



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:13 PM UTC

PDB ID : 5ST5 / pdb_00005st5
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P02D06 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 : 1.61 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

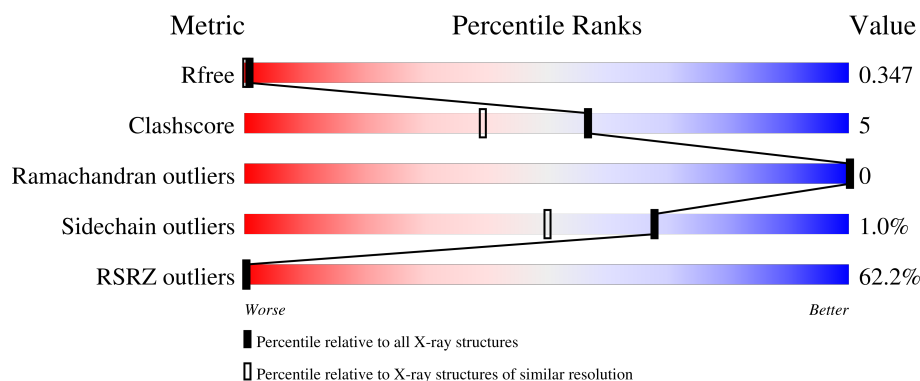
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.61 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	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (1.64-1.60)

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	62% 83% 9% 8%
2	B	308	57% 84% 12% ..

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	UXB	B	401	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9235 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:

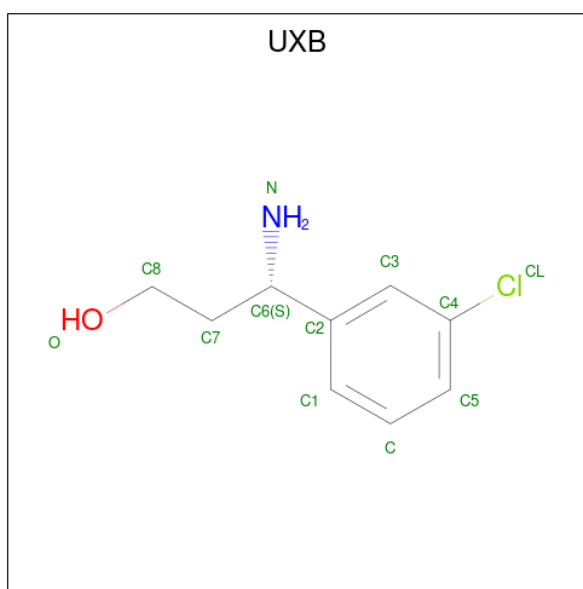
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN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

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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 (3S)-3-amino-3-(3-chlorophenyl)propan-1-ol (CCD ID: UXB) (formula: C₉H₁₂ClNO).



