



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:46 PM EDT

PDB ID : 5R0I / pdb_00005r0i
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment F2X-Entry E12, DMSO-free
Authors : Wollenhaupt, J.; Metz, A.; Barthel, T.; Lima, G.M.A.; Heine, A.; Mueller, U.; Klebe, G.; Weiss, M.S.
Deposited on : 2020-02-12
Resolution : 1.86 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:

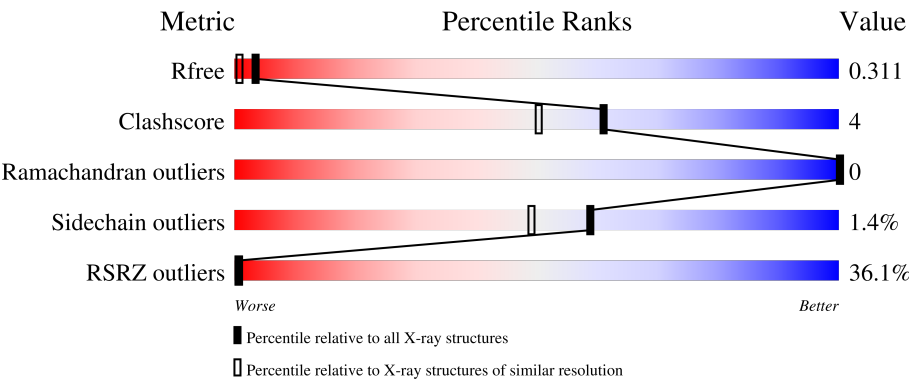
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.86 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	38% 82%9%8%
2	B	308	31% 86%10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4683 atoms, of which 0 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	N	O	S			
1	A	237	2002	1283	335	372	12	0	12	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	N	O	S			
2	B	300	2580	1654	421	485	20	0	9	0

There are 20 discrepancies between the modelled and reference sequences:

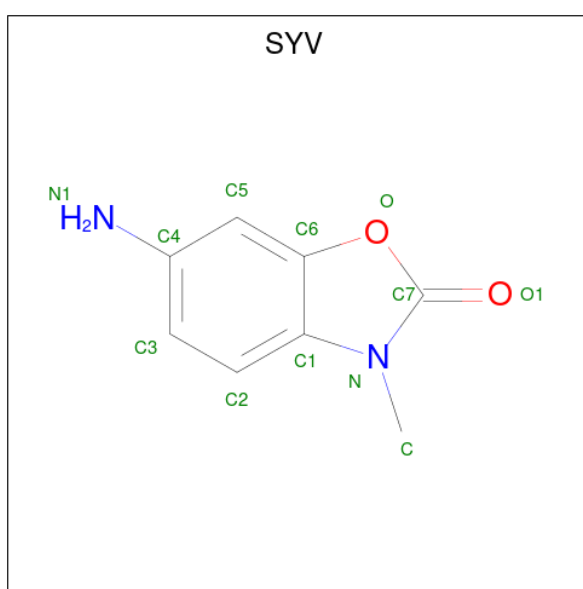
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	170	SER	LEU	conflict	UNP P32357
B	?	-	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	?	-	ASP	deletion	UNP P32357

- Molecule 3 is 6-azanyl-3-methyl-1,3-benzoxazol-2-one (CCD ID: SYV) (formula: C₈H₈N₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	8	2	2		

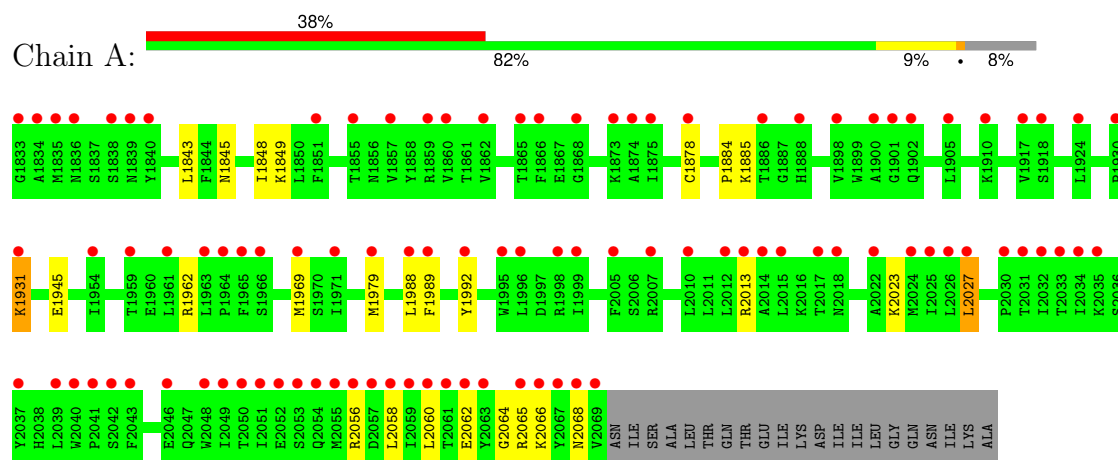
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	56	Total	O	0	0
			56	56		
4	B	33	Total	O	0	0
			33	33		

