



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:18 PM EDT

PDB ID : 5STK / pdb_00005stk
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P02H12 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 : 1.80 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

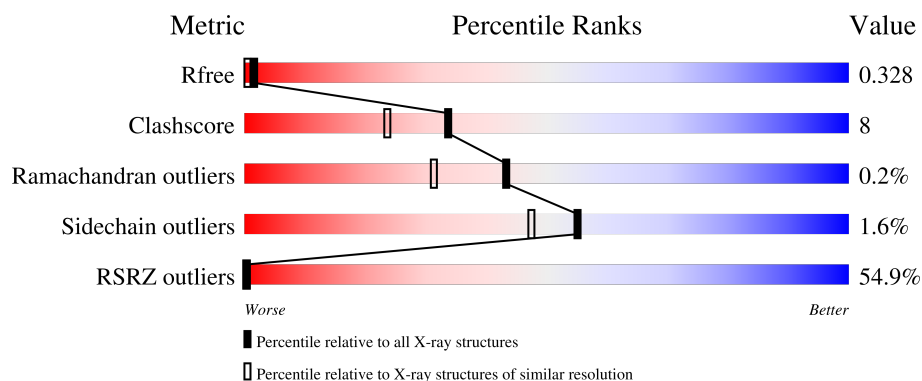
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	50% 78% 12% 8%
2	B	308	54% 74% 22% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9188 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:

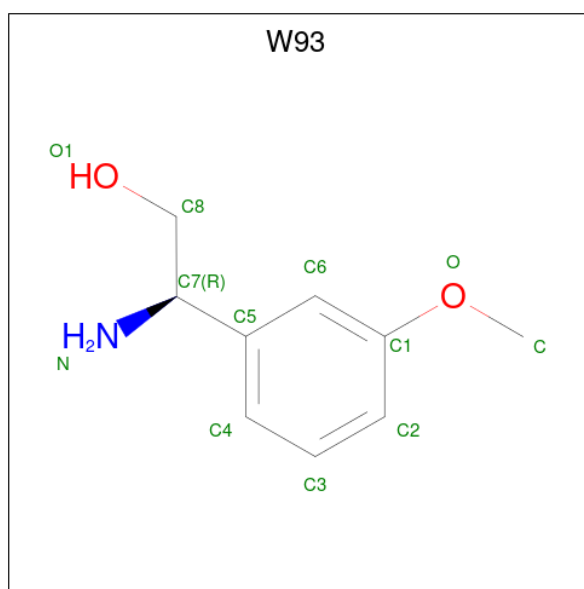
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN	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 (2R)-2-amino-2-(3-methoxyphenyl)ethan-1-ol (CCD ID: W93) (formula: $C_9H_{13}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			12	9	1	2		

