



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:57 PM UTC

PDB ID : 7FN2 / pdb_00007fn2
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment P06G08 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 : 1.62 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

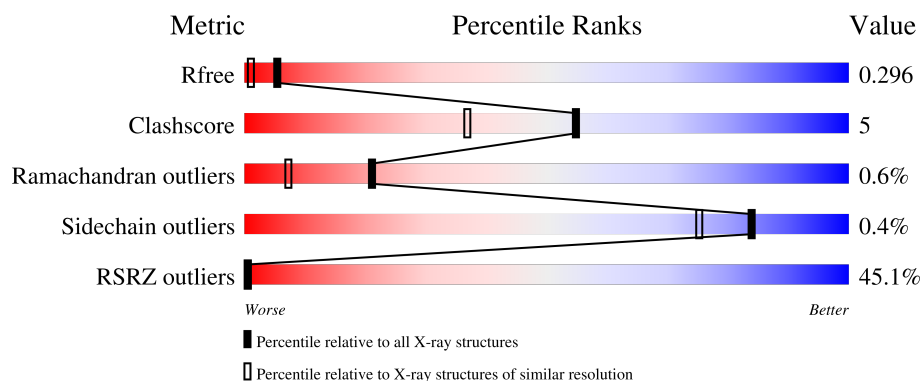
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.62 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	
2	B	308	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9218 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	36	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	11	17	0

There are 20 discrepancies between the modelled and reference sequences:

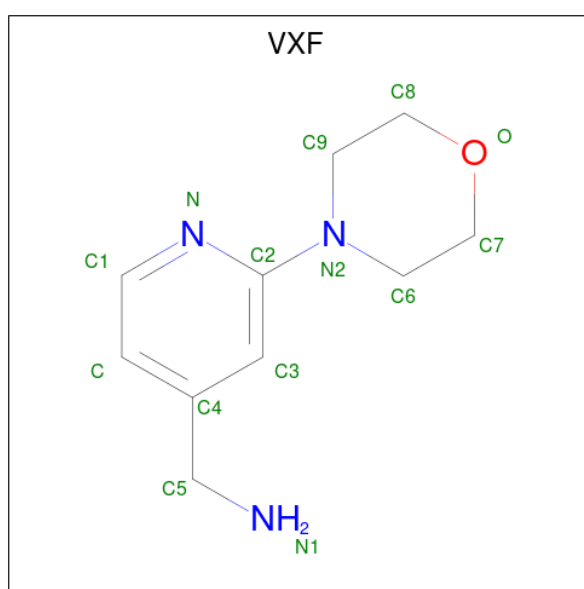
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	?	-	LEU	deletion	UNP P32357
B	?	-	GLN	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 1-[2-(morpholin-4-yl)pyridin-4-yl]methanamine (CCD ID: VXF) (formula: C₁₀H₁₅N₃O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	10	3	1		