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

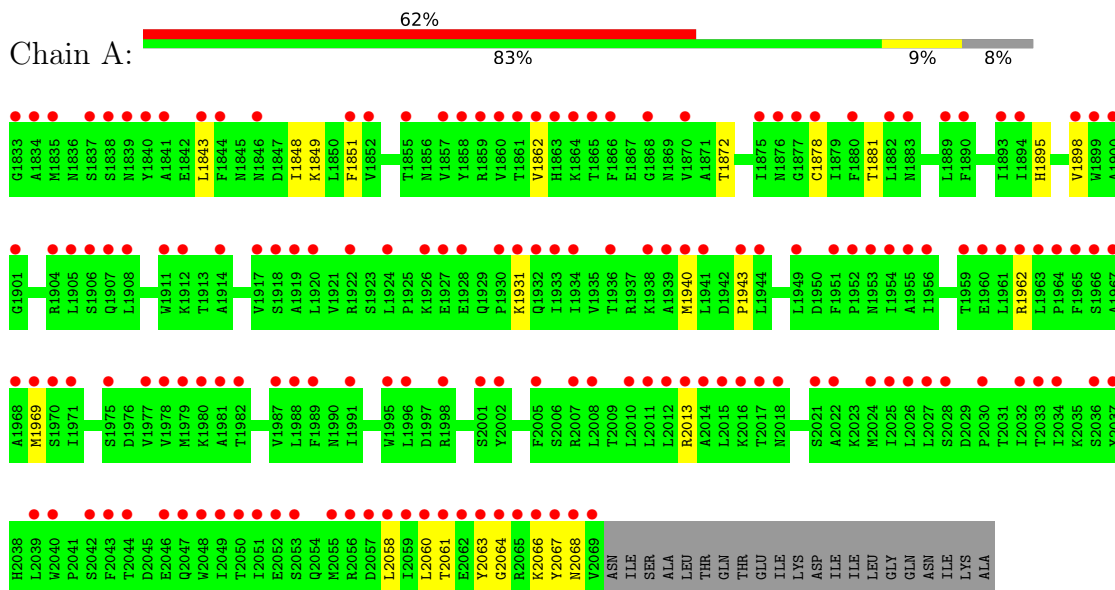
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total	O	0	0
			49	49		
4	B	50	Total	O	0	0
			50	50		

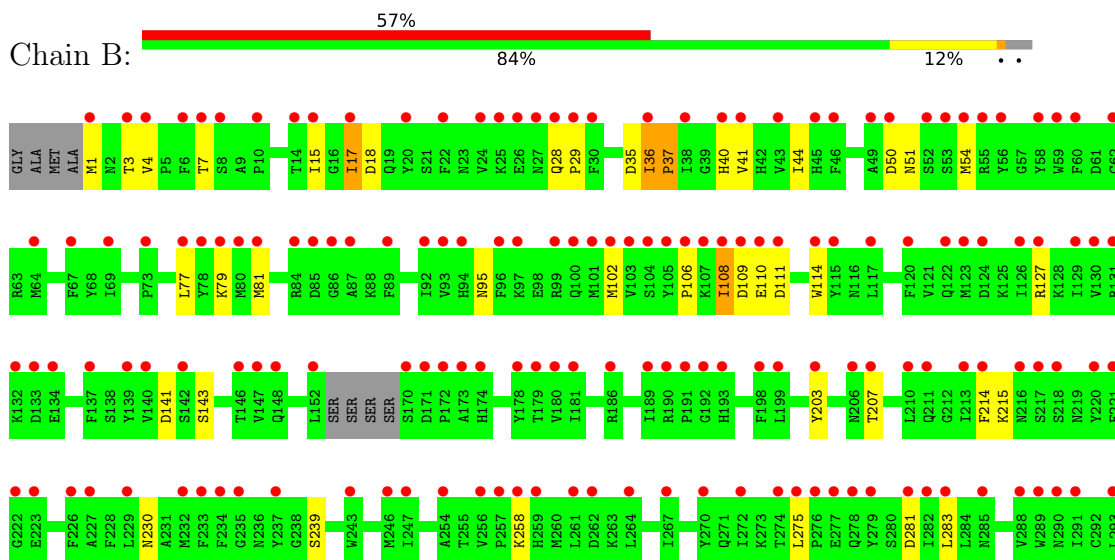
3 Residue-property plots

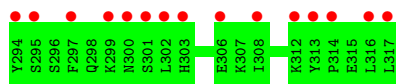
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	89.06Å 81.77Å 93.56Å 90.00° 108.61° 90.00°	Depositor
Resolution (Å)	44.61 – 1.61 44.61 – 1.61	Depositor EDS
% Data completeness (in resolution range)	98.9 (44.61-1.61) 99.0 (44.61-1.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 1.62Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.284 , 0.333 0.303 , 0.347	Depositor DCC
R_{free} test set	2099 reflections (2.59%)	wwPDB-VP
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 54.1	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	9235	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 5.67% 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: UXB

