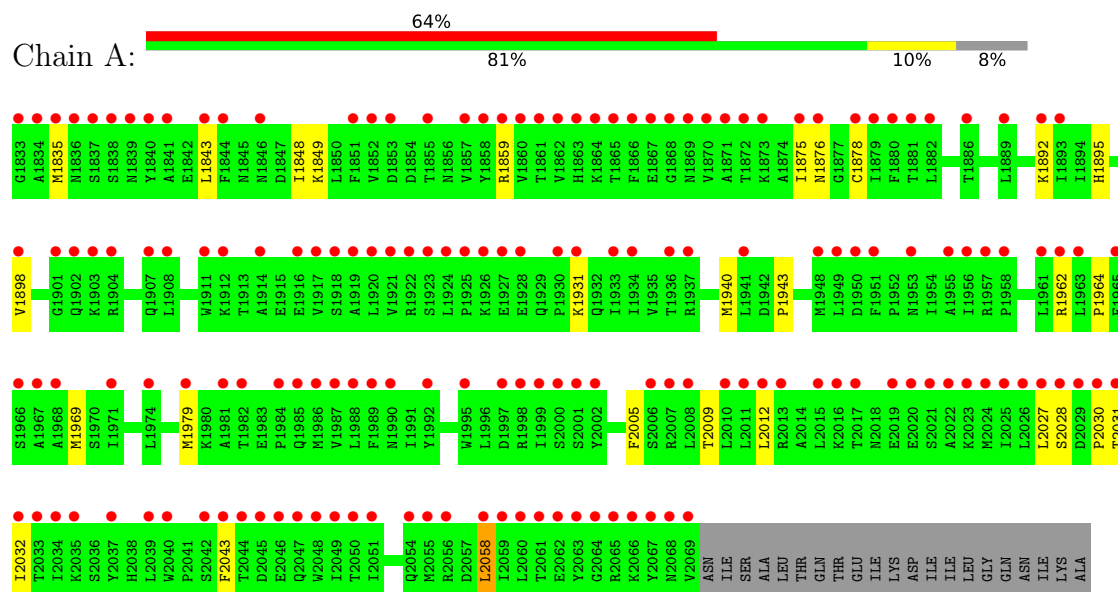
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		
4	B	25	Total	O	0	0
			25	25		

