



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:37 PM UTC

PDB ID : 7FK0 / pdb_00007fk0
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P04A05 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

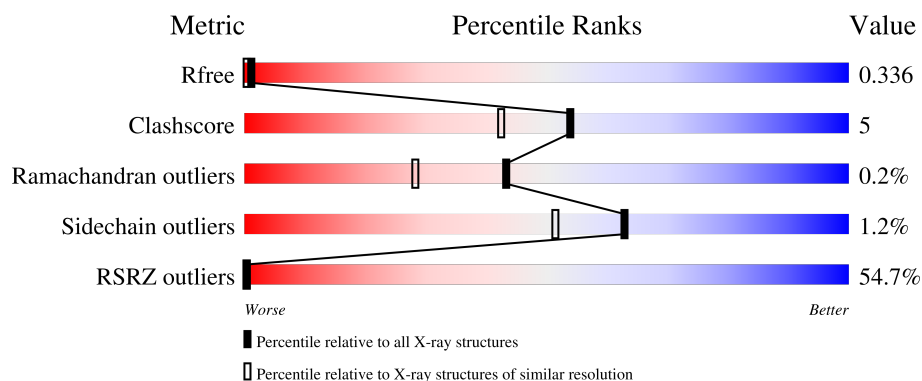
1 Overall quality at a glance

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	52% 80% 10% 8%
2	B	308	52% 83% 14%

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	W36	B	401	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9207 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:

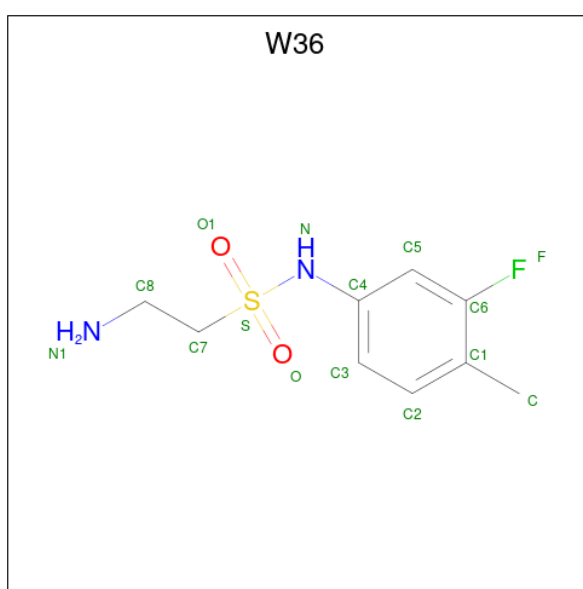
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN	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 2-amino-N-(3-fluoro-4-methylphenyl)ethane-1-sulfonamide (CCD ID: W36) (formula: C₉H₁₃FN₂O₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	S	0	0
			15	9	1	2	2	1		

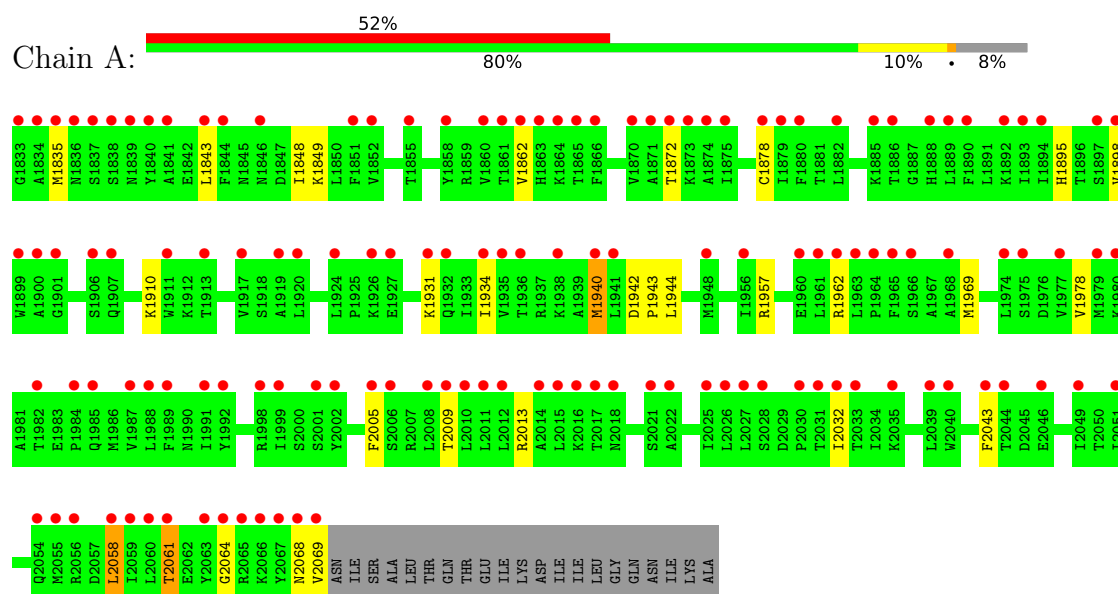
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		
4	B	41	Total	O	0	0
			41	41		