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	0.73	0/2149	0.78	0/2911
2	B	0.80	4/2739 (0.1%)	0.93	4/3699 (0.1%)
All	All	0.77	4/4888 (0.1%)	0.87	4/6610 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	17	ILE	C-O	-6.43	1.17	1.24
2	B	37	PRO	C-N	-6.04	1.26	1.33
2	B	95	ASN	C-O	-5.51	1.17	1.24
2	B	7	THR	C-O	-5.15	1.18	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	36	ILE	N-CA-C	5.77	114.60	108.95
2	B	111	ASP	N-CA-C	5.31	116.96	108.41
2	B	15	ILE	CA-C-N	-5.07	118.63	122.33
2	B	15	ILE	C-N-CA	-5.07	118.63	122.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	14	0
2	B	2580	2464	2398	28	0
3	B	24	0	0	0	0
4	A	49	0	0	0	0
4	B	50	0	0	3	0
All	All	4711	4524	4372	42	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 5.

All (42) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1962:ARG:O	1:A:2013:ARG:NH1	2.17	0.77
2:B:110:GLU:HG2	2:B:110:GLU:O	1.91	0.71
2:B:3:THR:HG21	2:B:102:MET:HE1	1.77	0.66
1:A:1895:HIS:O	1:A:1898[A]:VAL:HG22	2.02	0.58
1:A:2064:GLY:O	1:A:2068:ASN:N	2.35	0.58
2:B:17:ILE:HD13	2:B:44[B]:ILE:HG12	1.85	0.57
1:A:2061:THR:O	1:A:2064:GLY:N	2.38	0.57
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	1.88	0.55
2:B:17:ILE:HD13	2:B:44[B]:ILE:CG1	2.38	0.54
2:B:18:ASP:HB3	2:B:114:TRP:CE3	2.43	0.54
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.55	0.53
1:A:1878:CYS:SG	1:A:1969:MET:HE3	2.50	0.52
2:B:1:MET:N	4:B:502:HOH:O	2.43	0.51
2:B:40:HIS:HD2	4:B:516:HOH:O	1.93	0.51
2:B:108:ILE:N	2:B:108:ILE:CD1	2.73	0.51
2:B:275:LEU:HD21	2:B:283:LEU:HD13	1.93	0.51
1:A:1862:VAL:HG22	1:A:1872:THR:HG22	1.93	0.50
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.37	0.50
2:B:1:MET:HB3	2:B:35:ASP:HA	1.93	0.50
2:B:77:LEU:HD21	2:B:79:LYS:HE3	1.94	0.48
2:B:50:ASP:OD1	2:B:51:ASN:N	2.46	0.47
2:B:108:ILE:N	2:B:108:ILE:HD12	2.29	0.47
2:B:258:LYS:HD2	2:B:258:LYS:H	1.80	0.46
2:B:17:ILE:CD1	2:B:44[B]:ILE:CG1	2.94	0.46
2:B:36:ILE:HA	2:B:37:PRO:HD3	1.83	0.45
1:A:1940:MET:C	1:A:1943:PRO:HD2	2.43	0.44
2:B:214:PHE:O	2:B:215:LYS:HB2	2.16	0.44
2:B:3:THR:CG2	2:B:102:MET:HE1	2.47	0.43
2:B:28:GLN:HG3	2:B:29:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54[B]:MET:HE1	2:B:143:SER:HB3	2.01	0.43
1:A:2060:LEU:O	1:A:2063:TYR:HB3	2.18	0.43
2:B:230[B]:ASN:ND2	2:B:239:SER:OG	2.51	0.43
2:B:203[A]:TYR:CZ	2:B:207:THR:HG21	2.53	0.43
2:B:41[A]:VAL:HG12	4:B:536:HOH:O	2.20	0.42
1:A:1851:PHE:O	1:A:1881:THR:HA	2.20	0.41
2:B:275:LEU:CD2	2:B:283:LEU:HD13	2.50	0.41
2:B:17:ILE:CD1	2:B:44[B]:ILE:HG12	2.48	0.41
1:A:1962:ARG:HD3	1:A:1962:ARG:H	1.86	0.40
1:A:2066:LYS:HD2	1:A:2067:TYR:CE1	2.56	0.40
2:B:4:VAL:HG23	2:B:36:ILE:CD1	2.51	0.40
2:B:141:ASP:C	2:B:141:ASP:OD1	2.65	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%)	249 (96%)	9 (4%)	0	100	100
2	B	315/308 (102%)	301 (96%)	14 (4%)	0	100	100
All	All	573/566 (101%)	550 (96%)	23 (4%)	0	100	100

There are no Ramachandran outliers to report.