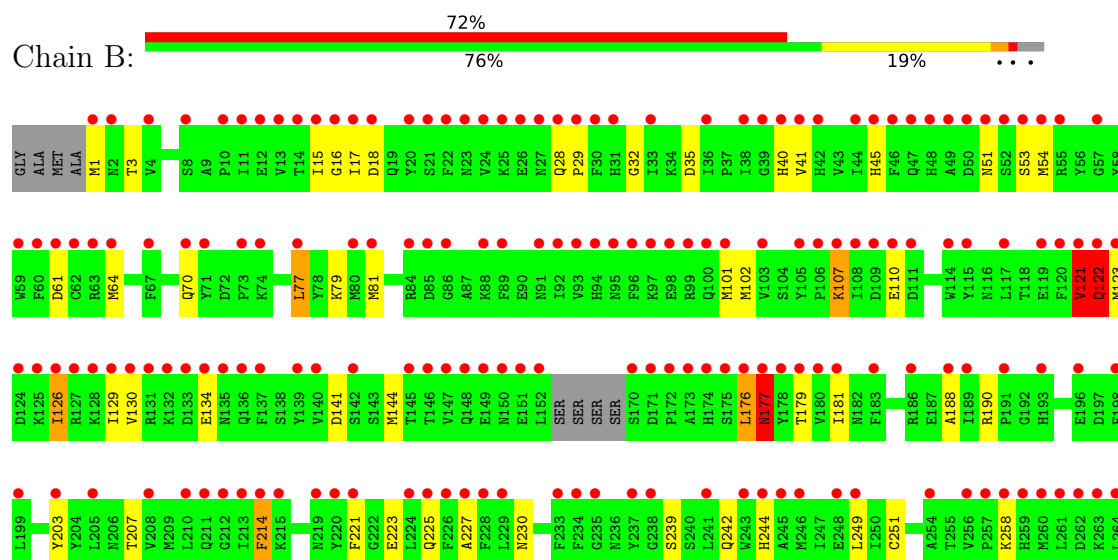
3 Residue-property plots

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



D265	E266	I267	L268	Y269	Y270	Q271	I272	K273	T274	L275	P276	E277	Q278	Y279	S280	D281	I282	L283	L284	N285	E286	R287	V288	W289	N290	I291	C292	L293	Y294	S295	S296	F297	Q298	K299	N300	S301	L302	H303	N304	T305	E306	K307	E310	N311	K312	Y313	P314	E315	L316	L317
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	89.40Å 81.78Å 93.43Å 90.00° 108.60° 90.00°	Depositor
Resolution (Å)	44.27 – 1.69 44.27 – 1.69	Depositor EDS
% Data completeness (in resolution range)	95.7 (44.27-1.69) 96.4 (44.27-1.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 1.69Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.297 , 0.336 0.316 , 0.343	Depositor DCC
R_{free} test set	2093 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9200	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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: W5U

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	0.78	0/2149	0.78	0/2911
2	B	0.91	7/2739 (0.3%)	1.09	26/3699 (0.7%)
All	All	0.86	7/4888 (0.1%)	0.96	26/6610 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	7

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	123[A]	MET	N-CA	7.63	1.55	1.46
2	B	123[B]	MET	N-CA	7.63	1.55	1.46
2	B	122[A]	GLN	C-N	6.74	1.43	1.33
2	B	122[B]	GLN	C-N	6.74	1.43	1.33
2	B	221	PHE	C-O	-6.46	1.16	1.24
2	B	227	ALA	C-O	-5.84	1.17	1.24
2	B	18	ASP	CG-OD2	-5.33	1.15	1.25

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	122[A]	GLN	CA-C-N	-8.07	108.83	120.29
2	B	122[A]	GLN	C-N-CA	-8.07	108.83	120.29
2	B	122[B]	GLN	CA-C-N	-8.07	108.83	120.29
2	B	122[B]	GLN	C-N-CA	-8.07	108.83	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	214	PHE	CA-C-O	-6.47	112.03	119.60
2	B	122[A]	GLN	CA-C-O	-6.46	113.78	121.66
2	B	122[B]	GLN	CA-C-O	-6.46	113.78	121.66
2	B	244	HIS	CA-CB-CG	-6.29	107.51	113.80
2	B	223	GLU	CA-C-N	6.13	128.78	120.38
2	B	223	GLU	C-N-CA	6.13	128.78	120.38
2	B	126	ILE	CA-C-N	6.01	130.76	120.72
2	B	126	ILE	C-N-CA	6.01	130.76	120.72
2	B	32	GLY	N-CA-C	5.96	119.33	111.52
2	B	16	GLY	CA-C-O	-5.90	115.16	120.94
2	B	15	ILE	CA-C-N	-5.80	116.98	122.66
2	B	15	ILE	C-N-CA	-5.80	116.98	122.66
2	B	123[A]	MET	CA-C-O	-5.61	114.47	120.42
2	B	123[B]	MET	CA-C-O	-5.61	114.47	120.42
2	B	121	VAL	CA-C-O	-5.37	114.58	120.97
2	B	16	GLY	CA-C-N	5.23	130.69	122.84
2	B	16	GLY	C-N-CA	5.23	130.69	122.84
2	B	225	GLN	CA-C-N	5.21	128.23	120.31
2	B	225	GLN	C-N-CA	5.21	128.23	120.31
2	B	107	LYS	CA-C-O	-5.13	115.44	120.98
2	B	129	ILE	CA-C-N	5.12	128.11	122.22
2	B	129	ILE	C-N-CA	5.12	128.11	122.22