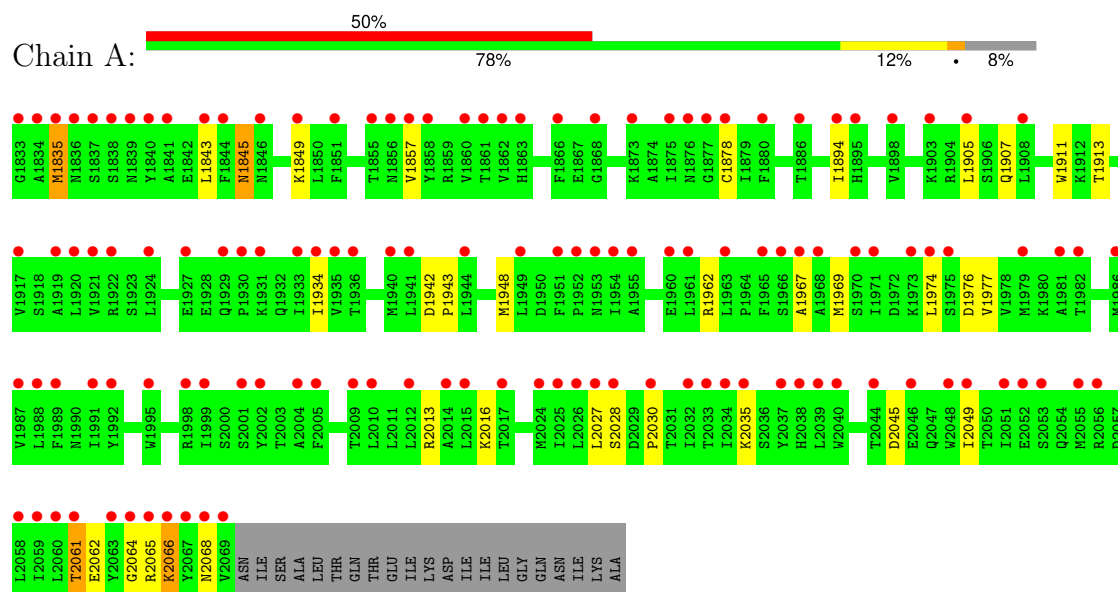
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total	O	0	0
			34	34		
4	B	30	Total	O	0	0
			30	30		

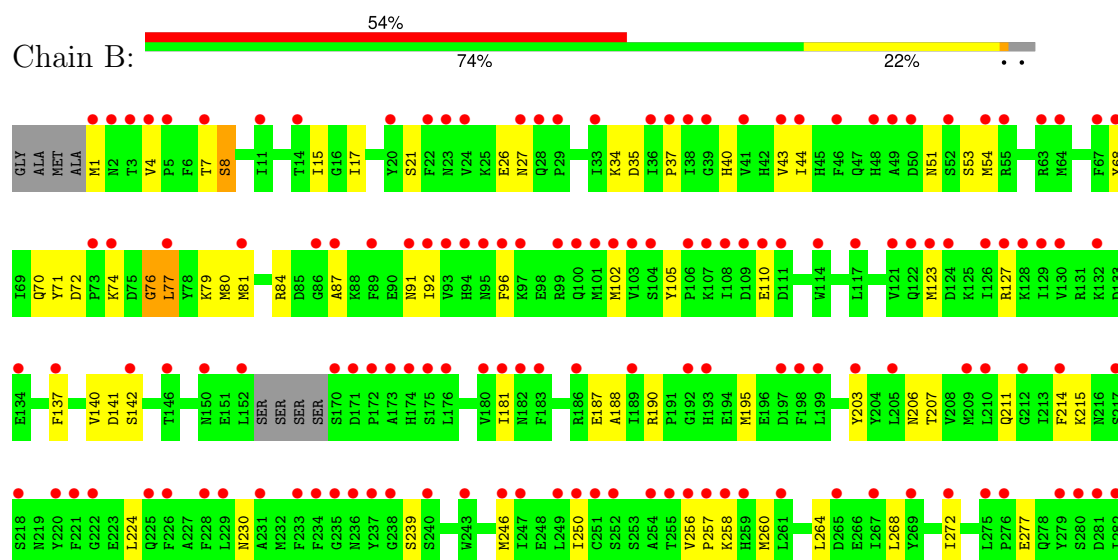
3 Residue-property plots

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



L283	L284	N285	E286	R287	Y288	W289	N290	I291	C292	L293	Y294	S295	S296	F297	Q298	S301	L302	H303	K307	I308	K312	Y313	P314	E315	L316	L317
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.69Å 81.67Å 92.94Å 90.00° 108.00° 90.00°	Depositor
Resolution (Å)	44.20 – 1.80 44.20 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (44.20-1.80) 99.2 (44.20-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 1.81Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.282 , 0.320 0.290 , 0.328	Depositor DCC
R_{free} test set	2098 reflections (3.63%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 56.9	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	0.93	EDS
Total number of atoms	9188	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% 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: W93