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%)	237 (100%)	0	100	100
2	B	294/284 (104%)	289 (98%)	5 (2%)	53	29
All	All	531/517 (103%)	526 (99%)	5 (1%)	68	54

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	81	MET
2	B	106	PRO
2	B	108	ILE
2	B	109	ASP
2	B	281	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1863	HIS
2	B	40	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	UXB	B	401	-	10,12,12	2.62	6 (60%)	13,15,15	2.93	8 (61%)
3	UXB	B	402	-	10,12,12	2.34	4 (40%)	13,15,15	2.11	2 (15%)

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	UXB	B	401	-	-	5/7/7/7	0/1/1/1
3	UXB	B	402	-	-	2/7/7/7	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	UXB	C6-N	4.37	1.56	1.47
3	B	401	UXB	C4-CL	-4.31	1.64	1.74
3	B	401	UXB	C3-C4	-4.24	1.31	1.38
3	B	402	UXB	C4-CL	-3.87	1.65	1.74
3	B	401	UXB	C1-C2	-3.49	1.33	1.39
3	B	402	UXB	C3-C4	-3.27	1.33	1.38
3	B	401	UXB	C6-N	2.51	1.52	1.47
3	B	401	UXB	C3-C2	-2.27	1.35	1.39
3	B	402	UXB	C-C1	-2.19	1.35	1.38
3	B	401	UXB	C-C1	-2.10	1.35	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	UXB	C7-C6-C2	-6.43	101.75	111.37
3	B	401	UXB	C7-C6-C2	5.85	120.12	111.37
3	B	401	UXB	C1-C2-C6	-4.52	112.37	120.52
3	B	401	UXB	C5-C4-CL	3.57	124.63	119.36
3	B	401	UXB	C4-C3-C2	3.17	123.20	119.43
3	B	401	UXB	C3-C2-C6	3.04	126.62	120.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	UXB	C-C1-C2	-2.72	117.40	120.65
3	B	401	UXB	C5-C-C1	2.54	123.51	120.24
3	B	401	UXB	C3-C4-CL	-2.35	116.22	119.17
3	B	402	UXB	O-C8-C7	-2.25	103.97	111.34

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	UXB	C6-C7-C8-O
3	B	401	UXB	C2-C6-C7-C8
3	B	401	UXB	N-C6-C7-C8
3	B	402	UXB	C6-C7-C8-O
3	B	401	UXB	C3-C2-C6-N
3	B	401	UXB	C1-C2-C6-N
3	B	402	UXB	C3-C2-C6-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%)	2.92	159 (67%) 0 0	27, 75, 150, 258	12 (5%)
2	B	300/308 (97%)	2.54	175 (58%) 0 0	21, 72, 140, 274	9 (3%)
All	All	537/566 (94%)	2.71	334 (62%) 0 0	21, 74, 148, 274	21 (3%)

All (334) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1840	TYR	11.5
2	B	308	ILE	9.8
1	A	1979[A]	MET	9.2
2	B	203[A]	TYR	8.8
1	A	1878	CYS	7.7
1	A	2069	VAL	7.7
2	B	54[A]	MET	7.7
1	A	1940	MET	7.3
1	A	1857	VAL	7.3
1	A	2043	PHE	7.3
2	B	275	LEU	7.0
1	A	1860	VAL	7.0
2	B	232	MET	7.0
1	A	2014	ALA	6.7
1	A	1894	ILE	6.5
2	B	108	ILE	6.3
1	A	2063	TYR	6.2
2	B	152	LEU	6.2
2	B	170	SER	6.2
2	B	80	MET	6.1
1	A	2065	ARG	6.0
2	B	123[A]	MET	5.9
2	B	77	LEU	5.8
1	A	1951	PHE	5.8