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	121	VAL	Mainchain
2	B	122[A]	GLN	Mainchain
2	B	122[B]	GLN	Mainchain
2	B	176	LEU	Mainchain
2	B	177[A]	ASN	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	17	0
2	B	2580	2464	2398	42	0
3	B	30	0	0	0	0
4	A	33	0	0	0	0
4	B	25	0	0	2	0
All	All	4676	4524	4372	59	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 (59) 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:41[A]:VAL:HG11	2:B:121:VAL:O	1.69	0.92
2:B:249:LEU:HD12	2:B:249:LEU:O	1.77	0.84
2:B:121:VAL:HG12	2:B:126:ILE:HD11	1.67	0.75
2:B:41[A]:VAL:CG1	2:B:121:VAL:O	2.40	0.69
2:B:1:MET:HB3	2:B:35:ASP:HA	1.76	0.66
2:B:258:LYS:HD2	2:B:258:LYS:H	1.66	0.61
2:B:70:GLN:HB3	2:B:81:MET:CE	2.32	0.60
2:B:230[B]:ASN:ND2	2:B:239:SER:OG	2.36	0.58
2:B:242:GLN:HA	2:B:242:GLN:OE1	2.03	0.58
2:B:41[B]:VAL:HG11	2:B:121:VAL:O	2.04	0.57
2:B:3:THR:HG21	2:B:102:MET:HE1	1.86	0.57
2:B:177[A]:ASN:HD22	2:B:177[A]:ASN:H	1.52	0.56
1:A:2005:PHE:O	1:A:2009:THR:HG23	2.05	0.56
1:A:1878:CYS:HA	1:A:1892:LYS:O	2.06	0.55
2:B:1:MET:N	4:B:501:HOH:O	2.38	0.55
2:B:3:THR:CG2	2:B:102:MET:HE1	2.37	0.55
2:B:41[B]:VAL:CG1	2:B:121:VAL:O	2.55	0.54
1:A:1895:HIS:O	1:A:1898[A]:VAL:HG22	2.08	0.53
2:B:249:LEU:HD12	2:B:249:LEU:C	2.28	0.51
1:A:1859:ARG:NH1	1:A:1979[B]:MET:HE3	2.25	0.51
1:A:1875:ILE:O	1:A:1876:ASN:C	2.54	0.51
2:B:179:THR:HG21	2:B:214:PHE:CE2	2.46	0.50
2:B:277:GLU:CD	2:B:277:GLU:H	2.18	0.50
2:B:306:GLU:O	2:B:310:GLU:HG3	2.13	0.49
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.38	0.48
1:A:2032:ILE:HG21	1:A:2043:PHE:CD1	2.49	0.48
1:A:1979[B]:MET:HA	1:A:1979[B]:MET:HE2	1.96	0.48
2:B:40:HIS:HD2	4:B:511:HOH:O	1.97	0.47
2:B:144:MET:HE2	2:B:176:LEU:HG	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	1.96	0.47
2:B:122[A]:GLN:HA	2:B:122[A]:GLN:OE1	2.15	0.47
1:A:1964:PRO:HG2	1:A:2012:LEU:HB2	1.96	0.47
2:B:28:GLN:HG3	2:B:29:PRO:HD2	1.96	0.46
2:B:110:GLU:HG2	2:B:110:GLU:O	2.16	0.45
2:B:51:ASN:OD1	2:B:53:SER:HB2	2.16	0.45
2:B:77:LEU:HD21	2:B:79:LYS:HE3	1.98	0.45
2:B:141:ASP:OD1	2:B:141:ASP:C	2.60	0.45
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.64	0.45
2:B:177[A]:ASN:HD22	2:B:177[A]:ASN:N	2.14	0.45
2:B:190:ARG:HG3	2:B:203[B]:TYR:CZ	2.52	0.45
1:A:1859:ARG:HH12	1:A:1979[A]:MET:CE	2.30	0.44
1:A:1962:ARG:HD3	1:A:1962:ARG:H	1.81	0.44
2:B:61:ASP:OD1	2:B:61:ASP:C	2.59	0.44
1:A:1969:MET:HA	1:A:1969:MET:HE2	1.99	0.44
2:B:287:ARG:O	2:B:291:ILE:HD13	2.18	0.44
2:B:17:ILE:O	2:B:17:ILE:HG23	2.17	0.44
2:B:134:GLU:OE1	2:B:134:GLU:N	2.43	0.43
2:B:70:GLN:HB3	2:B:81:MET:HE2	2.01	0.43
1:A:1940:MET:C	1:A:1943:PRO:HD2	2.45	0.42
2:B:1:MET:HE3	2:B:35:ASP:O	2.19	0.41
1:A:2028:SER:O	1:A:2030:PRO:HD3	2.21	0.41
2:B:53:SER:O	2:B:54[A]:MET:HB3	2.21	0.41
2:B:251:CYS:SG	2:B:292:CYS:SG	3.19	0.41
2:B:203[A]:TYR:CZ	2:B:207:THR:HG21	2.56	0.40
2:B:275:LEU:CD2	2:B:283:LEU:HD13	2.51	0.40
2:B:275:LEU:HD23	2:B:275:LEU:HA	1.98	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%)	9 (4%)	0	100	100
2	B	315/308 (102%)	298 (95%)	15 (5%)	2 (1%)	21	9
All	All	573/566 (101%)	547 (96%)	24 (4%)	2 (0%)	43	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	177[A]	ASN
2	B	177[B]	ASN