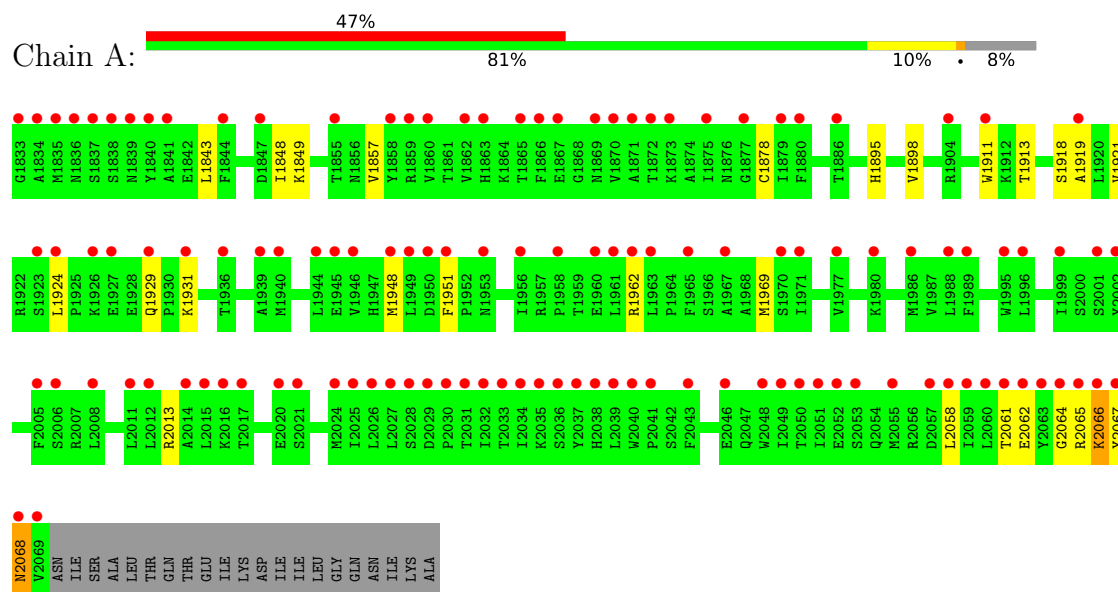
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	50	Total	O	0	0
			50	50		

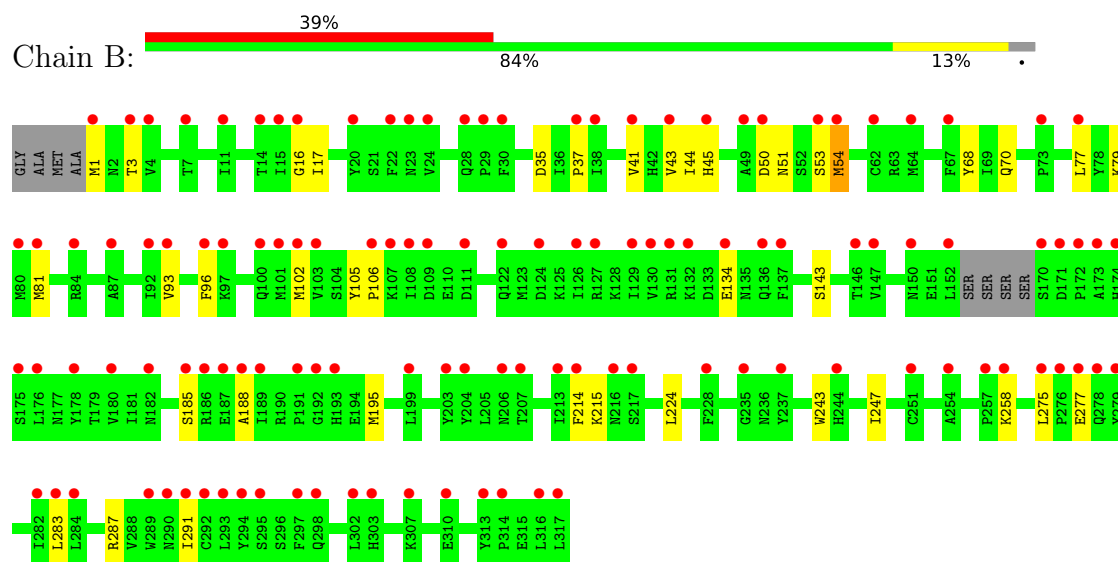
3 Residue-property plots

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	88.73Å 81.84Å 93.04Å 90.00° 108.13° 90.00°	Depositor
Resolution (Å)	44.21 – 1.62 44.21 – 1.62	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.21-1.62) 99.7 (44.21-1.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 1.62Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.256 , 0.294 0.262 , 0.296	Depositor DCC
R_{free} test set	2099 reflections (2.62%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 48.6	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	0.95	EDS
Total number of atoms	9218	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% 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: VXF