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Mol	Chain	Res	Type	RSRZ
2	B	50	ASP	5.7
1	A	2015	LEU	5.7
1	A	2060	LEU	5.7
1	A	1870	VAL	5.7
1	A	1866	PHE	5.7
2	B	172	PRO	5.7
2	B	129	ILE	5.6
1	A	1975	SER	5.6
1	A	1834	ALA	5.5
1	A	2058	LEU	5.5
2	B	316	LEU	5.5
1	A	1833	GLY	5.5
2	B	193	HIS	5.5
1	A	1835	MET	5.5
2	B	313	TYR	5.4
1	A	2040	TRP	5.2
2	B	282	ILE	5.2
2	B	1	MET	5.1
2	B	102	MET	5.1
2	B	64[A]	MET	5.0
2	B	246	MET	5.0
1	A	1955	ALA	5.0
1	A	2064	GLY	5.0
2	B	10	PRO	4.9
1	A	1939	ALA	4.9
2	B	92	ILE	4.9
2	B	101	MET	4.9
2	B	173	ALA	4.9
2	B	264	LEU	4.9
1	A	1954	ILE	4.8
1	A	2059	ILE	4.8
2	B	43	VAL	4.8
1	A	2017[A]	THR	4.8
1	A	1877	GLY	4.8
2	B	49	ALA	4.8
1	A	1961[A]	LEU	4.8
1	A	2013	ARG	4.8
1	A	1941	LEU	4.7
1	A	2012	LEU	4.7
2	B	283	LEU	4.7
1	A	2024[A]	MET	4.7
2	B	142	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	1928	GLU	4.7
1	A	2037	TYR	4.7
1	A	2068	ASN	4.7
2	B	146	THR	4.7
1	A	1931[A]	LYS	4.6
2	B	317	LEU	4.6
2	B	181	ILE	4.6
2	B	130	VAL	4.6
1	A	1875	ILE	4.6
1	A	1969	MET	4.5
2	B	81	MET	4.5
1	A	2051	ILE	4.5
1	A	2067	TYR	4.5
1	A	1966	SER	4.5
1	A	1965	PHE	4.4
1	A	1914	ALA	4.4
1	A	1930	PRO	4.4
2	B	261	LEU	4.4
2	B	281	ASP	4.4
1	A	2056[A]	ARG	4.3
2	B	148	GLN	4.3
2	B	36	ILE	4.3
1	A	1956	ILE	4.2
2	B	216	ASN	4.2
2	B	134	GLU	4.2
1	A	1949	LEU	4.2
2	B	291	ILE	4.2
2	B	198	PHE	4.2
2	B	192	GLY	4.1
1	A	1927	GLU	4.1
1	A	1841	ALA	4.1
1	A	2026	LEU	4.1
1	A	2061	THR	4.0
2	B	105	TYR	4.0
2	B	17	ILE	3.9
1	A	2055	MET	3.9
2	B	24	VAL	3.9
2	B	207	THR	3.9
1	A	2044	THR	3.8
2	B	272	ILE	3.8
1	A	2022	ALA	3.8
2	B	270	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	276	PRO	3.8
1	A	2049	ILE	3.8
1	A	1908	LEU	3.7
2	B	210	LEU	3.7
2	B	180	VAL	3.7
1	A	1953	ASN	3.7
2	B	254	ALA	3.7
1	A	1838	SER	3.7
1	A	1890	PHE	3.7
2	B	96	PHE	3.7
2	B	277	GLU	3.7
1	A	1943	PRO	3.7
1	A	1863	HIS	3.7
2	B	237	TYR	3.7
2	B	53	SER	3.7
2	B	214	PHE	3.6
1	A	1862	VAL	3.6
2	B	174	HIS	3.6
1	A	2016	LYS	3.6
2	B	221	PHE	3.6
2	B	122[A]	GLN	3.6