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	0.72	1/2149 (0.0%)	0.92	3/2911 (0.1%)
2	B	0.78	0/2739	1.03	6/3699 (0.2%)
All	All	0.75	1/4888 (0.0%)	0.98	9/6610 (0.1%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1934	ILE	C-N	5.15	1.41	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	8	SER	CA-C-N	7.87	131.50	122.85
2	B	8	SER	C-N-CA	7.87	131.50	122.85
1	A	1845	ASN	N-CA-C	-5.73	102.44	110.35
1	A	1976	ASP	CA-C-N	-5.65	110.57	120.29
1	A	1976	ASP	C-N-CA	-5.65	110.57	120.29
2	B	76	GLY	N-CA-C	-5.51	106.05	115.08
2	B	87	ALA	CA-C-N	5.15	127.18	120.28
2	B	87	ALA	C-N-CA	5.15	127.18	120.28
2	B	7	THR	CB-CA-C	-5.13	102.27	110.79

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	8	SER	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	23	0
2	B	2580	2464	2398	49	0
3	B	12	0	0	0	0
4	A	34	0	0	1	0
4	B	30	0	0	4	0
All	All	4664	4524	4372	70	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 8.

All (70) 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:1:MET:N	4:B:501:HOH:O	2.15	0.78
2:B:77:LEU:HD21	2:B:79:LYS:HE3	1.71	0.73
2:B:72:ASP:OD2	2:B:79:LYS:NZ	2.23	0.69
2:B:203[A]:TYR:CZ	2:B:207:THR:HG21	2.30	0.67
1:A:2064:GLY:O	1:A:2068:ASN:N	2.31	0.62
2:B:91:ASN:O	2:B:91:ASN:ND2	2.32	0.62
2:B:51:ASN:OD1	2:B:53:SER:HB2	2.00	0.61
2:B:206:ASN:O	2:B:211[A]:GLN:HG3	2.02	0.59
2:B:53:SER:O	2:B:54[A]:MET:HB3	2.04	0.58
1:A:1962:ARG:O	1:A:2013:ARG:NH1	2.37	0.57
1:A:1845:ASN:OD1	1:A:1849:LYS:NZ	2.39	0.55
2:B:4:VAL:HG21	2:B:44[B]:ILE:CD1	2.38	0.53
2:B:287:ARG:O	2:B:291:ILE:HD13	2.10	0.52
2:B:40:HIS:CD2	4:B:512:HOH:O	2.61	0.52
2:B:70:GLN:HB3	2:B:81:MET:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:ILE:O	2:B:17:ILE:HG23	2.09	0.51
2:B:26:GLU:O	2:B:27:ASN:HB2	2.10	0.51
2:B:43:VAL:HG13	2:B:43:VAL:O	2.11	0.50
2:B:34:LYS:O	2:B:35:ASP:HB2	2.12	0.49
2:B:96:PHE:HB2	2:B:102:MET:HE3	1.92	0.49
2:B:230[B]:ASN:ND2	2:B:239:SER:OG	2.46	0.49
2:B:258:LYS:HD2	2:B:258:LYS:H	1.78	0.49
1:A:2061:THR:O	1:A:2064:GLY:N	2.39	0.49
2:B:15:ILE:O	2:B:21:SER:HA	2.13	0.48
2:B:250:ILE:HG21	2:B:264:LEU:HD22	1.95	0.48
2:B:187:GLU:H	2:B:187:GLU:CD	2.22	0.48
1:A:1974:LEU:O	1:A:1977:VAL:HG12	2.13	0.48
1:A:1907:GLN:HG2	2:B:195:MET:HE3	1.96	0.47
1:A:1878:CYS:SG	1:A:1969:MET:HE3	2.54	0.47
2:B:68:TYR:CE2	2:B:81:MET:HE3	2.49	0.47
1:A:1962:ARG:HD3	1:A:1962:ARG:H	1.79	0.47
2:B:190:ARG:HG3	2:B:203[B]:TYR:CZ	2.49	0.46
