



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:47 PM UTC

PDB ID : 7FO5 / pdb_00007fo5
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P07G11 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 : 1.71 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:

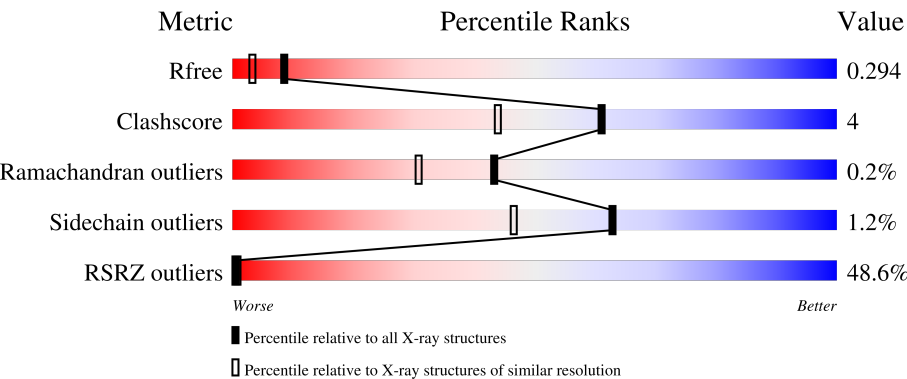
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.71 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	41% 81% 10% 8%
2	B	308	50% 84% 12% ••

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9213 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:

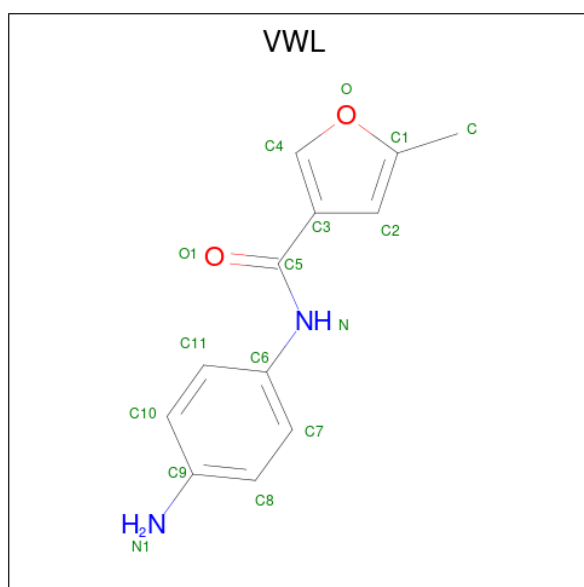
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN	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-(4-aminophenyl)-5-methylfuran-3-carboxamide (CCD ID: VWL) (formula: $C_{12}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			16	12	2	2		

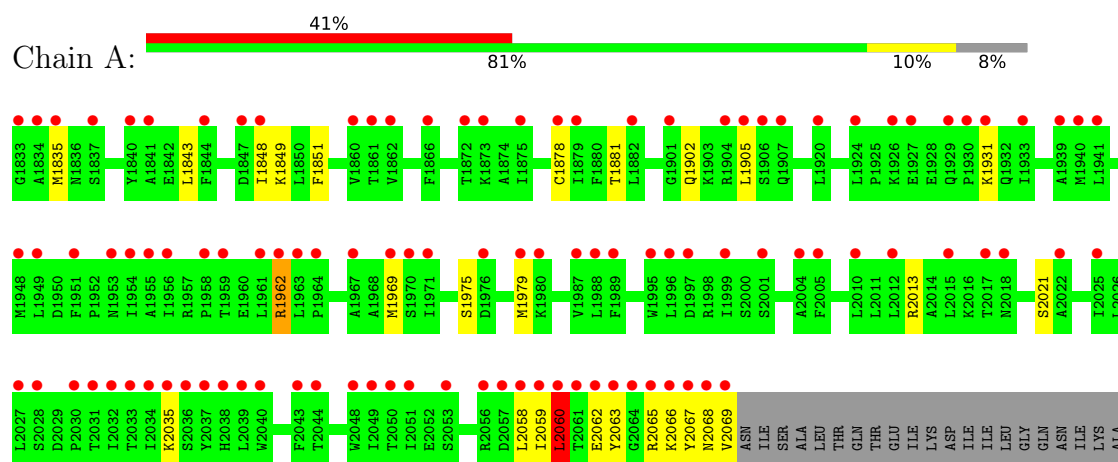
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total	O	0	0
			44	44		
4	B	41	Total	O	0	0
			41	41		