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%)	234 (99%)	3 (1%)	61	48
2	B	294/284 (104%)	283 (96%)	11 (4%)	30	14
All	All	531/517 (103%)	517 (97%)	14 (3%)	43	23

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2027	LEU
1	A	2031	THR
1	A	2058	LEU
2	B	45[A]	HIS
2	B	45[B]	HIS
2	B	77	LEU
2	B	101	MET
2	B	107	LYS
2	B	130	VAL
2	B	177[A]	ASN
2	B	177[B]	ASN
2	B	181	ILE
2	B	281	ASP
2	B	317	LEU

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	1907	GLN
2	B	40	HIS
2	B	206	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	W5U	B	402	-	15,15,15	2.32	6 (40%)	19,19,19	2.12	6 (31%)
3	W5U	B	401	-	15,15,15	2.41	7 (46%)	19,19,19	2.71	9 (47%)

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	W5U	B	402	-	-	1/10/10/10	0/1/1/1
3	W5U	B	401	-	-	5/10/10/10	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	W5U	F-C8	-5.22	1.23	1.36
3	B	401	W5U	C3-N1	-4.61	1.35	1.46
3	B	401	W5U	C6-C7	-4.12	1.32	1.38
3	B	402	W5U	C6-C7	-3.96	1.32	1.38
3	B	402	W5U	O-C4	-3.70	1.14	1.23
3	B	401	W5U	C6-C5	-3.63	1.33	1.39
3	B	401	W5U	F-C8	-3.08	1.28	1.36
3	B	401	W5U	C7-C8	-2.83	1.31	1.37
3	B	402	W5U	C7-C8	-2.46	1.32	1.37
3	B	402	W5U	C3-N1	-2.24	1.41	1.46
3	B	401	W5U	C5-C4	-2.14	1.45	1.50
3	B	402	W5U	C9-C8	2.07	1.41	1.37
3	B	401	W5U	C9-C8	2.04	1.41	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	W5U	C2-C3-N1	-6.99	98.06	111.56
3	B	402	W5U	C2-C3-N1	-5.20	101.53	111.56
3	B	401	W5U	O-C4-N1	-4.39	114.03	122.59
3	B	401	W5U	F-C8-C9	3.68	124.44	118.55
3	B	402	W5U	F-C8-C9	3.32	123.87	118.55
3	B	401	W5U	C6-C5-C4	-3.19	110.26	120.60
3	B	402	W5U	C7-C6-C5	3.17	124.19	120.80
3	B	401	W5U	C5-C4-N1	2.99	123.34	117.12
3	B	401	W5U	C3-N1-C4	2.84	128.53	122.11
3	B	402	W5U	C9-C10-C5	-2.71	117.90	120.80
3	B	402	W5U	F-C8-C7	-2.70	114.22	118.55
3	B	402	W5U	O-C4-N1	-2.63	117.47	122.59
3	B	401	W5U	C9-C10-C5	-2.59	118.03	120.80
3	B	401	W5U	F-C8-C7	-2.57	114.43	118.55
3	B	401	W5U	C10-C5-C4	2.33	128.14	120.60

