



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2021 – 11:29 AM EST

PDB ID : 5R0G
Title : PanDDA analysis group deposition – Aar2/RNaseH in complex with fragment F2X-Entry D07, 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 : 1.73 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.17.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.17.1

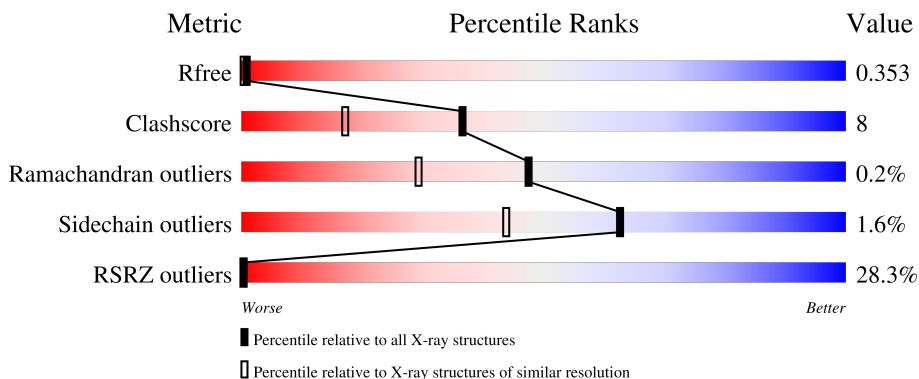
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	

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	SYJ	A	2501	-	-	X	-

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4675 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	1995	1278	334	371	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:

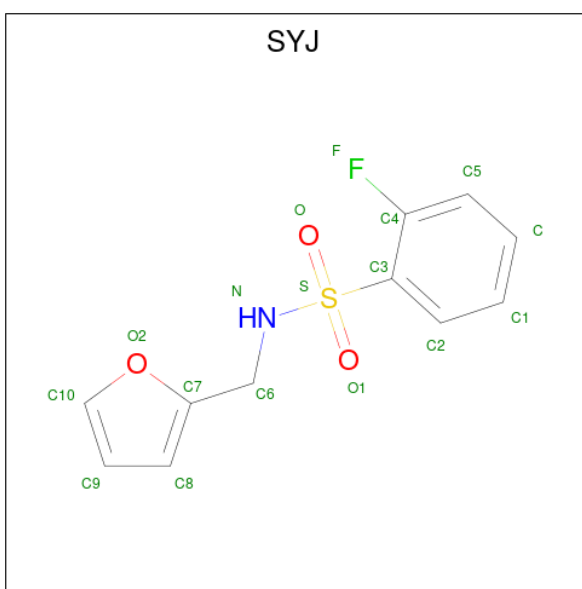
Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P32357
B	-2	ALA	-	expression tag	UNP P32357
B	-1	MET	-	expression tag	UNP P32357
B	0	ALA	-	expression tag	UNP P32357
B	166	SER	LEU	conflict	UNP P32357
B	167	SER	LYS	conflict	UNP P32357
B	170	SER	LEU	conflict	UNP P32357
B	?	-	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 2-fluoranyl- {N}-(furan-2-ylmethyl)benzenesulfonamide (three-letter code: SYJ) (formula: C₁₁H₁₀FNO₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
3	A	1	17	11	1	1	3	1	0	0

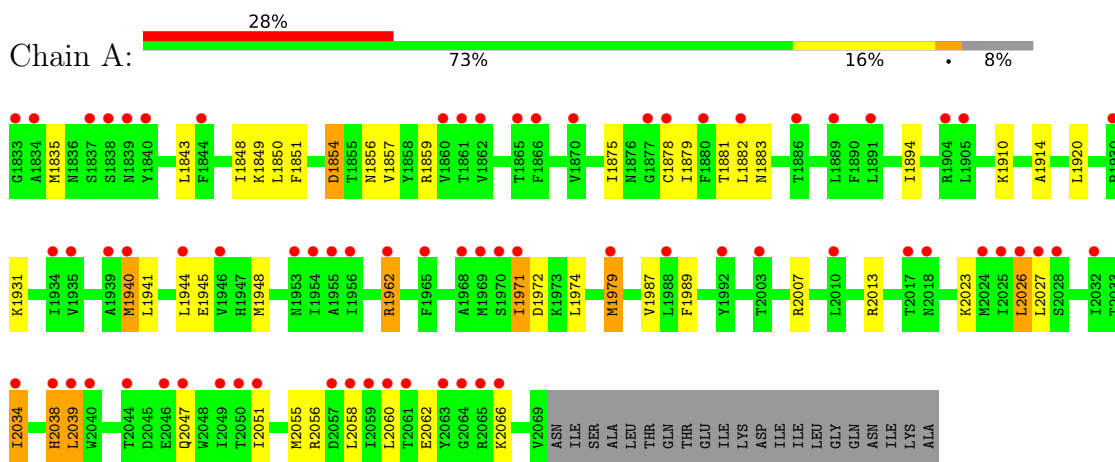
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total	O	0	0
			50	50		
4	B	33	Total	O	0	0
			33	33		