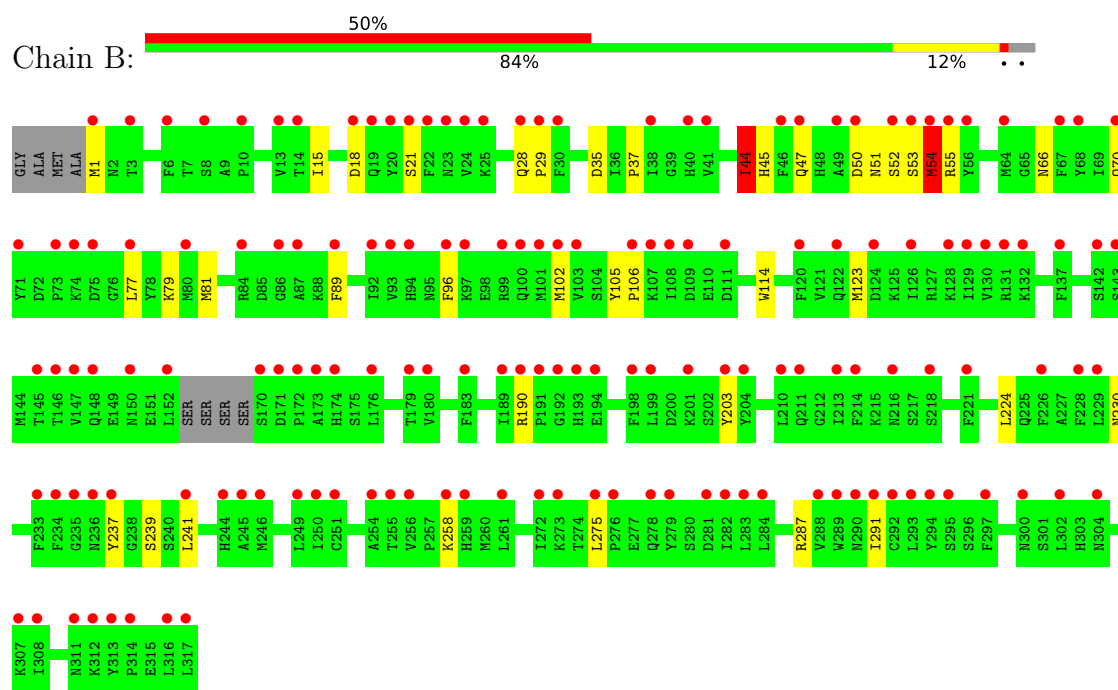
3 Residue-property plots

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	89.34Å 82.25Å 92.91Å 90.00° 107.85° 90.00°	Depositor
Resolution (Å)	44.22 – 1.71 44.22 – 1.71	Depositor EDS
% Data completeness (in resolution range)	98.8 (44.22-1.71) 98.8 (44.22-1.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 1.71Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.262 , 0.289 0.272 , 0.294	Depositor DCC
R_{free} test set	2098 reflections (3.08%)	wwPDB-VP
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9213	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	2/2149 (0.1%)	1.00	10/2911 (0.3%)
2	B	0.81	8/2739 (0.3%)	1.01	14/3699 (0.4%)
All	All	0.79	10/4888 (0.2%)	1.00	24/6610 (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	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2060	LEU	C-O	-7.38	1.15	1.24
2	B	55[A]	ARG	N-CA	7.13	1.55	1.46
2	B	55[B]	ARG	N-CA	7.13	1.55	1.46
2	B	44[A]	ILE	C-N	6.56	1.41	1.33
2	B	44[B]	ILE	C-N	6.56	1.41	1.33
2	B	45[A]	HIS	N-CA	6.52	1.54	1.46
2	B	45[B]	HIS	N-CA	6.52	1.54	1.46
2	B	54[A]	MET	C-N	5.91	1.41	1.33
2	B	54[B]	MET	C-N	5.91	1.41	1.33
1	A	2060	LEU	N-CA	5.13	1.52	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54[A]	MET	CA-C-N	-10.75	106.05	121.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	54[A]	MET	C-N-CA	-10.75	106.05	121.42
2	B	54[B]	MET	CA-C-N	-10.75	106.05	121.42
2	B	54[B]	MET	C-N-CA	-10.75	106.05	121.42
1	A	2067	TYR	CA-C-N	9.92	136.25	122.07
1	A	2067	TYR	C-N-CA	9.92	136.25	122.07
1	A	2067	TYR	CB-CA-C	7.71	123.46	111.28
2	B	44[A]	ILE	CA-C-O	-6.97	112.63	121.48
2	B	44[B]	ILE	CA-C-O	-6.97	112.63	121.48
2	B	44[A]	ILE	CA-C-N	-6.57	107.17	121.87
2	B	44[A]	ILE	C-N-CA	-6.57	107.17	121.87
2	B	44[B]	ILE	CA-C-N	-6.57	107.17	121.87
2	B	44[B]	ILE	C-N-CA	-6.57	107.17	121.87
1	A	2060	LEU	CB-CA-C	-6.22	100.85	110.81
1	A	2059	ILE	CA-C-N	5.58	128.08	120.54
1	A	2059	ILE	C-N-CA	5.58	128.08	120.54
1	A	2062	GLU	CB-CA-C	5.50	120.28	109.72
1	A	2063	TYR	CA-C-O	5.49	125.69	119.27
2	B	44[A]	ILE	N-CA-C	-5.45	100.76	109.20
2	B	44[B]	ILE	N-CA-C	-5.45	100.76	109.20
1	A	2063	TYR	N-CA-C	-5.39	106.55	113.23
1	A	2066	LYS	CA-C-O	-5.12	114.08	119.97