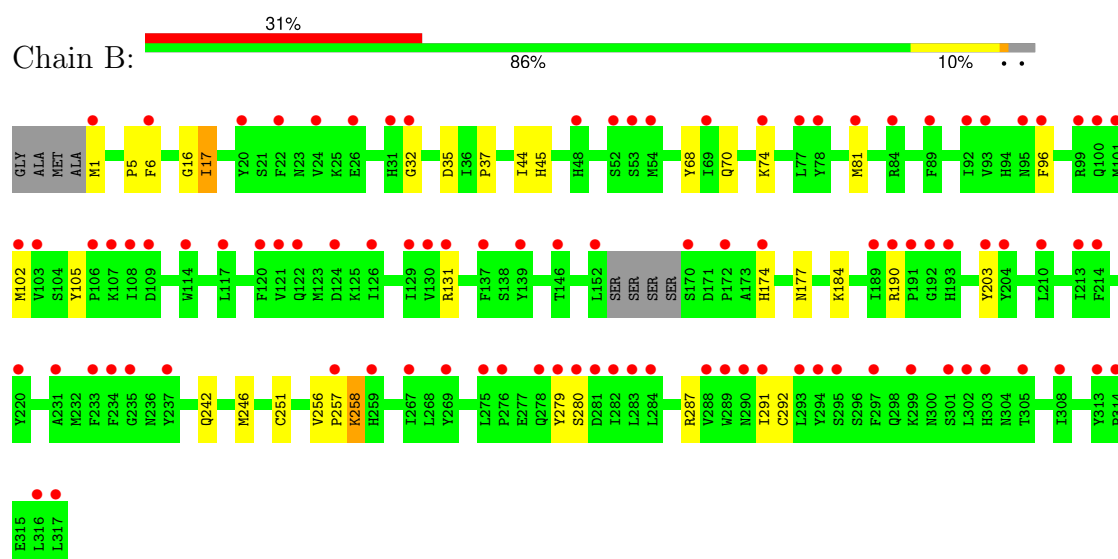
3 Residue-property plots

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	88.68Å 82.46Å 93.14Å 90.00° 108.04° 90.00°	Depositor
Resolution (Å)	22.71 – 1.86 22.71 – 1.86	Depositor EDS
% Data completeness (in resolution range)	99.5 (22.71-1.86) 99.9 (22.71-1.86)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.259 , 0.295 0.274 , 0.311	Depositor DCC
R_{free} test set	2100 reflections (3.89%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.5	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	4683	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% 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: SYV

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	1/2049 (0.0%)	0.93	3/2775 (0.1%)
2	B	0.65	0/2651	0.78	0/3581
All	All	0.70	1/4700 (0.0%)	0.85	3/6356 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1992	TYR	C-O	-7.72	1.13	1.24

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1884	PRO	CA-C-N	5.35	129.65	120.71
1	A	1884	PRO	C-N-CA	5.35	129.65	120.71
1	A	1989	PHE	CA-CB-CG	5.07	118.87	113.80