2:B:37:PRO:HD3	2:B:105:TYR:CD1	2.50	0.46
1:A:2045:ASP:O	1:A:2049:ILE:HG12	2.15	0.46
2:B:268:LEU:O	2:B:272:ILE:HG12	2.15	0.46
2:B:1:MET:HB3	2:B:35:ASP:HA	1.96	0.46
2:B:190:ARG:HG3	2:B:203[B]:TYR:CE2	2.51	0.46
2:B:4:VAL:HG21	2:B:44[B]:ILE:HD11	1.98	0.45
2:B:224:LEU:C	2:B:224:LEU:HD23	2.40	0.45
1:A:1967:ALA:HB2	1:A:2016:LYS:HB2	1.98	0.45
2:B:40:HIS:HD2	4:B:512:HOH:O	1.95	0.45
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	1.98	0.45
1:A:2062:GLU:OE1	1:A:2065:ARG:NH1	2.50	0.45
1:A:1894:ILE:HA	4:A:2101:HOH:O	2.17	0.45
2:B:298:GLN:HA	2:B:298:GLN:OE1	2.17	0.44
2:B:71:TYR:OH	2:B:76:GLY:HA2	2.17	0.44
2:B:277:GLU:CD	2:B:277:GLU:H	2.26	0.44
2:B:51:ASN:CG	2:B:53:SER:HB2	2.43	0.44
2:B:80:MET:SD	2:B:137:PHE:CG	3.11	0.44
2:B:260:MET:HE2	2:B:260:MET:HB3	1.77	0.44
2:B:110:GLU:HG2	2:B:110:GLU:O	2.18	0.43
2:B:214:PHE:O	2:B:215:LYS:HB2	2.18	0.43
1:A:1948:MET:HE3	1:A:1948:MET:HB3	1.90	0.42
1:A:2035:LYS:HD3	1:A:2035:LYS:HA	1.77	0.42
2:B:181:ILE:CD1	2:B:246:MET:HG2	2.49	0.42
1:A:2062:GLU:O	1:A:2066:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2028:SER:O	1:A:2030:PRO:HD3	2.19	0.42
2:B:17:ILE:HD13	2:B:44[B]:ILE:CG1	2.49	0.42
1:A:1911:TRP:CD2	2:B:195:MET:HB2	2.55	0.41
2:B:314:PRO:HD2	2:B:315:GLU:OE1	2.20	0.41
1:A:1905:LEU:HD23	1:A:1905:LEU:HA	1.81	0.41
2:B:256:VAL:O	2:B:257:PRO:C	2.61	0.41
1:A:1942:ASP:HB2	1:A:1943:PRO:HD3	2.02	0.41
2:B:140:VAL:HG12	2:B:141:ASP:N	2.36	0.41
1:A:1857:VAL:HG21	1:A:1913:THR:OG1	2.21	0.41
2:B:74:LYS:NZ	4:B:507:HOH:O	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	258/258 (100%)	248 (96%)	9 (4%)	1 (0%)	30	19
2	B	315/308 (102%)	298 (95%)	17 (5%)	0	100	100
All	All	573/566 (101%)	546 (95%)	26 (4%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2061	THR

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	237/233 (102%)	234 (99%)	3 (1%)	61	54
2	B	294/284 (104%)	288 (98%)	6 (2%)	48	38
All	All	531/517 (103%)	522 (98%)	9 (2%)	55	45

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1835	MET
1	A	2027	LEU
1	A	2066	LYS
2	B	77	LEU
2	B	84	ARG
2	B	92	ILE
2	B	123[A]	MET
2	B	123[B]	MET
2	B	142	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1869	ASN
1	A	1907	GLN
2	B	40	HIS
2	B	91	ASN
2	B	135	ASN
2	B	150	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 [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	W93	B	401	-	10,12,12	0.50	0	12,15,15	1.13	2 (16%)