2	B	45[A]	HIS	CA-CB-CG	5.01	118.81	113.80
2	B	45[B]	HIS	CA-CB-CG	5.01	118.81	113.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	44[A]	ILE	Mainchain
2	B	44[B]	ILE	Mainchain
2	B	54[A]	MET	Mainchain
2	B	54[B]	MET	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	16	11
2	B	2580	2464	2398	22	11
3	B	16	0	0	0	0
4	A	44	0	0	0	0
4	B	41	0	0	1	0
All	All	4689	4524	4372	38	11

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 (38) 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:2021:SER:HB3	1:A:2058:LEU:HD11	1.41	1.02
1:A:2021:SER:CB	1:A:2058:LEU:HD11	2.08	0.83
1:A:1962:ARG:O	1:A:2013:ARG:NH1	2.12	0.83
2:B:1:MET:N	4:B:501:HOH:O	2.17	0.77
1:A:2021:SER:HB3	1:A:2058:LEU:CD1	2.15	0.75
2:B:70:GLN:HB3	2:B:81:MET:CE	2.21	0.69
1:A:2060:LEU:HD12	1:A:2060:LEU:O	1.94	0.68
2:B:96:PHE:HB2	2:B:102:MET:HE3	1.78	0.64
2:B:230[B]:ASN:ND2	2:B:239:SER:OG	2.32	0.63
2:B:54[A]:MET:HG2	2:B:54[A]:MET:O	1.98	0.62
2:B:96:PHE:CB	2:B:102:MET:HE3	2.31	0.61
2:B:287:ARG:O	2:B:291:ILE:HD13	2.04	0.57
2:B:258:LYS:HD2	2:B:258:LYS:H	1.70	0.56
2:B:1:MET:HB3	2:B:35:ASP:HA	1.90	0.54
2:B:70:GLN:HB3	2:B:81:MET:HE2	1.89	0.53
2:B:77:LEU:HD21	2:B:79:LYS:HE3	1.90	0.52
1:A:2058:LEU:HD23	1:A:2058:LEU:O	2.10	0.52
2:B:50:ASP:OD1	2:B:51:ASN:N	2.44	0.50
1:A:2058:LEU:HD23	1:A:2058:LEU:C	2.37	0.50
2:B:237:TYR:CE2	2:B:241:LEU:HD11	2.47	0.49
1:A:2060:LEU:HD12	1:A:2060:LEU:C	2.38	0.49
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	1.95	0.48
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.60	0.48
2:B:224:LEU:C	2:B:224:LEU:HD23	2.38	0.48
2:B:70:GLN:HB3	2:B:81:MET:HE1	1.94	0.47
1:A:1962:ARG:HD3	1:A:1962:ARG:H	1.79	0.47
2:B:37:PRO:HD3	2:B:105:TYR:CD1	2.50	0.46
2:B:190:ARG:HD3	2:B:203[A]:TYR:CE2	2.50	0.46
1:A:1878:CYS:SG	1:A:1969:MET:HE3	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1975:SER:O	1:A:1979[A]:MET:SD	2.77	0.43
1:A:2035:LYS:HD3	1:A:2035:LYS:HA	1.84	0.42
2:B:28:GLN:HG3	2:B:29:PRO:HD2	2.02	0.42
2:B:44[A]:ILE:O	2:B:44[A]:ILE:HG23	2.20	0.41
2:B:18:ASP:HB3	2:B:114:TRP:CE3	2.55	0.41
1:A:1902:GLN:HB2	1:A:1905:LEU:HD21	2.02	0.41
1:A:1851:PHE:O	1:A:1881:THR:HA	2.21	0.41
2:B:66:ASN:HB3	2:B:89:PHE:CE1	2.55	0.41
2:B:15:ILE:O	2:B:21:SER:HA	2.21	0.40