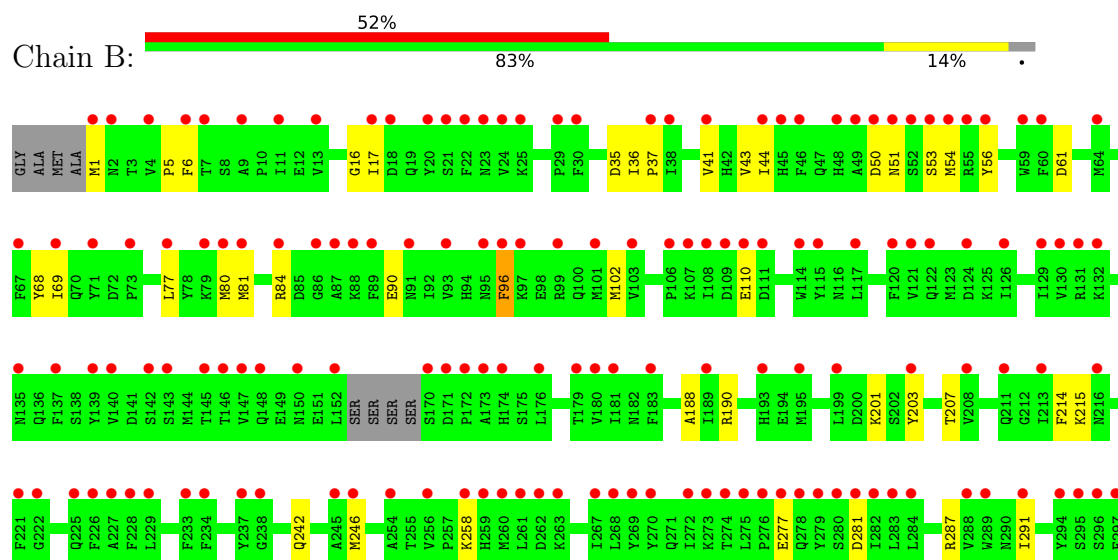
3 Residue-property plots

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	88.59Å 81.63Å 93.29Å 90.00° 108.58° 90.00°	Depositor
Resolution (Å)	44.21 – 1.69 44.21 – 1.69	Depositor EDS
% Data completeness (in resolution range)	98.7 (44.21-1.69) 98.8 (44.21-1.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.271 , 0.331 0.284 , 0.336	Depositor DCC
R_{free} test set	2091 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9207	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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: W36

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	0.75	2/2149 (0.1%)	0.82	0/2911
2	B	0.78	1/2739 (0.0%)	0.91	3/3699 (0.1%)
All	All	0.77	3/4888 (0.1%)	0.87	3/6610 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1940	MET	SD-CE	-6.32	1.63	1.79
1	A	1978	VAL	CA-C	5.73	1.59	1.52
2	B	90	GLU	C-O	-5.54	1.17	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6	PHE	CA-C-O	-5.50	114.76	120.70
2	B	201	LYS	CA-C-O	-5.14	113.16	120.51
2	B	96	PHE	CA-CB-CG	5.12	118.92	113.80

There are no chirality outliers.

There are no planarity outliers.