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	0.90	7/2149 (0.3%)	0.98	11/2911 (0.4%)
2	B	0.73	1/2739 (0.0%)	0.84	1/3699 (0.0%)
All	All	0.81	8/4888 (0.2%)	0.90	12/6610 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1951	PHE	C-N	14.38	1.52	1.34
1	A	1929	GLN	C-N	14.04	1.51	1.33
1	A	1924	LEU	C-N	13.06	1.50	1.33
2	B	16	GLY	CA-C	-8.44	1.46	1.52
1	A	1919[A]	ALA	N-CA	6.71	1.54	1.46
1	A	1919[B]	ALA	N-CA	6.71	1.54	1.46
1	A	1918[A]	SER	C-N	6.03	1.42	1.34
1	A	1918[B]	SER	C-N	6.03	1.42	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1951	PHE	CA-C-N	8.79	128.44	119.56
1	A	1951	PHE	C-N-CA	8.79	128.44	119.56
1	A	1929	GLN	CA-C-N	8.50	128.44	119.85
1	A	1929	GLN	C-N-CA	8.50	128.44	119.85
1	A	1918[A]	SER	CA-C-N	-8.19	107.86	120.31
1	A	1918[A]	SER	C-N-CA	-8.19	107.86	120.31
1	A	1918[B]	SER	CA-C-N	-8.19	107.86	120.31
1	A	1918[B]	SER	C-N-CA	-8.19	107.86	120.31
1	A	1924	LEU	CA-C-N	7.68	127.72	119.89
1	A	1924	LEU	C-N-CA	7.68	127.72	119.89
1	A	1951	PHE	O-C-N	-5.40	116.51	121.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	185	SER	N-CA-C	5.07	116.70	109.14

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	14	0
2	B	2580	2464	2398	31	0
3	B	14	0	0	0	0
4	A	42	0	0	0	0
4	B	50	0	0	2	0
All	All	4694	4524	4372	44	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 (44) 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:70:GLN:HB3	2:B:81:MET:HE2	1.62	0.82
2:B:77:LEU:HD21	2:B:79:LYS:HE3	1.68	0.75
1:A:2061:THR:O	1:A:2064:GLY:N	2.20	0.75
2:B:68:TYR:CE2	2:B:81:MET:HE3	2.28	0.68
2:B:1:MET:N	4:B:501:HOH:O	2.26	0.68
2:B:96:PHE:CB	2:B:102:MET:HE3	2.24	0.67
2:B:96:PHE:HB2	2:B:102:MET:HE3	1.75	0.67
2:B:258:LYS:HD2	2:B:258:LYS:H	1.60	0.66
1:A:1962:ARG:O	1:A:2013:ARG:NH1	2.35	0.59
2:B:1:MET:HB3	2:B:35:ASP:HA	1.85	0.58
1:A:1878:CYS:SG	1:A:1969:MET:HE3	2.44	0.58
2:B:50:ASP:OD1	2:B:51:ASN:N	2.37	0.57
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	1.90	0.54
2:B:287:ARG:O	2:B:291:ILE:HD13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1895:HIS:O	1:A:1898[A]:VAL:HG22	2.07	0.54
1:A:2064:GLY:O	1:A:2068:ASN:N	2.42	0.53
2:B:54[B]:MET:HE1	2:B:143:SER:HB3	1.91	0.52
1:A:2062:GLU:OE1	1:A:2065:ARG:NH1	2.44	0.50
1:A:1921:VAL:HG21	1:A:1948:MET:HE1	1.97	0.47
1:A:1911:TRP:CG	2:B:195:MET:HG3	2.51	0.46
2:B:77:LEU:H	2:B:77:LEU:HD23	1.80	0.46
2:B:17:ILE:HD13	2:B:44[B]:ILE:CG1	2.46	0.46
2:B:277:GLU:CD	2:B:277:GLU:H	2.24	0.46
2:B:243:TRP:O	2:B:247:ILE:HG13	2.17	0.45
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.64	0.45
2:B:77:LEU:HD23	2:B:77:LEU:N	2.31	0.45
2:B:51:ASN:OD1	2:B:53:SER:HB2	2.17	0.44
2:B:70:GLN:CB	2:B:81:MET:HE2	2.38	0.44
2:B:134:GLU:OE1	2:B:134:GLU:N	2.36	0.44
2:B:43:VAL:HG13	2:B:43:VAL:O	2.18	0.44
1:A:1857:VAL:HG21	1:A:1913:THR:OG1	2.19	0.43
2:B:3:THR:HG21	2:B:93:VAL:HG13	2.02	0.42
2:B:37:PRO:HD3	2:B:105:TYR:CD1	2.54	0.42
2:B:214:PHE:O	2:B:215:LYS:HB2	2.19	0.42
1:A:2066:LYS:HD2	1:A:2067:TYR:CE1	2.54	0.42
2:B:96:PHE:HB3	2:B:102:MET:HE3	1.99	0.42
1:A:1962:ARG:HD3	1:A:1962:ARG:H	1.84	0.41
2:B:275:LEU:CD2	2:B:283:LEU:HD13	2.50	0.41
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.46	0.41
2:B:41[A]:VAL:HG12	4:B:537:HOH:O	2.19	0.41
2:B:224:LEU:HD23	2:B:224:LEU:C	2.45	0.41
2:B:258:LYS:H	2:B:258:LYS:CD	2.31	0.40
2:B:17:ILE:HD13	2:B:44[B]:ILE:HG12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	258/258 (100%)	250 (97%)	7 (3%)	1 (0%)	30	14
2	B	315/308 (102%)	304 (96%)	8 (2%)	3 (1%)	12	2
All	All	573/566 (101%)	554 (97%)	15 (3%)	4 (1%)	21	6