All (11) 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:2065:ARG:HH11	2:B:47:GLN:HE22[2_655]	0.77	0.83
1:A:2065:ARG:HG2	2:B:52:SER:HB2[2_655]	1.14	0.46
1:A:2069:VAL:O	2:B:53:SER:OG[2_655]	1.76	0.44
1:A:2065:ARG:HD3	2:B:52:SER:HB2[2_655]	1.19	0.41
1:A:2065:ARG:CG	2:B:52:SER:HB2[2_655]	1.30	0.30
1:A:2065:ARG:CD	2:B:52:SER:HB2[2_655]	1.41	0.19
1:A:2069:VAL:O	2:B:53:SER:HG[2_655]	1.45	0.15
1:A:2065:ARG:HH11	2:B:47:GLN:NE2[2_655]	1.46	0.14
1:A:2065:ARG:CG	2:B:52:SER:CB[2_655]	2.09	0.11
1:A:2065:ARG:NH1	2:B:47:GLN:HE22[2_655]	1.55	0.05
1:A:2065:ARG:CD	2:B:52:SER:CB[2_655]	2.16	0.04

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%)	251 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	315/308 (102%)	305 (97%)	9 (3%)	1 (0%)	36 24
All	All	573/566 (101%)	556 (97%)	16 (3%)	1 (0%)	43 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	106	PRO

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%)	233 (98%)	4 (2%)	53 31
2	B	294/284 (104%)	291 (99%)	3 (1%)	68 53
All	All	531/517 (103%)	524 (99%)	7 (1%)	63 43

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1835	MET
1	A	1962	ARG
1	A	2060	LEU
1	A	2068	ASN
2	B	123[A]	MET
2	B	123[B]	MET
2	B	275	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	1907	GLN
1	A	2038	HIS
2	B	40	HIS

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Mol	Chain	Res	Type
2	B	48	HIS
2	B	135	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 ⓘ

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	VWL	B	401	-	17,17,17	1.77	5 (29%)	18,23,23	1.16	1 (5%)

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	VWL	B	401	-	-	0/8/8/8	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	VWL	C-C1	-3.40	1.42	1.50
3	B	401	VWL	O1-C5	-3.37	1.17	1.23
3	B	401	VWL	C3-C5	-2.64	1.41	1.49
3	B	401	VWL	C10-C9	-2.43	1.34	1.40
3	B	401	VWL	C7-C6	-2.09	1.35	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	VWL	O-C1-C2	2.33	111.81	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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%)	2.18	106 (44%) 0 1	25, 71, 126, 214	12 (5%)
2	B	300/308 (97%)	2.22	155 (51%) 0 0	22, 76, 123, 203	9 (3%)
All	All	537/566 (94%)	2.20	261 (48%) 0 1	22, 74, 126, 214	21 (3%)