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	W5U	N-C2-C3-N1
3	B	401	W5U	C5-C4-N1-C3
3	B	401	W5U	O-C4-N1-C3
3	B	401	W5U	C3-C2-N-C
3	B	402	W5U	C3-C2-N-C
3	B	401	W5U	C3-C2-N-C1

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%)	3.32	165 (69%) 0 0	22, 71, 159, 236	12 (5%)
2	B	300/308 (97%)	3.25	221 (73%) 0 0	26, 70, 162, 225	9 (3%)
All	All	537/566 (94%)	3.28	386 (71%) 0 0	22, 71, 162, 236	21 (3%)

All (386) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	275	LEU	12.2
1	A	1860	VAL	11.2
1	A	2063	TYR	9.7
2	B	49	ALA	9.3
1	A	1955	ALA	9.2
2	B	316	LEU	9.1
2	B	129	ILE	8.8
2	B	24	VAL	8.7
2	B	227	ALA	8.4
2	B	288	VAL	8.4
1	A	2069	VAL	8.3
2	B	111	ASP	8.2
1	A	1951	PHE	8.2
2	B	213	ILE	8.1
2	B	130	VAL	8.1
2	B	54[A]	MET	8.0
2	B	276	PRO	8.0
2	B	152	LEU	8.0
1	A	1879	ILE	7.9
1	A	1878	CYS	7.8
1	A	2002[A]	TYR	7.8
1	A	1852	VAL	7.7
2	B	283	LEU	7.5
2	B	246	MET	7.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	108	ILE	7.3
1	A	1834	ALA	7.3
1	A	1923	SER	7.3
1	A	1840	TYR	7.3
1	A	1979[A]	MET	7.2
2	B	274	THR	7.2
1	A	2027	LEU	7.1
2	B	291	ILE	7.1
1	A	1989	PHE	7.0
2	B	282	ILE	6.8
2	B	313	TYR	6.8
1	A	1866	PHE	6.8
1	A	1833	GLY	6.7
2	B	44[A]	ILE	6.7
1	A	2001[A]	SER	6.7
1	A	1961[A]	LEU	6.6
2	B	121	VAL	6.6
1	A	1965	PHE	6.4
2	B	203[A]	TYR	6.4
1	A	2065	ARG	6.4
1	A	2048	TRP	6.4
1	A	1988	LEU	6.3
1	A	2015	LEU	6.3
2	B	107	LYS	6.3
1	A	1859	ARG	6.3
1	A	2060	LEU	6.3
2	B	22	PHE	6.3
2	B	77	LEU	6.2
1	A	2059	ILE	6.2
2	B	119	GLU	6.1
1	A	1893	ILE	6.1
2	B	41[A]	VAL	6.0
1	A	1835	MET	6.0
1	A	2017[A]	THR	5.9
2	B	122[A]	GLN	5.9
2	B	13	VAL	5.9
2	B	284	LEU	5.9
2	B	212[A]	GLY	5.8
2	B	270	TYR	5.7
2	B	101	MET	5.7
1	A	1870	VAL	5.5
1	A	1855[A]	THR	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	266	GLU	5.5
1	A	1868	GLY	5.4
2	B	1	MET	5.4
1	A	2032	ILE	5.3
1	A	2061	THR	5.2
1	A	2058	LEU	5.2
1	A	2040	TRP	5.2
1	A	1876	ASN	5.2
2	B	173	ALA	5.2
2	B	11	ILE	5.1
2	B	117	LEU	5.1