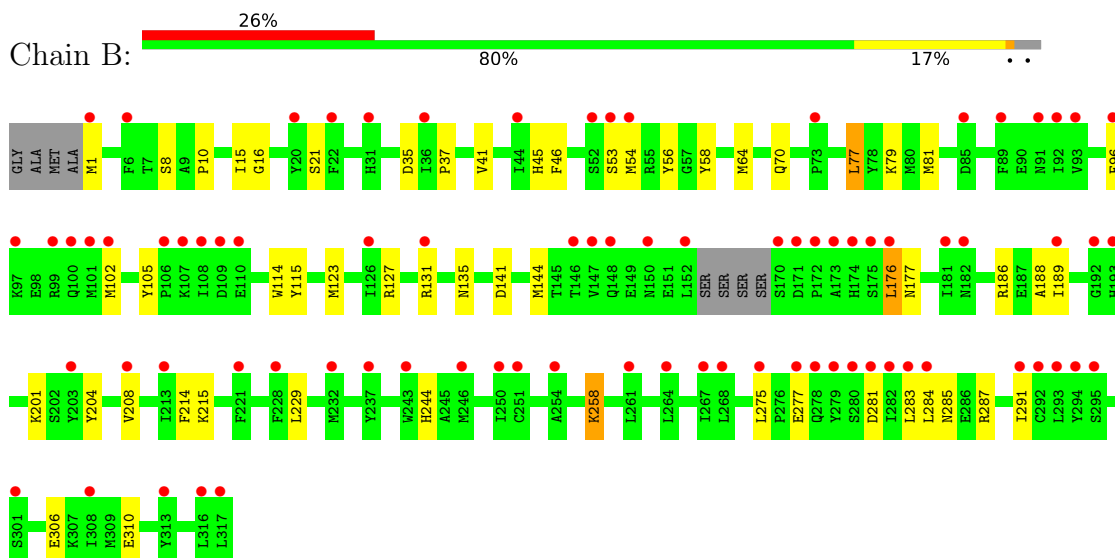
3 Residue-property plots [i](#)

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	88.20Å 82.30Å 93.11Å 90.00° 108.08° 90.00°	Depositor
Resolution (Å)	21.22 – 1.73 44.67 – 1.73	Depositor EDS
% Data completeness (in resolution range)	97.9 (21.22-1.73) 98.0 (44.67-1.73)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.98 (at 1.73Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.289 , 0.340 0.301 , 0.353	Depositor DCC
R_{free} test set	2100 reflections (3.23%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtrriage
Anisotropy	0.349	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4675	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% 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: SYJ

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	0.79	2/2042 (0.1%)	1.06	10/2765 (0.4%)
2	B	0.74	3/2651 (0.1%)	0.83	6/3581 (0.2%)
All	All	0.76	5/4693 (0.1%)	0.93	16/6346 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1972	ASP	C-O	-12.05	1.00	1.23
1	A	1883	ASN	CB-CG	6.43	1.65	1.51
2	B	114	TRP	CE3-CZ3	5.95	1.48	1.38
2	B	58	TYR	CD2-CE2	5.51	1.47	1.39
2	B	115	TYR	CD1-CE1	5.34	1.47	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1940	MET	CG-SD-CE	-16.72	73.44	100.20
2	B	284	LEU	CB-CG-CD2	8.44	125.34	111.00
1	A	2007	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	A	2007	ARG	NE-CZ-NH1	7.56	124.08	120.30
2	B	284	LEU	CB-CG-CD1	-7.18	98.80	111.00
1	A	2026	LEU	CB-CA-C	6.77	123.06	110.20
2	B	141	ASP	CB-CG-OD1	6.71	124.34	118.30
1	A	2038	HIS	CB-CA-C	-6.63	97.14	110.40
2	B	229	LEU	CB-CG-CD1	-6.61	99.76	111.00
1	A	1854	ASP	CB-CG-OD2	6.33	124.00	118.30
2	B	229	LEU	CB-CG-CD2	6.05	121.29	111.00
2	B	176	LEU	CB-CG-CD1	-5.90	100.97	111.00
1	A	1882	LEU	CB-CG-CD2	-5.84	101.08	111.00
1	A	1850	LEU	CB-CG-CD2	5.58	120.49	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1883	ASN	CB-CG-ND2	-5.12	104.41	116.70
1	A	1920	LEU	CB-CG-CD2	-5.07	102.37	111.00