All (261) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	203[A]	TYR	9.2
1	A	1979[A]	MET	8.3
1	A	2017[A]	THR	8.3
1	A	2069	VAL	7.8
1	A	2060	LEU	7.4
1	A	2058	LEU	6.7
2	B	152	LEU	6.6
2	B	316	LEU	6.5
1	A	2040	TRP	6.1
1	A	2039	LEU	6.0
1	A	2065	ARG	5.9
2	B	276	PRO	5.8
2	B	101	MET	5.7
2	B	275	LEU	5.6
2	B	122[A]	GLN	5.6
2	B	54[A]	MET	5.4
1	A	2063	TYR	5.4
1	A	1940	MET	5.3
1	A	1878	CYS	5.2
2	B	288	VAL	5.1
2	B	279	TYR	5.1
1	A	2061	THR	5.0
1	A	1840	TYR	5.0
2	B	55[A]	ARG	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	2067	TYR	4.8
2	B	77	LEU	4.8
2	B	256	VAL	4.8
2	B	170	SER	4.6
2	B	189	ILE	4.6
1	A	2059	ILE	4.6
1	A	2064	GLY	4.5
2	B	174	HIS	4.4
2	B	183	PHE	4.4
2	B	317	LEU	4.4
1	A	2030	PRO	4.3
2	B	1	MET	4.3
2	B	108	ILE	4.3
1	A	2066	LYS	4.3
1	A	1848	ILE	4.3
2	B	172	PRO	4.2
2	B	289	TRP	4.2
1	A	1833	GLY	4.1
1	A	1860	VAL	4.1
2	B	254	ALA	4.0
1	A	2028	SER	4.0
1	A	1939	ALA	4.0
1	A	2051	ILE	4.0
1	A	1866	PHE	4.0
2	B	74	LYS	3.9
1	A	1988	LEU	3.9
1	A	2048	TRP	3.9
2	B	67	PHE	3.9
2	B	214	PHE	3.9
1	A	2032	ILE	3.9
2	B	259	HIS	3.9
1	A	2034	ILE	3.8
2	B	38	ILE	3.8
1	A	2037	TYR	3.8
1	A	1961[A]	LEU	3.8
2	B	284	LEU	3.8
2	B	52	SER	3.8
2	B	246	MET	3.7
1	A	2027	LEU	3.7
2	B	73	PRO	3.7
1	A	2022	ALA	3.7
2	B	53	SER	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	29	PRO	3.7
2	B	146	THR	3.7
1	A	1964	PRO	3.6
1	A	1963	LEU	3.6
1	A	2010	LEU	3.6
2	B	297	PHE	3.6
1	A	1924	LEU	3.5
1	A	2068	ASN	3.5
2	B	294	TYR	3.5
2	B	96	PHE	3.5
2	B	199	LEU	3.5
2	B	210	LEU	3.4
2	B	41[A]	VAL	3.4
2	B	191	PRO	3.4
2	B	314	PRO	3.4
2	B	313	TYR	3.4
1	A	2056[A]	ARG	3.4
1	A	2043	PHE	3.4
2	B	283	LEU	3.4
1	A	1956	ILE	3.3
1	A	1999	ILE	3.3
2	B	282	ILE	3.3
2	B	192	GLY	3.3
1	A	1834	ALA	3.3
2	B	87	ALA	3.3
1	A	1976	ASP	3.3
2	B	272	ILE	3.3
1	A	1949	LEU	3.3
1	A	1970	SER	3.3
2	B	93	VAL	3.3
2	B	258	LYS	3.3
2	B	46	PHE	3.3
2	B	204[A]	TYR	3.2
2	B	241	LEU	3.2
2	B	235	GLY	3.2
2	B	307	LYS	3.2
2	B	193	HIS	3.2
2	B	249	LEU	3.1
2	B	295	SER	3.1
2	B	14	THR	3.1
1	A	1907	GLN	3.1
2	B	24	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1931[A]	LYS	3.1
1	A	1927	GLU	3.1
1	A	2038	HIS	3.1
2	B	173	ALA	3.1
2	B	30	PHE	3.1
2	B	250	ILE	3.1
2	B	234	PHE	3.1
1	A	2049	ILE	3.0
2	B	89	PHE	3.0
1	A	2062	GLU	3.0
2	B	68	TYR	3.0
1	A	1967	ALA	3.0
2	B	201	LYS	3.0
1	A	1997	ASP	3.0
2	B	106	PRO	3.0
2	B	137	PHE	3.0
2	B	198	PHE	3.0
1	A	1835	MET	2.9
1	A	1969	MET	2.9
2	B	291	ILE	2.9
2	B	19	GLN	2.9
2	B	228	PHE	2.9
1	A	1862	VAL	2.9
1	A	1872	THR	2.9
1	A	1873	LYS	2.9