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	2002	0	2029	14	1
2	B	2580	0	2450	25	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	0	0	0
4	A	56	0	0	0	0
4	B	33	0	0	2	0
All	All	4683	0	4479	38	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (38) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.35	0.74
1:A:2062:GLU:O	1:A:2066:LYS:HG2	1.88	0.74
1:A:1962:ARG:O	1:A:2013:ARG:NH1	2.23	0.72
2:B:1:MET:N	4:B:401:HOH:O	2.24	0.70
1:A:1845:ASN:O	1:A:1885:LYS:HD3	1.95	0.66
2:B:70:GLN:HB3	2:B:81:MET:HE2	1.79	0.64
1:A:1979[B]:MET:HA	1:A:1979[B]:MET:HE2	1.84	0.59
2:B:68:TYR:CE2	2:B:81:MET:HE3	2.38	0.58
1:A:2062:GLU:HB3	1:A:2066:LYS:HE3	1.86	0.58
2:B:6:PHE:HZ	2:B:44[A]:ILE:HD11	1.70	0.56
2:B:258:LYS:HD2	2:B:258:LYS:H	1.71	0.54
2:B:242:GLN:O	2:B:246:MET:HG3	2.08	0.54
2:B:96:PHE:HB2	2:B:102:MET:HE3	1.88	0.54
2:B:1:MET:HB3	2:B:35:ASP:HA	1.90	0.53
2:B:74:LYS:NZ	4:B:402:HOH:O	2.41	0.53
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.34	0.52
1:A:2056[B]:ARG:O	1:A:2060:LEU:HG	2.09	0.52
2:B:131:ARG:NH2	2:B:177[B]:ASN:OD1	2.36	0.52
2:B:37:PRO:HD3	2:B:105:TYR:CD1	2.45	0.52
2:B:190:ARG:HG3	2:B:203[B]:TYR:CE2	2.45	0.51
2:B:287:ARG:O	2:B:291:ILE:HD13	2.12	0.50
1:A:2023:LYS:O	1:A:2027:LEU:HG	2.14	0.48
2:B:16:GLY:HA3	2:B:45:HIS:CE1	2.50	0.47
2:B:70:GLN:OE1	2:B:81:MET:HE1	2.14	0.46
1:A:1945:GLU:OE2	2:B:184:LYS:NZ	2.35	0.45
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	1.99	0.45
2:B:6:PHE:CZ	2:B:44[A]:ILE:HD11	2.49	0.45
2:B:251:CYS:SG	2:B:292:CYS:HB3	2.57	0.44
2:B:70:GLN:CB	2:B:81:MET:HE2	2.47	0.44
1:A:2056[A]:ARG:O	1:A:2060:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:VAL:O	2:B:257:PRO:C	2.59	0.43
2:B:258:LYS:H	2:B:258:LYS:CD	2.30	0.43
1:A:1878:CYS:SG	1:A:1969:MET:HE3	2.60	0.42
1:A:2064:GLY:O	1:A:2068:ASN:N	2.51	0.41
2:B:96:PHE:CB	2:B:102:MET:HE3	2.51	0.41
2:B:190:ARG:HG3	2:B:203[B]:TYR:CZ	2.55	0.41
2:B:17:ILE:HD12	2:B:44[B]:ILE:HG13	2.03	0.41
2:B:5:PRO:HA	2:B:32:GLY:HA3	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2065:ARG:NH1	2:B:279:TYR:OH[2_655]	2.16	0.04

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/258 (96%)	242 (98%)	6 (2%)	0	100	100
2	B	306/308 (99%)	295 (96%)	11 (4%)	0	100	100
All	All	554/566 (98%)	537 (97%)	17 (3%)	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	226/233 (97%)	222 (98%)	4 (2%)	51	40
2	B	287/284 (101%)	283 (99%)	4 (1%)	59	49
All	All	513/517 (99%)	505 (98%)	8 (2%)	59	44

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1931[A]	LYS
1	A	1931[B]	LYS
1	A	1988	LEU
1	A	2027	LEU
2	B	17	ILE
2	B	174	HIS
2	B	258	LYS
2	B	280	SER

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

Mol	Chain	Res	Type
2	B	45	HIS
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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SYV	A	2501	-	12,13,13	1.07	0	15,19,19	0.85	0

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	SYV	A	2501	-	-	-	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