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2068	ASN
2	B	54[A]	MET
2	B	54[B]	MET
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%)	236 (100%)	1 (0%)	84	75
2	B	294/284 (104%)	292 (99%)	2 (1%)	76	62
All	All	531/517 (103%)	528 (99%)	3 (1%)	84	66

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2066	LYS
2	B	45[A]	HIS
2	B	45[B]	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2038	HIS
2	B	47	GLN
2	B	150	ASN

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	VXF	B	401	-	15,15,15	1.21	1 (6%)	19,19,19	1.12	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	VXF	B	401	-	-	0/6/14/14	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	401	VXF	C3-C4	-2.70	1.34	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	401	VXF	C-C4-C3	2.12	121.47	118.55

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	236/258 (91%)	2.24	121 (51%) 0 0	23, 68, 116, 189	11 (4%)
2	B	300/308 (97%)	1.91	121 (40%) 0 0	22, 66, 115, 180	9 (3%)
All	All	536/566 (94%)	2.06	242 (45%) 0 0	22, 67, 116, 189	20 (3%)

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2060	LEU	10.1
1	A	2069	VAL	8.6
2	B	54[A]	MET	8.4
2	B	152	LEU	6.6
2	B	203[A]	TYR	6.5
1	A	2017[A]	THR	6.3
2	B	170	SER	6.3
2	B	29	PRO	5.8
1	A	1841	ALA	5.8
1	A	1862	VAL	5.4
1	A	2058	LEU	5.4
1	A	2040	TRP	5.3
1	A	2005	PHE	5.1
1	A	2064	GLY	5.1
2	B	101	MET	5.0
1	A	2039	LEU	4.9
1	A	1860	VAL	4.8
2	B	279	TYR	4.7
1	A	1949	LEU	4.7
1	A	2048	TRP	4.7
1	A	2061	THR	4.6
2	B	276	PRO	4.6
1	A	2043	PHE	4.6
2	B	172	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
2	B	316	LEU	4.5
2	B	67	PHE	4.5
2	B	22	PHE	4.4
2	B	108	ILE	4.4
1	A	2059	ILE	4.4
1	A	2068	ASN	4.3
1	A	1951	PHE	4.3
1	A	1958	PRO	4.3
1	A	1863	HIS	4.3
1	A	2033	THR	4.2
1	A	2063	TYR	4.2
2	B	30	PHE	4.2
2	B	122[A]	GLN	4.2
2	B	134	GLU	4.2
1	A	2032	ILE	4.1
2	B	111	ASP	4.1
2	B	307	LYS	4.0
1	A	2049	ILE	4.0
2	B	291	ILE	4.0