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	W93	B	401	-	-	5/8/8/8	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	W93	O-C1-C2	-2.11	109.79	119.82
3	B	401	W93	C4-C5-C7	-2.03	116.85	120.52

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	W93	C6-C5-C7-C8
3	B	401	W93	C4-C5-C7-C8
3	B	401	W93	C5-C7-C8-O1
3	B	401	W93	C6-C5-C7-N

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Mol	Chain	Res	Type	Atoms
3	B	401	W93	C4-C5-C7-N

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%)	2.35	128 (54%) 0 0	29, 78, 149, 186	12 (5%)
2	B	300/308 (97%)	2.31	167 (55%) 0 0	27, 81, 146, 234	9 (3%)
All	All	537/566 (94%)	2.33	295 (54%) 0 0	27, 80, 147, 234	21 (3%)

All (295) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1979[A]	MET	8.5
1	A	2060	LEU	7.4
2	B	54[A]	MET	7.4
2	B	111	ASP	6.8
1	A	2069	VAL	6.7
2	B	152	LEU	6.4
1	A	2051	ILE	6.2
1	A	1940	MET	6.2
2	B	316	LEU	6.2
2	B	101	MET	5.8
1	A	1834	ALA	5.7
2	B	89	PHE	5.5
1	A	1988	LEU	5.4
1	A	1860	VAL	5.4
2	B	203[A]	TYR	5.3
1	A	1840	TYR	5.2
1	A	2040	TRP	5.1
1	A	1894	ILE	5.0
1	A	1898[A]	VAL	5.0
2	B	124	ASP	4.8
1	A	1967	ALA	4.8
1	A	1855[A]	THR	4.8
2	B	221	PHE	4.7
1	A	2053[A]	SER	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	104	SER	4.7
1	A	2001[A]	SER	4.7
2	B	217	SER	4.7
1	A	1886	THR	4.6
1	A	1841	ALA	4.5
1	A	2002[A]	TYR	4.5
1	A	2067	TYR	4.5
2	B	106	PRO	4.5
2	B	41[A]	VAL	4.5
1	A	1878	CYS	4.4
1	A	2039	LEU	4.4
2	B	68	TYR	4.4
1	A	2027	LEU	4.4
1	A	1835	MET	4.3
2	B	256	VAL	4.3
1	A	2061	THR	4.2
2	B	275	LEU	4.2
1	A	2004	ALA	4.2
2	B	97	LYS	4.2
2	B	282	ILE	4.2
2	B	130	VAL	4.2
1	A	1954	ILE	4.2
2	B	73	PRO	4.2
1	A	1862	VAL	4.1
1	A	1987	VAL	4.1
2	B	235	GLY	4.1
2	B	126	ILE	4.0
1	A	2066	LYS	4.0
1	A	1861	THR	4.0
1	A	2025	ILE	4.0
2	B	132	LYS	4.0
2	B	174	HIS	4.0
1	A	1866	PHE	3.9
2	B	103	VAL	3.9
1	A	1833	GLY	3.9
2	B	170	SER	3.9
1	A	2059	ILE	3.9
1	A	1920	LEU	3.8
2	B	291	ILE	3.8
2	B	283	LEU	3.8
1	A	2038	HIS	3.8
2	B	11	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	175	SER	3.8
1	A	2037	TYR	3.8
2	B	108	ILE	3.8
2	B	308	ILE	3.8
2	B	38	ILE	3.7