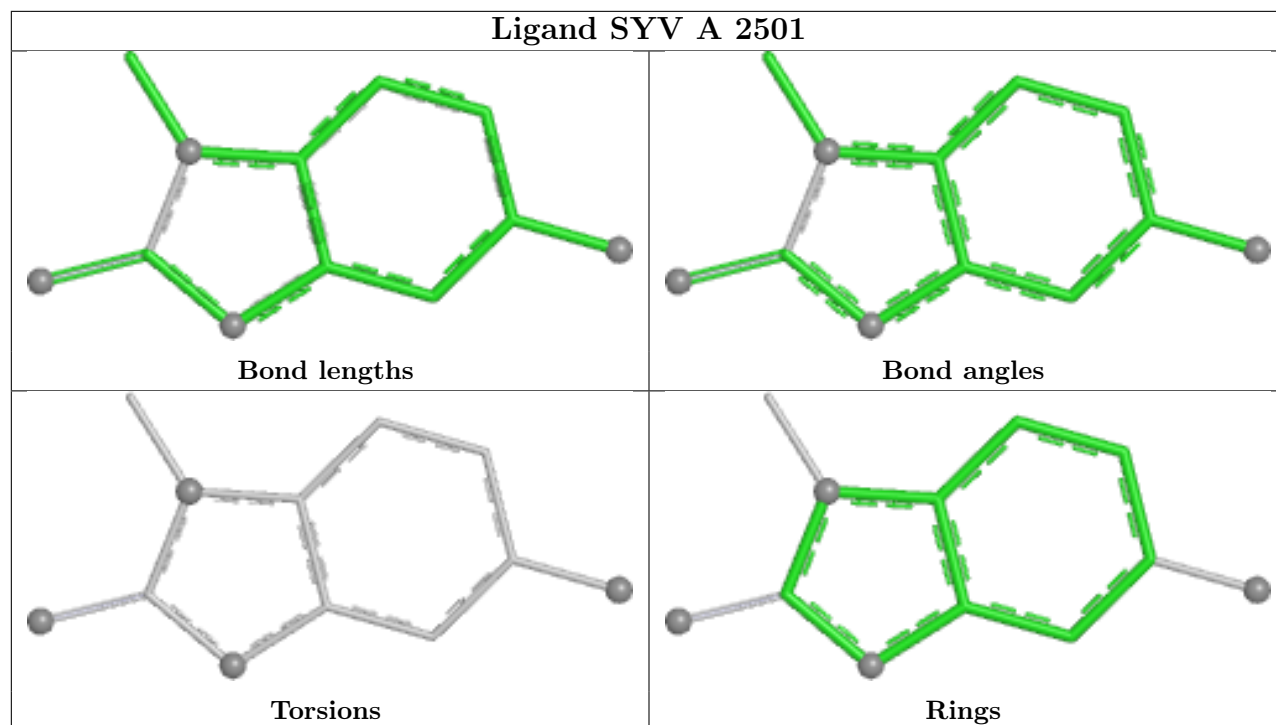
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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%)	2.04	98 (41%) 0 0	32, 68, 124, 174	12 (5%)
2	B	300/308 (97%)	1.63	96 (32%) 1 1	24, 73, 131, 251	9 (3%)
All	All	537/566 (94%)	1.81	194 (36%) 1 1	24, 70, 131, 251	21 (3%)