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	1995	0	2020	37	0
2	B	2580	0	2450	34	0
3	A	17	0	0	8	0
4	A	50	0	0	3	0
4	B	33	0	0	3	0
All	All	4675	0	4470	72	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (72) 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:2026:LEU:HD11	1:A:2055:MET:CE	1.60	1.30
1:A:2023:LYS:HE2	3:A:2501:SYJ:C6	1.80	1.10
1:A:2026:LEU:HD11	1:A:2055:MET:HE2	1.19	1.10
1:A:2026:LEU:CD1	1:A:2055:MET:CE	2.31	1.07
1:A:2026:LEU:CD1	1:A:2055:MET:HE1	1.93	0.95
1:A:2023:LYS:CE	3:A:2501:SYJ:C6	2.55	0.84
1:A:1848:ILE:H	1:A:1931[A]:LYS:HZ2	1.37	0.70
2:B:70:GLN:HB3	2:B:81:MET:HE2	1.80	0.63
1:A:2038:HIS:CE1	4:A:2613:HOH:O	2.51	0.62
1:A:2062:GLU:O	1:A:2066:LYS:HG2	2.00	0.60
1:A:2038:HIS:HE1	4:A:2613:HOH:O	1.84	0.59
1:A:1962:ARG:O	1:A:2013:ARG:NH1	2.29	0.59
2:B:188:ALA:HA	2:B:204:TYR:CD1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1987:VAL:HG12	1:A:1989:PHE:CE1	2.39	0.58
2:B:306:GLU:O	2:B:310:GLU:HG3	2.05	0.56
3:A:2501:SYJ:C6	3:A:2501:SYJ:C2	2.83	0.56
1:A:1910:LYS:HG2	1:A:1940:MET:SD	2.46	0.55
1:A:1875:ILE:HD12	1:A:1979[B]:MET:HE3	1.88	0.55
1:A:2034:ILE:HG13	3:A:2501:SYJ:C5	2.38	0.54
1:A:1941:LEU:O	1:A:1945:GLU:HB2	2.08	0.53
2:B:186:ARG:NH1	2:B:189:ILE:O	2.41	0.52
2:B:96:PHE:HB2	2:B:102:MET:HE3	1.90	0.52
2:B:1:MET:N	4:B:402:HOH:O	2.41	0.52
1:A:1843:LEU:HA	1:A:1849:LYS:HD2	1.92	0.52
1:A:2047:GLN:O	1:A:2051:ILE:HG12	2.10	0.51
1:A:2056[B]:ARG:O	1:A:2060:LEU:HG	2.11	0.51
2:B:70:GLN:HB3	2:B:81:MET:CE	2.40	0.51
2:B:214:PHE:O	2:B:215:LYS:HB2	2.12	0.49
2:B:123:MET:O	2:B:127:ARG:HG3	2.13	0.49
1:A:1856:ASN:O	1:A:1878:CYS:N	2.37	0.48
2:B:144:MET:HE2	2:B:176:LEU:HG	1.93	0.48
1:A:2062:GLU:HB3	1:A:2066:LYS:HE3	1.95	0.48
1:A:1854:ASP:OD2	1:A:1940:MET:SD	2.71	0.48
2:B:15:ILE:O	2:B:21:SER:HA	2.12	0.48
1:A:1857:VAL:HG22	1:A:1879:ILE:HG13	1.96	0.47