1	A	2063	TYR	3.7
2	B	107	LYS	3.7
2	B	102	MET	3.7
1	A	2009	THR	3.7
1	A	1963	LEU	3.7
1	A	2012	LEU	3.7
2	B	77	LEU	3.7
1	A	1992	TYR	3.7
2	B	313	TYR	3.7
2	B	123[A]	MET	3.7
1	A	1995	TRP	3.7
2	B	269	TYR	3.6
2	B	172	PRO	3.6
2	B	276	PRO	3.6
2	B	205	LEU	3.6
2	B	192	GLY	3.6
2	B	27	ASN	3.5
2	B	231	ALA	3.5
2	B	1	MET	3.5
2	B	289	TRP	3.5
2	B	20	TYR	3.5
2	B	29	PRO	3.4
2	B	181	ILE	3.4
1	A	1851	PHE	3.4
2	B	64[A]	MET	3.4
2	B	303	HIS	3.3
2	B	122[A]	GLN	3.3
1	A	1837	SER	3.3
1	A	2028	SER	3.3
2	B	254	ALA	3.3
2	B	22	PHE	3.3
2	B	183	PHE	3.3
2	B	297	PHE	3.3
1	A	1975	SER	3.3
2	B	129	ILE	3.3
1	A	2058	LEU	3.3
2	B	96	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	2034	ILE	3.2
2	B	267	ILE	3.2
2	B	279	TYR	3.2
2	B	67	PHE	3.2
2	B	246	MET	3.2
2	B	257	PRO	3.2
2	B	210	LEU	3.2
2	B	94	HIS	3.2
1	A	2049	ILE	3.2
2	B	294	TYR	3.2
1	A	1955	ALA	3.1
1	A	1849	LYS	3.1
1	A	1944	LEU	3.1
2	B	288	VAL	3.1
2	B	228	PHE	3.1
2	B	100	GLN	3.1
2	B	314	PRO	3.1
1	A	1924	LEU	3.1
2	B	226	PHE	3.1
2	B	92	ILE	3.0
2	B	229	LEU	3.0
2	B	249	LEU	3.0
1	A	1839	ASN	3.0
1	A	1953	ASN	3.0
1	A	1998	ARG	3.0
1	A	1905	LEU	3.0
2	B	173	ALA	3.0
1	A	1875	ILE	3.0
2	B	317	LEU	3.0
2	B	237	TYR	3.0
1	A	1838	SER	3.0
1	A	2055	MET	2.9
1	A	1876	ASN	2.9
1	A	1919[A]	ALA	2.9
2	B	225	GLN	2.9
2	B	74	LYS	2.9
2	B	186	ARG	2.9
2	B	7	THR	2.9
2	B	222	GLY	2.9
1	A	2068	ASN	2.9
2	B	233	PHE	2.9
1	A	1999	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	197	ASP	2.9
1	A	1935	VAL	2.9
2	B	171	ASP	2.9
1	A	2017[A]	THR	2.8
2	B	251	CYS	2.8
1	A	1856[A]	ASN	2.8
2	B	28	GLN	2.8
2	B	4	VAL	2.8
1	A	1965	PHE	2.8
1	A	1991	ILE	2.8
1	A	1931[A]	LYS	2.8
1	A	1930	PRO	2.8
2	B	99	ARG	2.8
2	B	193	HIS	2.8
1	A	1934	ILE	2.8
1	A	2048	TRP	2.8
2	B	280	SER	2.7
2	B	182	ASN	2.7
1	A	1844	PHE	2.7
2	B	134	GLU	2.7
1	A	2015	LEU	2.7
2	B	199	LEU	2.7
2	B	281	ASP	2.7
1	A	1968	ALA	2.7
2	B	128	LYS	2.7
1	A	1868	GLY	2.7
1	A	1970	SER	2.7
2	B	180	VAL	2.7
2	B	212[A]	GLY	2.7
2	B	5	PRO	2.7
2	B	295	SER	2.7
2	B	121	VAL	2.7
1	A	1895	HIS	2.6
1	A	1933	ILE	2.6
2	B	33	ILE	2.6
2	B	49	ALA	2.6
2	B	63	ARG	2.6
1	A	2046	GLU	2.6
1	A	1863	HIS	2.6