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1878	CYS	12.3
1	A	1969	MET	8.0
1	A	1979[A]	MET	7.7
2	B	130	VAL	7.3
1	A	1898[A]	VAL	7.2
1	A	2041	PRO	7.1
1	A	2034	ILE	6.9
1	A	2039	LEU	6.7
1	A	2058	LEU	6.4
2	B	203[A]	TYR	6.0
1	A	2015	LEU	6.0
1	A	2040	TRP	5.9
2	B	22	PHE	5.9
1	A	2037	TYR	5.8
2	B	54[A]	MET	5.8
1	A	2060	LEU	5.7
1	A	2059	ILE	5.6
2	B	283	LEU	5.4
1	A	1918[A]	SER	5.4
1	A	1917	VAL	5.2
2	B	101	MET	5.1
1	A	2048	TRP	4.7
2	B	313	TYR	4.7
1	A	1961	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	1996	LEU	4.5
1	A	2033	THR	4.4
1	A	2043	PHE	4.3
1	A	2017[A]	THR	4.2
2	B	53	SER	4.2
1	A	1833	GLY	4.2
1	A	1860	VAL	4.1
1	A	1875	ILE	4.1
1	A	2026	LEU	4.1
1	A	1857	VAL	4.1
2	B	317	LEU	4.1
1	A	1930	PRO	4.0
1	A	2053[A]	SER	4.0
1	A	1834	ALA	4.0
1	A	1862	VAL	4.0
1	A	2014	ALA	4.0
2	B	129	ILE	4.0
1	A	2030	PRO	4.0
1	A	2051	ILE	4.0
2	B	126	ILE	4.0
2	B	214	PHE	4.0
1	A	1840	TYR	3.9
2	B	316	LEU	3.9
1	A	2025	ILE	3.9
2	B	174	HIS	3.8
2	B	279	TYR	3.8
1	A	2010	LEU	3.7
1	A	2065	ARG	3.7
2	B	234	PHE	3.7
1	A	2066	LYS	3.7
2	B	92	ILE	3.7
1	A	1998	ARG	3.7
2	B	152	LEU	3.7
1	A	2022	ALA	3.6
2	B	257	PRO	3.6
2	B	282	ILE	3.6
2	B	69	ILE	3.5
1	A	2069	VAL	3.5
1	A	1988	LEU	3.4
1	A	2063	TYR	3.4
2	B	137	PHE	3.4
1	A	1924	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	1963	LEU	3.4
1	A	1835	MET	3.3
2	B	96	PHE	3.3
1	A	1954	ILE	3.3
2	B	297	PHE	3.3
2	B	52	SER	3.3
1	A	2052	GLU	3.3
2	B	103	VAL	3.3
2	B	106	PRO	3.3
2	B	170	SER	3.3
2	B	281	ASP	3.2
1	A	2061	THR	3.2
1	A	2012	LEU	3.2
2	B	77	LEU	3.2
1	A	1965	PHE	3.1
1	A	2032	ILE	3.1
2	B	284	LEU	3.1
2	B	1	MET	3.0
2	B	89	PHE	3.0
2	B	146	THR	3.0
2	B	305	THR	3.0
2	B	31	HIS	3.0
2	B	294	TYR	3.0
1	A	2042	SER	3.0
1	A	1839	ASN	3.0
2	B	122[A]	GLN	2.9
2	B	109	ASP	2.9
1	A	1838	SER	2.9
1	A	2049	ILE	2.9
1	A	2027	LEU	2.9
2	B	32	GLY	2.9
2	B	193	HIS	2.9
2	B	100	GLN	2.8
1	A	2035	LYS	2.8
2	B	131	ARG	2.8
2	B	301	SER	2.8
1	A	2018	ASN	2.8
1	A	2054	GLN	2.8
2	B	192	GLY	2.8
2	B	48	HIS	2.7
1	A	1901	GLY	2.7
2	B	275	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	2067	TYR	2.7
2	B	269	TYR	2.7
1	A	1851	PHE	2.7
2	B	6	PHE	2.7
2	B	189	ILE	2.7
1	A	1966	SER	2.7
1	A	1866	PHE	2.7
2	B	117	LEU	2.7
2	B	78	TYR	2.6
2	B	289	TRP	2.6
1	A	1971	ILE	2.6
1	A	2046	GLU	2.6
1	A	2062	GLU	2.6
1	A	1873	LYS	2.6
2	B	172	PRO	2.6
2	B	99	ARG	2.5
1	A	1989	PHE	2.5
2	B	107	LYS	2.5
2	B	93	VAL	2.5
2	B	20	TYR	2.5
2	B	74	LYS	2.5
2	B	108	ILE	2.5
2	B	290	ASN	2.5
2	B	120	PHE	2.5
1	A	2007	ARG	2.5
2	B	308	ILE	2.5
1	A	1995	TRP	2.5
2	B	121	VAL	2.5
2	B	124	ASP	2.5
1	A	1964	PRO	2.4
1	A	1900	ALA	2.4
2	B	191	PRO	2.4
1	A	1836	ASN	2.4
2	B	81	MET	2.4
1	A	1905	LEU	2.4
2	B	314	PRO	2.4
2	B	237	TYR	2.3
2	B	278	GLN	2.3
2	B	231	ALA	2.3
1	A	1902	GLN	2.3
1	A	2050	THR	2.3
2	B	220	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	213	ILE	2.3
2	B	295	SER	2.3
2	B	24	VAL	2.3
2	B	114	TRP	2.3
1	A	1888	HIS	2.3
1	A	2031	THR	2.3
2	B	102	MET	2.3
2	B	299	LYS	2.3
1	A	1868	GLY	2.3
1	A	1865	THR	2.3
2	B	302	LEU	2.3
1	A	2013	ARG	2.2
2	B	280	SER	2.2
1	A	2024[A]	MET	2.2
1	A	2056[A]	ARG	2.2
2	B	235	GLY	2.2
1	A	2055	MET	2.2
1	A	1874	ALA	2.2
1	A	1910	LYS	2.2
1	A	1931[A]	LYS	2.2
1	A	2068	ASN	2.2
2	B	84	ARG	2.2
2	B	190	ARG	2.2
1	A	1999	ILE	2.1
1	A	1886	THR	2.1
1	A	1959	THR	2.1
2	B	293	LEU	2.1
2	B	303	HIS	2.1
1	A	2057[A]	ASP	2.1
2	B	291	ILE	2.1
2	B	26	GLU	2.1
2	B	259	HIS	2.1
2	B	210	LEU	2.1
1	A	2005	PHE	2.0
1	A	1992	TYR	2.0
2	B	204	TYR	2.0
1	A	1855[A]	THR	2.0
2	B	288	VAL	2.0
1	A	1859	ARG	2.0
2	B	233	PHE	2.0
2	B	267	ILE	2.0
2	B	95	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	139	TYR	2.0
2	B	276	PRO	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](#)