1:A:1859:ARG:HH12	1:A:1979[A]:MET:CE	2.27	0.47
1:A:1971:ILE:HD12	1:A:1974:LEU:HD12	1.97	0.47
2:B:244:HIS:CD2	2:B:285:ASN:HB3	2.50	0.47
1:A:2023:LYS:CG	3:A:2501:SYJ:C8	2.93	0.47
1:A:2023:LYS:HG3	3:A:2501:SYJ:C8	2.46	0.46
2:B:77:LEU:HD21	2:B:79:LYS:HE3	1.96	0.46
1:A:2039:LEU:HD23	1:A:2039:LEU:N	2.30	0.46
2:B:37:PRO:HD3	2:B:105:TYR:CD1	2.51	0.46
2:B:204:TYR:O	2:B:208:VAL:HB	2.15	0.46
2:B:131:ARG:HH21	2:B:177[B]:ASN:ND2	2.14	0.46
1:A:2034:ILE:HG21	3:A:2501:SYJ:F	2.06	0.46
2:B:277:GLU:CD	2:B:277:GLU:H	2.20	0.45
2:B:258:LYS:HD2	2:B:258:LYS:H	1.81	0.45
1:A:1944:LEU:O	1:A:1948:MET:HG2	2.16	0.45
2:B:287:ARG:O	2:B:291:ILE:HD13	2.16	0.45
2:B:64[A]:MET:SD	2:B:123:MET:HG2	2.57	0.44
2:B:188:ALA:HB2	2:B:204:TYR:CZ	2.52	0.44
1:A:1848:ILE:H	1:A:1931[A]:LYS:NZ	2.12	0.44
1:A:2058:LEU:C	1:A:2058:LEU:HD23	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1987:VAL:CG1	1:A:1989:PHE:CE1	3.02	0.43
2:B:46:PHE:HB2	2:B:56:TYR:CZ	2.54	0.43
2:B:16:GLY:HA3	2:B:45:HIS:CE1	2.54	0.42
1:A:1851:PHE:O	1:A:1881:THR:HA	2.19	0.42
2:B:41[A]:VAL:HG12	4:B:410:HOH:O	2.19	0.42
2:B:127:ARG:NH1	2:B:135:ASN:O	2.49	0.42
2:B:275:LEU:CD2	2:B:283:LEU:HD13	2.50	0.42
2:B:275:LEU:HD22	2:B:283:LEU:HD13	2.02	0.42
2:B:281:ASP:OD1	2:B:281:ASP:N	2.42	0.42
1:A:1914:ALA:HB1	1:A:1944:LEU:HA	2.02	0.41
2:B:1:MET:HB3	2:B:35:ASP:HA	2.02	0.41
2:B:8:SER:C	2:B:10:PRO:HD3	2.41	0.41
1:A:1894:ILE:HA	4:A:2623:HOH:O	2.21	0.41
1:A:2023:LYS:HG2	3:A:2501:SYJ:C8	2.50	0.41
2:B:244:HIS:HE1	2:B:283:LEU:O	2.04	0.40
2:B:53:SER:O	2:B:54[A]:MET:HB3	2.21	0.40
2:B:96:PHE:HB2	2:B:102:MET:CE	2.52	0.40
2:B:201:LYS:NZ	4:B:403:HOH:O	2.42	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	247/258 (96%)	239 (97%)	7 (3%)	1 (0%)	34	17
2	B	306/308 (99%)	290 (95%)	16 (5%)	0	100	100
All	All	553/566 (98%)	529 (96%)	23 (4%)	1 (0%)	47	29