1	A	1984	PRO	5.0
1	A	1901	GLY	5.0
1	A	1927	GLU	5.0
1	A	1998	ARG	4.9
2	B	281	ASP	4.9
2	B	170	SER	4.9
1	A	2049	ILE	4.9
1	A	2012	LEU	4.9
2	B	89	PHE	4.9
2	B	93	VAL	4.9
1	A	2067	TYR	4.8
2	B	174	HIS	4.8
2	B	279	TYR	4.8
2	B	50	ASP	4.8
2	B	100	GLN	4.8
2	B	221	PHE	4.8
1	A	1926	LYS	4.7
1	A	2068	ASN	4.7
2	B	53	SER	4.7
1	A	1838	SER	4.6
2	B	4	VAL	4.6
2	B	307	LYS	4.6
2	B	80	MET	4.6
1	A	1992	TYR	4.6
2	B	29	PRO	4.6
1	A	2051	ILE	4.6
2	B	226	PHE	4.5
2	B	317	LEU	4.5
2	B	30	PHE	4.5
1	A	1995	TRP	4.5
1	A	2020	GLU	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	128	LYS	4.5
1	A	2056[A]	ARG	4.5
2	B	55[A]	ARG	4.5
2	B	20	TYR	4.4
1	A	2008	LEU	4.4
2	B	25	LYS	4.4
1	A	1853	ASP	4.4
1	A	2039	LEU	4.4
1	A	1861	THR	4.4
2	B	114	TRP	4.4
2	B	26	GLU	4.4
2	B	150	ASN	4.4
1	A	1862	VAL	4.4
1	A	2066	LYS	4.4
1	A	1934	ILE	4.4
2	B	2	ASN	4.3
1	A	1867	GLU	4.3
2	B	124	ASP	4.3
1	A	2025	ILE	4.3
2	B	94	HIS	4.3
1	A	1924	LEU	4.2
1	A	1925	PRO	4.2
1	A	1851	PHE	4.2
2	B	47	GLN	4.1
2	B	171	ASP	4.1
2	B	137	PHE	4.1
2	B	233	PHE	4.1
1	A	2024[A]	MET	4.1
2	B	103	VAL	4.1
2	B	234	PHE	4.1
1	A	2064	GLY	4.0
2	B	110	GLU	4.0
2	B	146	THR	4.0
2	B	297	PHE	4.0
1	A	2016	LYS	4.0
2	B	294	TYR	4.0
2	B	254	ALA	4.0
2	B	16	GLY	4.0
2	B	38	ILE	3.9
2	B	172	PRO	3.9
2	B	123[A]	MET	3.9
1	A	1882	LEU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	2026	LEU	3.9
2	B	245	ALA	3.9
1	A	1907	GLN	3.9
2	B	131	ARG	3.9
2	B	64[A]	MET	3.9
2	B	48	HIS	3.9
1	A	1844	PHE	3.9
1	A	1881	THR	3.8
1	A	2046	GLU	3.8
2	B	287	ARG	3.8
1	A	2037	TYR	3.8
1	A	2030	PRO	3.8
1	A	1933	ILE	3.8
2	B	125	LYS	3.8
1	A	2042	SER	3.8
2	B	278	GLN	3.8
1	A	2044	THR	3.8
1	A	2021	SER	3.8
1	A	1892	LYS	3.7
2	B	132	LYS	3.7
1	A	1999	ILE	3.7
2	B	42[A]	HIS	3.7
1	A	1836	ASN	3.7
2	B	238	GLY	3.7
1	A	1843	LEU	3.7
2	B	176	LEU	3.7
1	A	2031	THR	3.7
2	B	27	ASN	3.7
1	A	1904	ARG	3.7
2	B	134	GLU	3.7
1	A	1841	ALA	3.6
2	B	17	ILE	3.6
1	A	2028	SER	3.6
2	B	177[A]	ASN	3.6