2	B	25	LYS	2.9
2	B	13	VAL	2.9
2	B	100	GLN	2.9
2	B	102	MET	2.9
2	B	292	CYS	2.9
2	B	6	PHE	2.8
2	B	131	ARG	2.8
2	B	147	VAL	2.8
1	A	1996	LEU	2.8
2	B	22	PHE	2.8
1	A	1841	ALA	2.8
1	A	1953	ASN	2.8
1	A	1954	ILE	2.8
1	A	2044	THR	2.8
2	B	273	LYS	2.8
1	A	2053[A]	SER	2.8
2	B	180	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	20	TYR	2.8
2	B	111	ASP	2.8
1	A	2036	SER	2.8
2	B	278	GLN	2.7
1	A	2035	LYS	2.7
2	B	64[A]	MET	2.7
2	B	251	CYS	2.7
2	B	237	TYR	2.7
1	A	2033	THR	2.7
1	A	2050	THR	2.7
1	A	1875	ILE	2.7
2	B	50	ASP	2.7
2	B	229	LEU	2.7
1	A	2018[A]	ASN	2.7
2	B	304	ASN	2.7
2	B	145	THR	2.6
2	B	308	ILE	2.6
2	B	109	ASP	2.6
1	A	2004	ALA	2.6
2	B	132	LYS	2.6
2	B	233	PHE	2.6
1	A	1920	LEU	2.6
1	A	1971	ILE	2.6
2	B	10	PRO	2.6
2	B	129	ILE	2.6
2	B	255	THR	2.5
1	A	1837	SER	2.5
2	B	71	TYR	2.5
1	A	1844	PHE	2.5
1	A	1941	LEU	2.5
1	A	1948	MET	2.5
1	A	1959	THR	2.5
2	B	99	ARG	2.5
2	B	216	ASN	2.4
2	B	128	LYS	2.4
2	B	176	LEU	2.4
1	A	1861	THR	2.4
1	A	1906	SER	2.4
1	A	2031	THR	2.4
2	B	8	SER	2.4
2	B	281	ASP	2.4
2	B	80	MET	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	86	GLY	2.4
2	B	221	PHE	2.4
2	B	49	ALA	2.4
2	B	290	ASN	2.4
1	A	2025	ILE	2.4
1	A	1929	GLN	2.4
1	A	1905	LEU	2.4
2	B	107	LYS	2.4
2	B	103	VAL	2.4
2	B	244	HIS	2.4
1	A	2057[A]	ASP	2.3
2	B	179	THR	2.3
2	B	300	ASN	2.3
1	A	1847	ASP	2.3
2	B	226	PHE	2.3
1	A	1933	ILE	2.3
2	B	213	ILE	2.3
1	A	1904	ARG	2.3
1	A	1987	VAL	2.3
2	B	75	ASP	2.3
2	B	28	GLN	2.3
1	A	2001[A]	SER	2.3
1	A	2005	PHE	2.3
2	B	312	LYS	2.3
1	A	1930	PRO	2.2
1	A	1958	PRO	2.2
2	B	94	HIS	2.2
1	A	1962	ARG	2.2
2	B	84	ARG	2.2
2	B	236	ASN	2.2
1	A	1980[A]	LYS	2.2
2	B	194	GLU	2.2
2	B	18	ASP	2.2
2	B	261	LEU	2.2
2	B	92	ILE	2.2
2	B	126	ILE	2.2
1	A	1955	ALA	2.2
1	A	1882	LEU	2.2
1	A	1951	PHE	2.2
1	A	1989	PHE	2.2
1	A	1879	ILE	2.2
2	B	130	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	47	GLN	2.1
2	B	70	GLN	2.1
1	A	2015	LEU	2.1
2	B	293	LEU	2.1
2	B	97	LYS	2.1
2	B	3	THR	2.1
2	B	56	TYR	2.1
2	B	148	GLN	2.1
2	B	245	ALA	2.1
2	B	302	LEU	2.1
2	B	124	ASP	2.1
2	B	218	SER	2.1
2	B	23	ASN	2.1
2	B	211[A]	GLN	2.1
2	B	21	SER	2.1
1	A	2012	LEU	2.1
2	B	190	ARG	2.1
1	A	1995	TRP	2.1
2	B	40	HIS	2.1
2	B	120	PHE	2.1
2	B	150	ASN	2.0
2	B	311	ASN	2.0
2	B	171	ASP	2.0
1	A	1901	GLY	2.0
2	B	142	SER	2.0
2	B	143	SER	2.0
1	A	1926	LYS	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	VWL	B	401	16/16	0.69	0.17	20,20,20,20	16

6.5 Other polymers [i](#)

There are no such residues in this entry.