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1971	ILE

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	225/233 (97%)	217 (96%)	8 (4%)	35 12
2	B	287/284 (101%)	285 (99%)	2 (1%)	84 75
All	All	512/517 (99%)	502 (98%)	10 (2%)	62 33

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1835	MET
1	A	1962	ARG
1	A	1979[A]	MET
1	A	1979[B]	MET
1	A	1979[C]	MET
1	A	2027	LEU
1	A	2034	ILE
1	A	2039	LEU
2	B	77	LEU
2	B	258	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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	SYJ	A	2501	-	15,18,18	1.40	1 (6%)	19,25,25	1.70	2 (10%)

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	SYJ	A	2501	-	-	6/10/12/12	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2501	SYJ	C8-C7	-4.55	1.33	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2501	SYJ	C7-C6-N	6.45	124.48	112.23
3	A	2501	SYJ	C6-C7-C8	2.26	132.77	129.01

There are no chirality outliers.

All (6) torsion outliers are listed below:

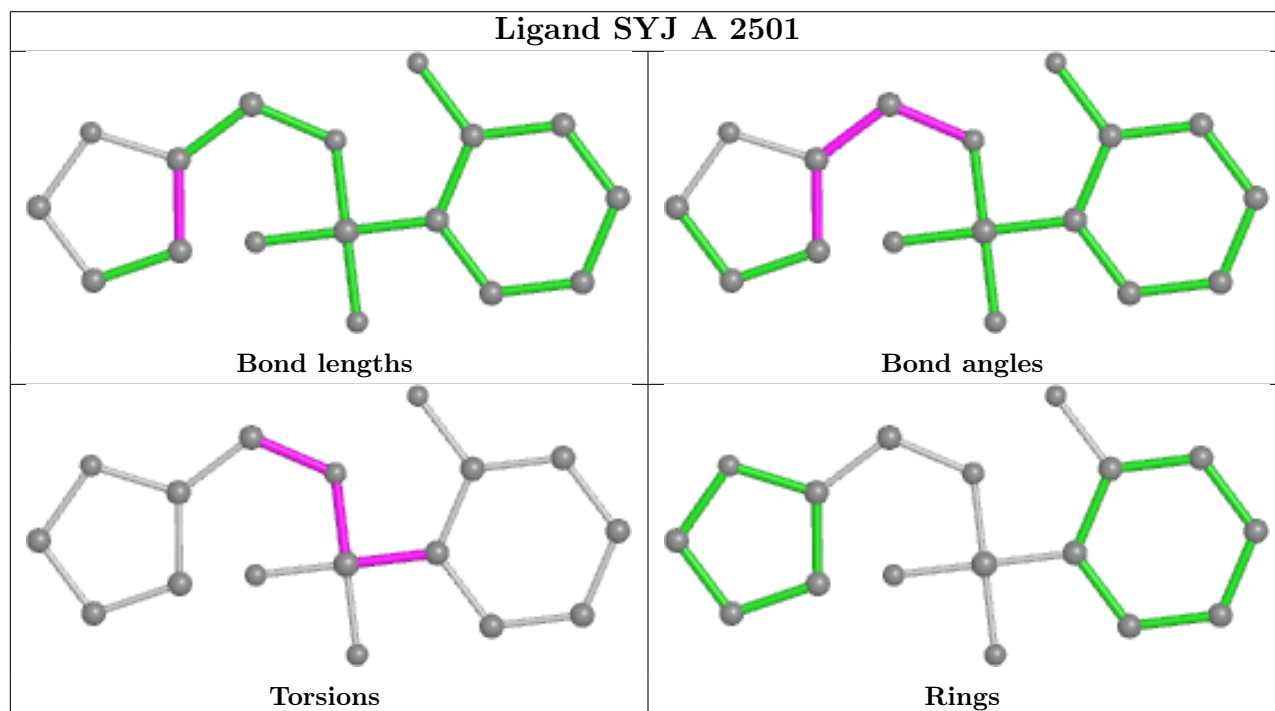
Mol	Chain	Res	Type	Atoms
3	A	2501	SYJ	C7-C6-N-S
3	A	2501	SYJ	C4-C3-S-N
3	A	2501	SYJ	C2-C3-S-N
3	A	2501	SYJ	C4-C3-S-O1
3	A	2501	SYJ	C6-N-S-O
3	A	2501	SYJ	C4-C3-S-O