1	A	1934	ILE	3.6
2	B	22	PHE	3.6
1	A	1839	ASN	3.6
1	A	1989	PHE	3.5
1	A	1977	VAL	3.5
2	B	294	TYR	3.5
1	A	1906	SER	3.5
2	B	104	SER	3.5
2	B	279	TYR	3.5
1	A	1898[A]	VAL	3.4
1	A	1967	ALA	3.4
1	A	2010	LEU	3.4
1	A	2027	LEU	3.4
2	B	147	VAL	3.4
1	A	1846	ASN	3.4
2	B	258	LYS	3.4
1	A	2005	PHE	3.4
1	A	2050	THR	3.4
2	B	117	LEU	3.3
2	B	259	HIS	3.3
2	B	206	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	229	LEU	3.3
2	B	293	LEU	3.3
1	A	2036	SER	3.3
1	A	1917	VAL	3.3
2	B	41[A]	VAL	3.3
1	A	1901	GLY	3.3
1	A	2066	LYS	3.3
1	A	1959	THR	3.2
1	A	1970	SER	3.2
2	B	217	SER	3.2
2	B	289	TRP	3.2
2	B	78	TYR	3.2
2	B	267	ILE	3.2
1	A	1904	ARG	3.2
2	B	131	ARG	3.2
1	A	2002[A]	TYR	3.2
2	B	106	PRO	3.2
2	B	52	SER	3.1
1	A	1865	THR	3.1
2	B	93	VAL	3.1
2	B	103	VAL	3.1
2	B	256	VAL	3.1
2	B	58	TYR	3.1
1	A	2032	ILE	3.1
1	A	2011	LEU	3.1
1	A	2048	TRP	3.0
2	B	171	ASP	3.1
2	B	20	TYR	3.0
1	A	1920	LEU	3.0
1	A	2030	PRO	3.0
2	B	73	PRO	3.0
1	A	1868	GLY	3.0
2	B	222	GLY	3.0
2	B	233	PHE	3.0
2	B	257	PRO	3.0
1	A	1932[A]	GLN	2.9
1	A	1926	LYS	2.9
2	B	179	THR	2.9
1	A	1968	ALA	2.9
1	A	1899[A]	TRP	2.9
1	A	1995	TRP	2.9
2	B	234	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	132	LYS	2.9
1	A	1882	LEU	2.9
2	B	213	ILE	2.9
2	B	40	HIS	2.9
2	B	56	TYR	2.9
2	B	220	TYR	2.9
2	B	99	ARG	2.9
1	A	1889	LEU	2.9
1	A	1924	LEU	2.9
2	B	302	LEU	2.9
2	B	247	ILE	2.9
1	A	2028	SER	2.9
2	B	274	THR	2.8
1	A	1963	LEU	2.8
2	B	114	TRP	2.8
2	B	7	THR	2.8
1	A	1864	LYS	2.8
2	B	87	ALA	2.8
1	A	2039	LEU	2.8
2	B	45[A]	HIS	2.8
1	A	1919[A]	ALA	2.8
2	B	262	ASP	2.8
2	B	227	ALA	2.7
1	A	1960[A]	GLU	2.7
2	B	29	PRO	2.7
2	B	191	PRO	2.7
2	B	139	TYR	2.7
1	A	2025	ILE	2.7
1	A	2062	GLU	2.7
2	B	107	LYS	2.7
2	B	124	ASP	2.7
2	B	127	ARG	2.7
1	A	1837	SER	2.7
1	A	1944	LEU	2.7
2	B	199	LEU	2.7
2	B	300	ASN	2.7
2	B	126	ILE	2.7
2	B	299	LYS	2.7
2	B	84	ARG	2.6
2	B	314	PRO	2.6
1	A	1851	PHE	2.6
2	B	97	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	1911	TRP	2.6
2	B	60	PHE	2.6
1	A	1971	ILE	2.6