2	B	41[A]	VAL	4.0
1	A	1840	TYR	3.9
2	B	11	ILE	3.9
2	B	275	LEU	3.9
1	A	2028	SER	3.9
1	A	2067	TYR	3.9
1	A	2034	ILE	3.8
2	B	1	MET	3.8
1	A	2015	LEU	3.8
1	A	1939	ALA	3.8
1	A	2027	LEU	3.8
2	B	174	HIS	3.7
1	A	2053[A]	SER	3.7
2	B	216	ASN	3.7
1	A	1833	GLY	3.7
1	A	1996	LEU	3.7
2	B	87	ALA	3.7
2	B	258	LYS	3.7
1	A	2001[A]	SER	3.7
1	A	2051	ILE	3.7
2	B	228	PHE	3.7
1	A	1834	ALA	3.6
2	B	186	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	193	HIS	3.6
1	A	1835	MET	3.6
1	A	2025	ILE	3.5
2	B	129	ILE	3.5
2	B	282	ILE	3.5
2	B	14	THR	3.5
2	B	146	THR	3.5
1	A	1999	ILE	3.5
1	A	1963	LEU	3.5
1	A	2037	TYR	3.5
2	B	173	ALA	3.4
1	A	2012	LEU	3.4
2	B	103	VAL	3.4
2	B	294	TYR	3.4
2	B	317	LEU	3.4
1	A	2031	THR	3.4
1	A	1931[A]	LYS	3.3
2	B	97	LYS	3.3
2	B	199	LEU	3.3
1	A	1866	PHE	3.3
1	A	2035	LYS	3.3
1	A	1940	MET	3.2
1	A	2055	MET	3.2
2	B	298	GLN	3.2
2	B	38	ILE	3.2
2	B	124	ASP	3.2
1	A	2065	ARG	3.2
2	B	293	LEU	3.2
1	A	2006	SER	3.2
1	A	1886	THR	3.2
1	A	1995	TRP	3.1
1	A	2038	HIS	3.1
1	A	2026	LEU	3.1
1	A	2030	PRO	3.0
2	B	176	LEU	3.0
2	B	53	SER	3.0
2	B	185	SER	3.0
2	B	16	GLY	3.0
2	B	147	VAL	3.0
1	A	1950	ASP	2.9
2	B	3	THR	2.9
2	B	102	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1927	GLU	2.9
2	B	20	TYR	2.9
2	B	284	LEU	2.9
1	A	2024[A]	MET	2.9
1	A	2020	GLU	2.9
2	B	43	VAL	2.9
1	A	1877	GLY	2.9
1	A	1961[A]	LEU	2.9
2	B	283	LEU	2.9
1	A	2041	PRO	2.9
2	B	107	LYS	2.9
1	A	1859	ARG	2.8
2	B	106	PRO	2.8
1	A	1880	PHE	2.8
2	B	37	PRO	2.8
2	B	290	ASN	2.8
2	B	80	MET	2.8
2	B	126	ILE	2.8
2	B	217	SER	2.8
1	A	1965	PHE	2.7
1	A	2011	LEU	2.7
2	B	178[A]	TYR	2.7
1	A	1944	LEU	2.7
2	B	7	THR	2.7
1	A	1879	ILE	2.7
1	A	1971	ILE	2.7
2	B	109	ASP	2.7
1	A	1989	PHE	2.7
2	B	96	PHE	2.7
2	B	297	PHE	2.7
1	A	1872	THR	2.7
2	B	235	GLY	2.7
1	A	1956	ILE	2.7
1	A	1837	SER	2.6
1	A	1844	PHE	2.6
1	A	1836	ASN	2.6
1	A	1870	VAL	2.6
2	B	213	ILE	2.6
1	A	1865	THR	2.6
1	A	1988	LEU	2.6
1	A	2052	GLU	2.6