1	A	1921	VAL	2.6
1	A	1836	ASN	2.6
2	B	23	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1951	PHE	2.6
2	B	250	ILE	2.6
1	A	2064	GLY	2.6
1	A	1966	SER	2.6
2	B	110	GLU	2.5
1	A	1941	LEU	2.5
2	B	302	LEU	2.5
2	B	258	LYS	2.5
2	B	220	TYR	2.5
2	B	214	PHE	2.5
2	B	52	SER	2.5
2	B	3	THR	2.5
1	A	2030	PRO	2.5
2	B	234	PHE	2.5
2	B	293	LEU	2.5
1	A	1922	ARG	2.5
1	A	1971	ILE	2.5
1	A	2032	ILE	2.5
2	B	109	ASP	2.5
2	B	284	LEU	2.4
2	B	298	GLN	2.4
2	B	240	SER	2.4
2	B	55[A]	ARG	2.4
1	A	2024[A]	MET	2.4
2	B	137	PHE	2.4
1	A	2065	ARG	2.4
1	A	1927	GLU	2.4
2	B	218	SER	2.4
2	B	301	SER	2.4
1	A	1858	TYR	2.4
1	A	2014	ALA	2.4
2	B	114	TRP	2.4
2	B	176	LEU	2.3
1	A	2033	THR	2.3
1	A	2044	THR	2.3
1	A	1981	ALA	2.3
2	B	236	ASN	2.3
1	A	1857	VAL	2.3
2	B	287	ARG	2.3
1	A	2052	GLU	2.3
2	B	14	THR	2.3
1	A	1880	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	198	PHE	2.3
2	B	2	ASN	2.3
2	B	91	ASN	2.3
2	B	247	ILE	2.3
2	B	238	GLY	2.3
2	B	265	ASP	2.3
2	B	290	ASN	2.3
1	A	2005	PHE	2.3
1	A	2035	LYS	2.3
1	A	1843	LEU	2.3
1	A	1873	LYS	2.3
1	A	1952	PRO	2.2
2	B	307	LYS	2.2
2	B	312	LYS	2.2
1	A	1936	THR	2.2
2	B	146	THR	2.2
1	A	1974	LEU	2.2
2	B	261	LEU	2.2
2	B	87	ALA	2.2
1	A	1989	PHE	2.2
2	B	259	HIS	2.2
2	B	81	MET	2.2
2	B	127	ARG	2.2
1	A	1929	GLN	2.2
2	B	36	ILE	2.2
2	B	24	VAL	2.2
2	B	50	ASP	2.2
2	B	95	ASN	2.1
2	B	243	TRP	2.1
1	A	1917	VAL	2.1
1	A	1982	THR	2.1
2	B	93	VAL	2.1
2	B	255	THR	2.1
1	A	2026	LEU	2.1
1	A	2056[A]	ARG	2.1
1	A	1877	GLY	2.1
2	B	43	VAL	2.1
1	A	1973	LYS	2.1
1	A	1986	MET	2.1
2	B	209	MET	2.1
1	A	2010	LEU	2.1
2	B	37	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	117	LEU	2.1
2	B	189	ILE	2.1
2	B	86	GLY	2.1
1	A	1908	LEU	2.1
1	A	1949	LEU	2.1
1	A	1961[A]	LEU	2.1
1	A	1960[A]	GLU	2.0
2	B	44[A]	ILE	2.0
2	B	46	PHE	2.0
2	B	252	SER	2.0
2	B	272	ILE	2.0
2	B	39	GLY	2.0
2	B	48	HIS	2.0
1	A	1846	ASN	2.0
2	B	285	ASN	2.0
2	B	286	GLU	2.0
1	A	1903	LYS	2.0
2	B	142	SER	2.0
2	B	150	ASN	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	W93	B	401	12/12	0.70	0.16	20,20,20,20	12

6.5 Other polymers [i](#)

There are no such residues in this entry.