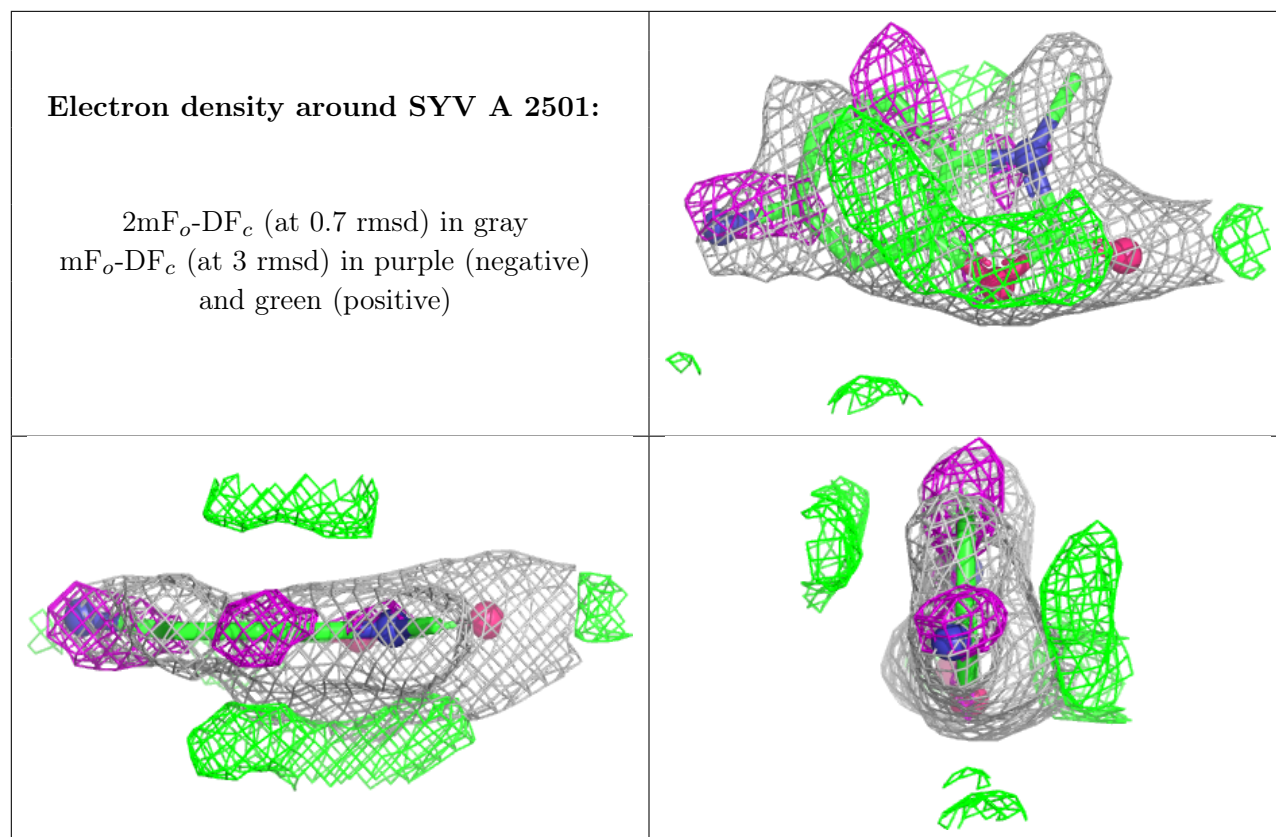
There are no oligosaccharides in this entry.

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	SYV	A	2501	12/12	0.73	0.13	20,20,20,20	12

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.