2	B	313	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	2029	ASP	2.6
2	B	214	PHE	2.6
2	B	62	CYS	2.6
1	A	1858	TYR	2.6
1	A	1945	GLU	2.6
2	B	131	ARG	2.6
2	B	302	LEU	2.5
1	A	2050	THR	2.5
1	A	1986	MET	2.5
2	B	64[A]	MET	2.5
2	B	127	ARG	2.5
1	A	2002[A]	TYR	2.5
2	B	204[A]	TYR	2.5
2	B	50	ASP	2.5
1	A	1871	ALA	2.5
1	A	1875	ILE	2.5
1	A	1855[A]	THR	2.5
1	A	1873	LYS	2.5
1	A	2016	LYS	2.5
1	A	1960[A]	GLU	2.5
2	B	207	THR	2.5
2	B	45[A]	HIS	2.4
2	B	303	HIS	2.4
1	A	1838	SER	2.4
2	B	93	VAL	2.4
2	B	310	GLU	2.4
2	B	84	ARG	2.4
1	A	1924	LEU	2.4
1	A	1936	THR	2.4
2	B	237	TYR	2.4
2	B	15	ILE	2.4
2	B	130	VAL	2.4
2	B	292	CYS	2.4
2	B	191	PRO	2.4
2	B	206	ASN	2.4
1	A	1911	TRP	2.4
2	B	4	VAL	2.4
1	A	1867	GLU	2.3
1	A	2046	GLU	2.3
1	A	1919[A]	ALA	2.3
1	A	1962	ARG	2.3
1	A	2066	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	150	ASN	2.3
2	B	277	GLU	2.3
2	B	314	PRO	2.3
2	B	137	PHE	2.3
2	B	192	GLY	2.3
1	A	1967	ALA	2.2
1	A	2008	LEU	2.2
2	B	171	ASP	2.2
2	B	100	GLN	2.2
2	B	244	HIS	2.2
1	A	1953	ASN	2.2
2	B	23	ASN	2.2
2	B	182	ASN	2.2
2	B	77	LEU	2.2
2	B	92	ILE	2.2
1	A	1977	VAL	2.2
2	B	132	LYS	2.2
1	A	1970	SER	2.2
1	A	2062	GLU	2.2
2	B	187	GLU	2.2
2	B	28	GLN	2.1
2	B	49	ALA	2.1
1	A	1923	SER	2.1
1	A	2057[A]	ASP	2.1
2	B	257	PRO	2.1
2	B	189	ILE	2.1
1	A	1946	VAL	2.1
2	B	24	VAL	2.1
1	A	1980[A]	LYS	2.1
1	A	1948	MET	2.1
1	A	1847	ASP	2.1
1	A	1929	GLN	2.1
1	A	2021	SER	2.1
2	B	188	ALA	2.1
1	A	1839	ASN	2.1
2	B	175	SER	2.1
1	A	1904	ARG	2.1
2	B	73	PRO	2.1
2	B	289	TRP	2.1
1	A	1926	LYS	2.1
2	B	81	MET	2.0
2	B	136	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	278	GLN	2.0
2	B	295	SER	2.0
1	A	1869	ASN	2.0
1	A	2014	ALA	2.0
2	B	254	ALA	2.0
1	A	2036	SER	2.0
2	B	180	VAL	2.0
2	B	251	CYS	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	VXF	B	401	14/14	0.66	0.18	20,20,20,20	14

6.5 Other polymers [i](#)

There are no such residues in this entry.