2	B	179	THR	3.6
2	B	148	GLN	3.6
1	A	1918[A]	SER	3.5
2	B	189	ILE	3.5
1	A	2010	LEU	3.5
2	B	109	ASP	3.5
1	A	1837	SER	3.5
2	B	39	GLY	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	2007	ARG	3.5
2	B	84	ARG	3.5
2	B	33	ILE	3.5
1	A	2006	SER	3.5
1	A	2034	ILE	3.4
2	B	92	ILE	3.4
2	B	267	ILE	3.4
2	B	315	GLU	3.4
2	B	46	PHE	3.4
2	B	52	SER	3.4
2	B	180	VAL	3.4
2	B	127	ARG	3.4
2	B	106	PRO	3.4
2	B	258	LYS	3.4
1	A	1963	LEU	3.4
2	B	12	GLU	3.4
2	B	256	VAL	3.4
2	B	257	PRO	3.4
1	A	1957	ARG	3.4
1	A	2055	MET	3.4
2	B	28	GLN	3.3
2	B	280	SER	3.3
2	B	31	HIS	3.3
2	B	237	TYR	3.3
1	A	1839	ASN	3.3
2	B	51	ASN	3.3
1	A	1864	LYS	3.3
2	B	301	SER	3.3
2	B	225	GLN	3.3
2	B	115	TYR	3.2
2	B	300	ASN	3.2
2	B	303	HIS	3.2
2	B	248	GLU	3.2
1	A	1931[A]	LYS	3.2
2	B	21	SER	3.2
1	A	1922	ARG	3.2
2	B	14	THR	3.2
2	B	193	HIS	3.2
1	A	1869	ASN	3.2
2	B	126	ILE	3.2
1	A	1902	GLN	3.2
1	A	1911	TRP	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	243	TRP	3.2
1	A	1974	LEU	3.1
1	A	1912	LYS	3.1
1	A	1962	ARG	3.1
1	A	1950	ASP	3.1
2	B	269	TYR	3.1
2	B	215	LYS	3.1
1	A	1967	ALA	3.1
1	A	2045	ASP	3.1
2	B	73	PRO	3.0
1	A	2047	GLN	3.0
2	B	293	LEU	3.0
2	B	211[A]	GLN	3.0
2	B	235	GLY	3.0
1	A	1982	THR	3.0
1	A	2000	SER	3.0
2	B	62	CYS	3.0
2	B	67	PHE	3.0
1	A	2062	GLU	3.0
2	B	91	ASN	3.0
1	A	2050	THR	3.0
2	B	142	SER	3.0
1	A	1981	ALA	3.0
2	B	60	PHE	3.0
1	A	1920	LEU	2.9
2	B	277	GLU	2.9
1	A	1846	ASN	2.9
1	A	1889	LEU	2.9
1	A	1936	THR	2.9
1	A	2023	LYS	2.9
1	A	1880	PHE	2.8
2	B	99	ARG	2.8
2	B	261	LEU	2.8
2	B	95	ASN	2.8
1	A	1873	LYS	2.8
2	B	96	PHE	2.8
2	B	299	LYS	2.8
1	A	1863	HIS	2.8
2	B	295	SER	2.8
1	A	1941	LEU	2.8
1	A	1953	ASN	2.8
1	A	1971	ILE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	36	ILE	2.8
2	B	86	GLY	2.8
1	A	1898[A]	VAL	2.8
2	B	151	GLU	2.8
2	B	224	LEU	2.8
2	B	305	THR	2.8
2	B	59	TRP	2.7
1	A	2054[A]	GLN	2.7
2	B	241	LEU	2.7
1	A	1886	THR	2.7
1	A	2029	ASP	2.7
1	A	1949	LEU	2.7
2	B	249	LEU	2.7