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	28	0
3	B	15	0	0	0	0
4	A	39	0	0	0	0
4	B	41	0	0	3	0
All	All	4683	4524	4372	45	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 (45) 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	2.15	0.80
1:A:1878:CYS:SG	1:A:1969:MET:HE3	2.35	0.66
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.46	0.64
1:A:2064:GLY:O	1:A:2068:ASN:N	2.30	0.61
1:A:1895:HIS:O	1:A:1898[A]:VAL:HG22	2.00	0.61
2:B:1:MET:HB3	2:B:35:ASP:HA	1.83	0.60
1:A:1862:VAL:HG22	1:A:1872:THR:HG22	1.85	0.58
2:B:287:ARG:O	2:B:291:ILE:HD13	2.05	0.57
2:B:50:ASP:OD1	2:B:51:ASN:N	2.38	0.55
1:A:1942:ASP:HB2	1:A:1943:PRO:HD3	1.89	0.55
2:B:54[A]:MET:HE2	4:B:537:HOH:O	2.07	0.53
2:B:41[A]:VAL:HG12	4:B:527:HOH:O	2.09	0.52
2:B:277:GLU:CD	2:B:277:GLU:H	2.19	0.51
2:B:110:GLU:HG2	2:B:110:GLU:O	2.10	0.51
2:B:1:MET:N	4:B:502:HOH:O	2.45	0.49
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.39	0.48
1:A:1910:LYS:O	1:A:1940:MET:HE1	2.13	0.48
2:B:17:ILE:HD13	2:B:44[B]:ILE:HG12	1.96	0.47
2:B:96:PHE:HB2	2:B:102:MET:HE3	1.97	0.47
2:B:77:LEU:N	2:B:77:LEU:HD23	2.30	0.47
1:A:2061:THR:O	1:A:2064:GLY:N	2.48	0.47
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	1.96	0.47
2:B:190:ARG:HG3	2:B:203[B]:TYR:CE2	2.50	0.46
1:A:1962:ARG:HD3	1:A:1962:ARG:H	1.80	0.46
2:B:203[A]:TYR:CZ	2:B:207:THR:HG21	2.50	0.45
2:B:56:TYR:CZ	2:B:77:LEU:HB2	2.52	0.45
1:A:2032:ILE:HG21	1:A:2043:PHE:CD1	2.52	0.45
2:B:51:ASN:HD21	2:B:53:SER:HB2	1.82	0.45
2:B:17:ILE:HD13	2:B:44[B]:ILE:CG1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:LYS:HD2	2:B:258:LYS:H	1.83	0.44
1:A:1835:MET:HE3	1:A:1835:MET:HB3	1.93	0.44
2:B:69:ILE:HD13	2:B:80:MET:HA	2.00	0.44
2:B:68:TYR:CE2	2:B:81:MET:HE3	2.54	0.43
2:B:36:ILE:HA	2:B:37:PRO:HD3	1.95	0.42
2:B:214:PHE:O	2:B:215:LYS:HB2	2.20	0.42
2:B:242:GLN:O	2:B:246:MET:HG3	2.20	0.41
2:B:306:GLU:O	2:B:310:GLU:HG3	2.21	0.41
2:B:43:VAL:O	2:B:43:VAL:HG13	2.20	0.41
2:B:77:LEU:HD23	2:B:77:LEU:H	1.85	0.41
1:A:1944:LEU:HD12	1:A:1944:LEU:HA	1.86	0.41
1:A:1934:ILE:HA	1:A:1957:ARG:O	2.20	0.41
1:A:2005:PHE:O	1:A:2009:THR:HG23	2.21	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%)	251 (97%)	6 (2%)	1 (0%)	30	16
2	B	315/308 (102%)	304 (96%)	11 (4%)	0	100	100
All	All	573/566 (101%)	555 (97%)	17 (3%)	1 (0%)	43	28

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%)	235 (99%)	2 (1%)	73	65
2	B	294/284 (104%)	290 (99%)	4 (1%)	59	46
All	All	531/517 (103%)	525 (99%)	6 (1%)	63	54

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2058	LEU
1	A	2069	VAL
2	B	5	PRO
2	B	84	ARG
2	B	281	ASP
2	B	315	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	40	HIS
2	B	91	ASN
2	B	135	ASN
2	B	259	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	W36	B	401	-	15,15,15	6.60	13 (86%)	19,21,21	3.80	12 (63%)