1	A	2052	GLU	2.6
1	A	1876	ASN	2.6
1	A	1980[A]	LYS	2.5
2	B	186	ARG	2.5
2	B	189	ILE	2.5
1	A	1998	ARG	2.5
1	A	1964	PRO	2.5
1	A	1936	THR	2.5
2	B	303	HIS	2.5
1	A	1905	LEU	2.5
1	A	1996	LEU	2.5
1	A	1858	TYR	2.5
1	A	1952	PRO	2.5
1	A	1978	VAL	2.5
2	B	38	ILE	2.5
2	B	100	GLN	2.4
2	B	120	PHE	2.4
1	A	1922	ARG	2.4
2	B	178[A]	TYR	2.4
1	A	1861	THR	2.4
1	A	1893	ILE	2.4
1	A	1982	THR	2.4
2	B	4	VAL	2.4
2	B	288	VAL	2.4
2	B	301	SER	2.4
1	A	2018[A]	ASN	2.4
1	A	1988	LEU	2.4
2	B	235	GLY	2.4
1	A	1844	PHE	2.4
1	A	1880	PHE	2.4
1	A	2053[A]	SER	2.4
1	A	2034	ILE	2.4
2	B	69	ILE	2.4
1	A	1912	LYS	2.4
1	A	1855[A]	THR	2.4
2	B	67	PHE	2.4
2	B	226	PHE	2.4
1	A	2007	ARG	2.4
1	A	1991	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	89	PHE	2.3
2	B	243	TRP	2.3
1	A	2046	GLU	2.3
2	B	27	ASN	2.3
1	A	2001[A]	SER	2.3
2	B	218	SER	2.3
2	B	295	SER	2.3
1	A	1852	VAL	2.3
2	B	190	ARG	2.3
2	B	312	LYS	2.3
2	B	14	THR	2.3
2	B	28	GLN	2.3
2	B	211[A]	GLN	2.3
1	A	1962	ARG	2.3
2	B	8	SER	2.3
1	A	2057[A]	ASP	2.3
2	B	59	TRP	2.2
2	B	3	THR	2.2
1	A	2008	LEU	2.2
2	B	79	LYS	2.2
2	B	46	PHE	2.2
2	B	137	PHE	2.2
2	B	115	TYR	2.2
1	A	1987	VAL	2.2
2	B	25	LYS	2.2
1	A	2047	GLN	2.2
2	B	6	PHE	2.2
1	A	1883	ASN	2.2
2	B	285	ASN	2.2
2	B	133	ASP	2.2
2	B	62	CYS	2.2
2	B	306	GLU	2.2
2	B	86	GLY	2.2
1	A	1938	LYS	2.2
2	B	15	ILE	2.2
2	B	85	ASP	2.1
2	B	110	GLU	2.1
1	A	1981	ALA	2.1
1	A	2033	THR	2.1
2	B	30	PHE	2.1
2	B	109	ASP	2.1
1	A	1907	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1933	ILE	2.1
1	A	1900	ALA	2.1
2	B	140	VAL	2.1
2	B	94	HIS	2.1
1	A	1918[A]	SER	2.1
1	A	1859	ARG	2.1
2	B	297	PHE	2.1
2	B	26	GLU	2.1
2	B	223	GLU	2.1
2	B	278	GLN	2.1
2	B	290	ASN	2.0
2	B	111	ASP	2.0
1	A	2042	SER	2.0
2	B	55[A]	ARG	2.0
1	A	1843	LEU	2.0
1	A	2021	SER	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(Å ²)	Q<0.9
3	UXB	B	401	12/12	0.85	0.17	20,20,20,20	12
3	UXB	B	402	12/12	0.87	0.18	20,20,20,20	12

6.5 Other polymers [i](#)

There are no such residues in this entry.