2	B	140	VAL	2.7
2	B	208	VAL	2.7
1	A	1858	TYR	2.7
2	B	74	LYS	2.7
2	B	61	ASP	2.7
1	A	2043	PHE	2.6
2	B	183	PHE	2.6
2	B	214	PHE	2.6
2	B	178[A]	TYR	2.6
1	A	1875	ILE	2.6
1	A	1985	GLN	2.6
2	B	70	GLN	2.6
2	B	219	ASN	2.6
1	A	1917	VAL	2.6
2	B	289	TRP	2.6
2	B	10	PRO	2.6
2	B	290	ASN	2.6
2	B	120	PHE	2.6
2	B	45[A]	HIS	2.6
2	B	210	LEU	2.6
2	B	23	ASN	2.6
2	B	191	PRO	2.6
2	B	85	ASP	2.5
1	A	1928	GLU	2.5
2	B	15	ILE	2.5
1	A	1968	ALA	2.5
2	B	57	GLY	2.5
2	B	40	HIS	2.5
2	B	260	MET	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1914	ALA	2.5
1	A	1921	VAL	2.5
1	A	1987	VAL	2.5
2	B	136	GLN	2.5
2	B	139	TYR	2.5
2	B	81	MET	2.5
1	A	1997	ASP	2.4
2	B	18	ASP	2.4
1	A	1903	LYS	2.4
2	B	228	PHE	2.4
2	B	264	LEU	2.4
1	A	1937	ARG	2.4
2	B	292	CYS	2.4
1	A	1930	PRO	2.4
1	A	1958	PRO	2.4
2	B	199	LEU	2.4
2	B	205	LEU	2.4
2	B	286	GLU	2.4
2	B	244	HIS	2.4
2	B	175	SER	2.4
2	B	285	ASN	2.4
2	B	133	ASP	2.4
1	A	1916	GLU	2.4
2	B	186	ARG	2.4
1	A	1956	ILE	2.4
1	A	1966	SER	2.3
2	B	8	SER	2.3
2	B	135	ASN	2.3
1	A	1865	THR	2.3
2	B	311	ASN	2.3
2	B	188	ALA	2.3
2	B	268	LEU	2.3
1	A	2019	GLU	2.3
2	B	149	GLU	2.3
1	A	1857	VAL	2.3
1	A	1948	MET	2.3
1	A	1986	MET	2.3
2	B	314	PRO	2.3
2	B	229	LEU	2.3
2	B	304	ASN	2.3
2	B	263	LYS	2.3
2	B	273	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1871	ALA	2.2
2	B	88	LYS	2.2
2	B	181	ILE	2.2
2	B	98	GLU	2.2
2	B	147	VAL	2.2
1	A	2011	LEU	2.2
2	B	271	GLN	2.2
2	B	63	ARG	2.2
1	A	1990	ASN	2.2
2	B	97	LYS	2.2
2	B	296	SER	2.2
1	A	1908	LEU	2.1
2	B	259	HIS	2.1
1	A	2035	LYS	2.1
2	B	196	GLU	2.1
2	B	262	ASP	2.1
1	A	1872	THR	2.1
1	A	2033	THR	2.1
2	B	220	TYR	2.1
1	A	2022	ALA	2.1
2	B	145	THR	2.0
1	A	2013	ARG	2.0
2	B	71	TYR	2.0
2	B	105	TYR	2.0
2	B	198	PHE	2.0
1	A	1919[A]	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	W5U	B	401	15/15	0.64	0.18	20,20,20,20	0
3	W5U	B	402	15/15	0.79	0.15	20,20,20,20	15

6.5 Other polymers [i](#)

There are no such residues in this entry.