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	W36	B	401	-	-	3/9/9/9	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	W36	O1-S	-14.13	1.24	1.43
3	B	401	W36	C4-N	-10.07	1.27	1.43
3	B	401	W36	O-S	-8.04	1.32	1.43
3	B	401	W36	C-C1	-7.23	1.37	1.51
3	B	401	W36	C2-C3	-6.61	1.28	1.38
3	B	401	W36	C7-S	-6.59	1.56	1.78
3	B	401	W36	C1-C6	6.26	1.45	1.37
3	B	401	W36	F-C6	-5.58	1.20	1.35
3	B	401	W36	C2-C1	-5.06	1.29	1.39
3	B	401	W36	S-N	-4.90	1.53	1.62
3	B	401	W36	C5-C6	-3.78	1.31	1.37
3	B	401	W36	C5-C4	-2.76	1.34	1.39
3	B	401	W36	C3-C4	-2.37	1.35	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	W36	O1-S-N	7.90	126.36	107.23
3	B	401	W36	O-S-N	-6.35	91.87	107.23
3	B	401	W36	C-C1-C6	5.62	129.32	121.94
3	B	401	W36	C4-C5-C6	-4.70	114.88	118.82
3	B	401	W36	C-C1-C2	-4.39	111.81	120.28
3	B	401	W36	C5-C6-C1	-4.22	121.39	124.36
3	B	401	W36	C5-C4-N	-3.91	110.41	119.92
3	B	401	W36	C7-S-N	-3.87	101.22	106.72
3	B	401	W36	C7-C8-N1	-3.77	102.59	112.39
3	B	401	W36	O-S-C7	3.01	112.64	107.86
3	B	401	W36	C3-C4-C5	2.99	123.27	119.66
3	B	401	W36	C3-C4-N	2.59	125.48	120.02

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	W36	C4-N-S-O1
3	B	401	W36	C4-N-S-O
3	B	401	W36	C4-N-S-C7

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%)	2.41	135 (56%) 0 0	21, 65, 121, 181	12 (5%)
2	B	300/308 (97%)	2.34	159 (53%) 0 0	19, 64, 116, 151	9 (3%)
All	All	537/566 (94%)	2.37	294 (54%) 0 0	19, 64, 118, 181	21 (3%)

All (294) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1878	CYS	11.8
1	A	1979[A]	MET	8.4
1	A	1860	VAL	7.9
1	A	2060	LEU	7.8
2	B	152	LEU	7.5
1	A	2069	VAL	7.4
2	B	54[A]	MET	7.3
2	B	170	SER	7.2
2	B	246	MET	6.4
2	B	267	ILE	6.1
2	B	316	LEU	5.8
2	B	59	TRP	5.8
2	B	282	ILE	5.7
2	B	1	MET	5.7
2	B	101	MET	5.7
1	A	1987	VAL	5.7
2	B	80	MET	5.5
2	B	313	TYR	5.5
1	A	1866	PHE	5.4
1	A	2017[A]	THR	5.3
2	B	22	PHE	5.1
1	A	1879	ILE	5.1
2	B	275	LEU	5.1
2	B	49	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	2061	THR	4.9
1	A	2064	GLY	4.9
2	B	111	ASP	4.8
2	B	103	VAL	4.8
1	A	1833	GLY	4.7
2	B	189	ILE	4.7
2	B	41[A]	VAL	4.6
2	B	117	LEU	4.6
1	A	2065	ARG	4.6
2	B	193	HIS	4.5
1	A	1843	LEU	4.5
1	A	1862	VAL	4.5
1	A	2001[A]	SER	4.5
1	A	2040	TRP	4.5
2	B	17	ILE	4.5
2	B	279	TYR	4.4
2	B	13	VAL	4.4
2	B	88	LYS	4.4
1	A	2068	ASN	4.3
2	B	180	VAL	4.3
2	B	137	PHE	4.3
1	A	2026	LEU	4.1
2	B	20	TYR	4.1
1	A	1963	LEU	4.1
1	A	2008	LEU	4.1
1	A	2027	LEU	4.1
2	B	108	ILE	4.0
2	B	276	PRO	4.0
1	A	2067	TYR	4.0
1	A	1992	TYR	4.0
1	A	2063	TYR	4.0
2	B	38	ILE	3.9
2	B	274	THR	3.9
1	A	1840	TYR	3.9
2	B	284	LEU	3.9
2	B	46	PHE	3.8
2	B	317	LEU	3.8
1	A	1890	PHE	3.8
1	A	1898[A]	VAL	3.8
2	B	107	LYS	3.8
1	A	2014	ALA	3.8
1	A	2028	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	1835	MET	3.7
1	A	2012	LEU	3.7
2	B	174	HIS	3.7
1	A	1977	VAL	3.7
1	A	1865	THR	3.7
1	A	1965	PHE	3.6
1	A	2030	PRO	3.6
1	A	1861	THR	3.6
1	A	2011	LEU	3.6
2	B	172	PRO	3.6
1	A	1917	VAL	3.6
2	B	126	ILE	3.6
1	A	2056[A]	ARG	3.6
1	A	2010	LEU	3.6
2	B	18	ASP	3.6
2	B	270	TYR	3.6
2	B	277	GLU	3.5
2	B	50	ASP	3.5
2	B	122[A]	GLN	3.5
2	B	130	VAL	3.5
1	A	1875	ILE	3.4
1	A	2025	ILE	3.4
2	B	268	LEU	3.4
2	B	114	TRP	3.4
2	B	238	GLY	3.4
1	A	1924	LEU	3.4
1	A	1927	GLU	3.4
1	A	2051	ILE	3.4
1	A	2058	LEU	3.4
1	A	1855[A]	THR	3.4
2	B	203[A]	TYR	3.3
2	B	258	LYS	3.3
1	A	1851	PHE	3.3
1	A	1863	HIS	3.3
2	B	211[A]	GLN	3.3
1	A	1991	ILE	3.3
2	B	129	ILE	3.3
2	B	67	PHE	3.3
1	A	1841	ALA	3.3
2	B	254	ALA	3.3
1	A	1834	ALA	3.3
2	B	228	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	273	LYS	3.2
1	A	1988	LEU	3.2
1	A	2002[A]	TYR	3.2
1	A	2049	ILE	3.2
1	A	1846	ASN	3.1
2	B	150	ASN	3.1
2	B	11	ILE	3.1
1	A	1941	LEU	3.1
2	B	229	LEU	3.1
2	B	261	LEU	3.1
2	B	48	HIS	3.1
2	B	234	PHE	3.1
1	A	1913	THR	3.1
1	A	2032	ILE	3.1
1	A	1897	SER	3.1
1	A	1940	MET	3.1
2	B	77	LEU	3.1
2	B	283	LEU	3.1
2	B	131	ARG	3.1
2	B	233	PHE	3.1
1	A	1899[A]	TRP	3.0
2	B	269	TYR	3.0
2	B	294	TYR	3.0
2	B	216	ASN	3.0
2	B	181	ILE	3.0
2	B	146	THR	3.0
2	B	30	PHE	3.0
1	A	1836	ASN	3.0
1	A	1838	SER	3.0
2	B	195	MET	3.0
2	B	25	LYS	3.0
2	B	55[A]	ARG	3.0
2	B	140	VAL	3.0
2	B	21	SER	3.0
2	B	96	PHE	3.0
2	B	256	VAL	2.9
2	B	53	SER	2.9
1	A	2031	THR	2.9
2	B	173	ALA	2.9
1	A	1839	ASN	2.9
2	B	86	GLY	2.9
1	A	1984	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1844	PHE	2.9
1	A	1837	SER	2.9
1	A	1926	LYS	2.9
2	B	97	LYS	2.9
1	A	1960[A]	GLU	2.9
1	A	2006	SER	2.9
2	B	227	ALA	2.9
2	B	56	TYR	2.9
2	B	278	GLN	2.9
2	B	171	ASP	2.9
1	A	1873	LYS	2.9
2	B	84	ARG	2.8
2	B	288	VAL	2.8
2	B	132	LYS	2.8
2	B	73	PRO	2.8
1	A	2005	PHE	2.8
2	B	297	PHE	2.8
2	B	222	GLY	2.8
2	B	45[A]	HIS	2.8
1	A	1935	VAL	2.8
2	B	93	VAL	2.8
1	A	2039	LEU	2.8
2	B	2	ASN	2.8
1	A	1980[A]	LYS	2.8
1	A	1982	THR	2.8
1	A	2055	MET	2.8
1	A	1906	SER	2.8
1	A	1893	ILE	2.8
1	A	1956	ILE	2.8
2	B	44[A]	ILE	2.8
1	A	2009	THR	2.8
2	B	87	ALA	2.7
2	B	289	TRP	2.7
2	B	29	PRO	2.7
2	B	24	VAL	2.7
1	A	1894	ILE	2.7
2	B	81	MET	2.7
2	B	303	HIS	2.7
1	A	1907	GLN	2.7
1	A	1968	ALA	2.7
2	B	6	PHE	2.7
2	B	142	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	71	TYR	2.7
1	A	1871	ALA	2.7
1	A	1985	GLN	2.6
1	A	1886	THR	2.6
1	A	2015	LEU	2.6
1	A	1852	VAL	2.6
2	B	115	TYR	2.6
2	B	139	TYR	2.6
1	A	2022	ALA	2.6
2	B	262	ASP	2.6
1	A	1858	TYR	2.6
2	B	147	VAL	2.6
2	B	208	VAL	2.6
1	A	2035	LYS	2.6
2	B	95	ASN	2.6
2	B	109	ASP	2.5
2	B	183	PHE	2.5
2	B	299	LYS	2.5
2	B	295	SER	2.5
2	B	291	ILE	2.5
2	B	308	ILE	2.5
2	B	245	ALA	2.5
1	A	1962	ARG	2.5
2	B	281	ASP	2.5
1	A	1874	ALA	2.5
2	B	305	THR	2.5
1	A	1901	GLY	2.5
1	A	1931[A]	LYS	2.5
1	A	2033	THR	2.5
2	B	145	THR	2.5
2	B	280	SER	2.5
2	B	176	LEU	2.4
2	B	69	ILE	2.4
1	A	1932[A]	GLN	2.4
2	B	124	ASP	2.4
2	B	99	ARG	2.4
2	B	259	HIS	2.4
1	A	1964	PRO	2.4
2	B	52	SER	2.4
2	B	7	THR	2.4
2	B	4	VAL	2.4
2	B	121	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	91	ASN	2.4
1	A	1989	PHE	2.4
1	A	2044	THR	2.4
1	A	2021	SER	2.3
2	B	51	ASN	2.3
2	B	296	SER	2.3
1	A	1974	LEU	2.3
1	A	1880	PHE	2.3
2	B	221	PHE	2.3
2	B	64[A]	MET	2.3
2	B	237	TYR	2.3
1	A	1999	ILE	2.3
1	A	1870	VAL	2.3
1	A	1900	ALA	2.3
2	B	260	MET	2.3
2	B	199	LEU	2.3
2	B	226	PHE	2.3
2	B	213	ILE	2.3
1	A	2016	LYS	2.3
2	B	110	GLU	2.3
2	B	89	PHE	2.3
2	B	120	PHE	2.3
2	B	272	ILE	2.3
1	A	1911	TRP	2.2
1	A	1936	THR	2.2
1	A	1975	SER	2.2
1	A	2054[A]	GLN	2.2
2	B	143	SER	2.2
1	A	2043	PHE	2.2
1	A	1998	ARG	2.2
1	A	2018[A]	ASN	2.2
1	A	2046	GLU	2.2
1	A	1920	LEU	2.2
2	B	263	LYS	2.2
1	A	1872	THR	2.2
2	B	37	PRO	2.2
1	A	1919[A]	ALA	2.1
2	B	9	ALA	2.1
1	A	1882	LEU	2.1
1	A	1889	LEU	2.1
1	A	1892	LYS	2.1
1	A	2066	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	225	GLN	2.1
2	B	135	ASN	2.1
2	B	148	GLN	2.1
2	B	179	THR	2.1
2	B	60	PHE	2.1
1	A	1934	ILE	2.1
1	A	1948	MET	2.1
1	A	1961[A]	LEU	2.1
2	B	106	PRO	2.1
1	A	1885	LYS	2.1
1	A	2059	ILE	2.1
1	A	1966	SER	2.0
1	A	1888	HIS	2.0
2	B	79	LYS	2.0
2	B	23	ASN	2.0
2	B	301	SER	2.0
1	A	1864	LYS	2.0
1	A	1938	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(Å ²)	Q<0.9
3	W36	B	401	15/15	0.59	0.22	20,20,20,20	15

6.5 Other polymers [i](#)

There are no such residues in this entry.