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2501	SYJ	8	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	1.63	71 (29%) 0 0	42, 75, 139, 198	0
2	B	300/308 (97%)	1.61	81 (27%) 0 0	38, 78, 140, 220	0
All	All	537/566 (94%)	1.62	152 (28%) 0 0	38, 77, 139, 220	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	53	SER	11.8
2	B	52	SER	8.5
1	A	2039	LEU	7.8
1	A	1840	TYR	7.1
1	A	2063	TYR	6.8
2	B	173	ALA	6.8
1	A	1833	GLY	6.2
2	B	22	PHE	5.8
2	B	1	MET	5.8
2	B	109	ASP	5.6
2	B	313	TYR	5.2
2	B	317	LEU	5.1
2	B	281	ASP	5.1
2	B	174	HIS	5.1
1	A	1969	MET	5.1
2	B	171	ASP	4.9
1	A	1878	CYS	4.9
1	A	1979[A]	MET	4.9
1	A	1954	ILE	4.9
2	B	91	ASN	4.6
1	A	2034	ILE	4.6
2	B	277	GLU	4.5
2	B	208	VAL	4.5
2	B	89	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	2046	GLU	4.5
1	A	2059	ILE	4.5
1	A	2040	TRP	4.5
1	A	1940	MET	4.4
1	A	1934	ILE	4.4
1	A	2060	LEU	4.4
2	B	243	TRP	4.4
1	A	2064	GLY	4.4
1	A	2026	LEU	4.2
2	B	108	ILE	4.2
1	A	2027	LEU	4.2
2	B	172	PRO	4.1
1	A	1877	GLY	4.1
1	A	1838	SER	4.0
2	B	175	SER	3.9
2	B	126	ILE	3.9
2	B	73	PRO	3.9
2	B	54[A]	MET	3.9
2	B	268	LEU	3.8
2	B	264	LEU	3.8
2	B	295	SER	3.8
2	B	170	SER	3.7
2	B	92	ILE	3.7
2	B	267	ILE	3.7
2	B	100	GLN	3.7
2	B	316	LEU	3.6
2	B	96	PHE	3.6
2	B	181	ILE	3.6
1	A	2032	ILE	3.5
1	A	2066	LYS	3.5
2	B	101	MET	3.4
2	B	110	GLU	3.4
1	A	1839	ASN	3.4
1	A	2017[A]	THR	3.4
1	A	1865	THR	3.4
2	B	20	TYR	3.3
1	A	1889	LEU	3.3
1	A	2038	HIS	3.3
2	B	275	LEU	3.3
1	A	2051	ILE	3.3
2	B	189	ILE	3.3
2	B	292	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	31	HIS	3.2
1	A	1962	ARG	3.2
2	B	146	THR	3.1
1	A	2057[A]	ASP	3.1
2	B	294	TYR	3.1
1	A	1971	ILE	3.1
1	A	2058	LEU	3.1
2	B	213	ILE	3.0
1	A	1844	PHE	3.0
1	A	1970	SER	3.0
1	A	1861	THR	3.0
1	A	1860	VAL	3.0
1	A	2049	ILE	3.0
2	B	107	LYS	3.0
1	A	1837	SER	2.9
2	B	147	VAL	2.9
2	B	284	LEU	2.9
1	A	2044	THR	2.9
1	A	2010	LEU	2.9
1	A	1935	VAL	2.8
2	B	228	PHE	2.8
1	A	2050	THR	2.8
2	B	99	ARG	2.7
1	A	2028	SER	2.7
2	B	237	TYR	2.7
2	B	291	ILE	2.7
1	A	1866	PHE	2.7
1	A	2047	GLN	2.7
2	B	36	ILE	2.7
2	B	279	TYR	2.7
1	A	1870	VAL	2.7
1	A	1834	ALA	2.7
1	A	1968	ALA	2.7
1	A	1988	LEU	2.7
1	A	2018	ASN	2.7
1	A	1956	ILE	2.6
2	B	280	SER	2.6
2	B	102	MET	2.6
1	A	1880	PHE	2.6
1	A	1905	LEU	2.6
2	B	131	ARG	2.5
1	A	2024[A]	MET	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	293	LEU	2.5
2	B	193	HIS	2.5
1	A	1946	VAL	2.5
2	B	282	ILE	2.5
1	A	1862	VAL	2.5
1	A	1882	LEU	2.5
1	A	1939	ALA	2.4
2	B	85	ASP	2.4
1	A	1886	THR	2.4
2	B	278	GLN	2.4
2	B	150	ASN	2.4
2	B	246	MET	2.4
2	B	148	GLN	2.4
2	B	152	LEU	2.4
2	B	182	ASN	2.4
1	A	1930	PRO	2.3
1	A	2061	THR	2.3
2	B	301	SER	2.3
2	B	176	LEU	2.3
1	A	1955	ALA	2.2
2	B	203[A]	TYR	2.2
2	B	254	ALA	2.2
2	B	308	ILE	2.2
2	B	221	PHE	2.2
2	B	93	VAL	2.2
2	B	44[A]	ILE	2.2
1	A	1965	PHE	2.2
1	A	1944	LEU	2.2
2	B	283	LEU	2.2
2	B	261	LEU	2.1
1	A	2003	THR	2.1
2	B	251	CYS	2.1
2	B	232	MET	2.1
2	B	97	LYS	2.1
1	A	2025	ILE	2.1
2	B	250	ILE	2.1
1	A	1992	TYR	2.1
2	B	6	PHE	2.1
2	B	192	GLY	2.0
1	A	1953	ASN	2.0
2	B	106	PRO	2.0
1	A	1904	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	2065	ARG	2.0
1	A	1891	LEU	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](#)

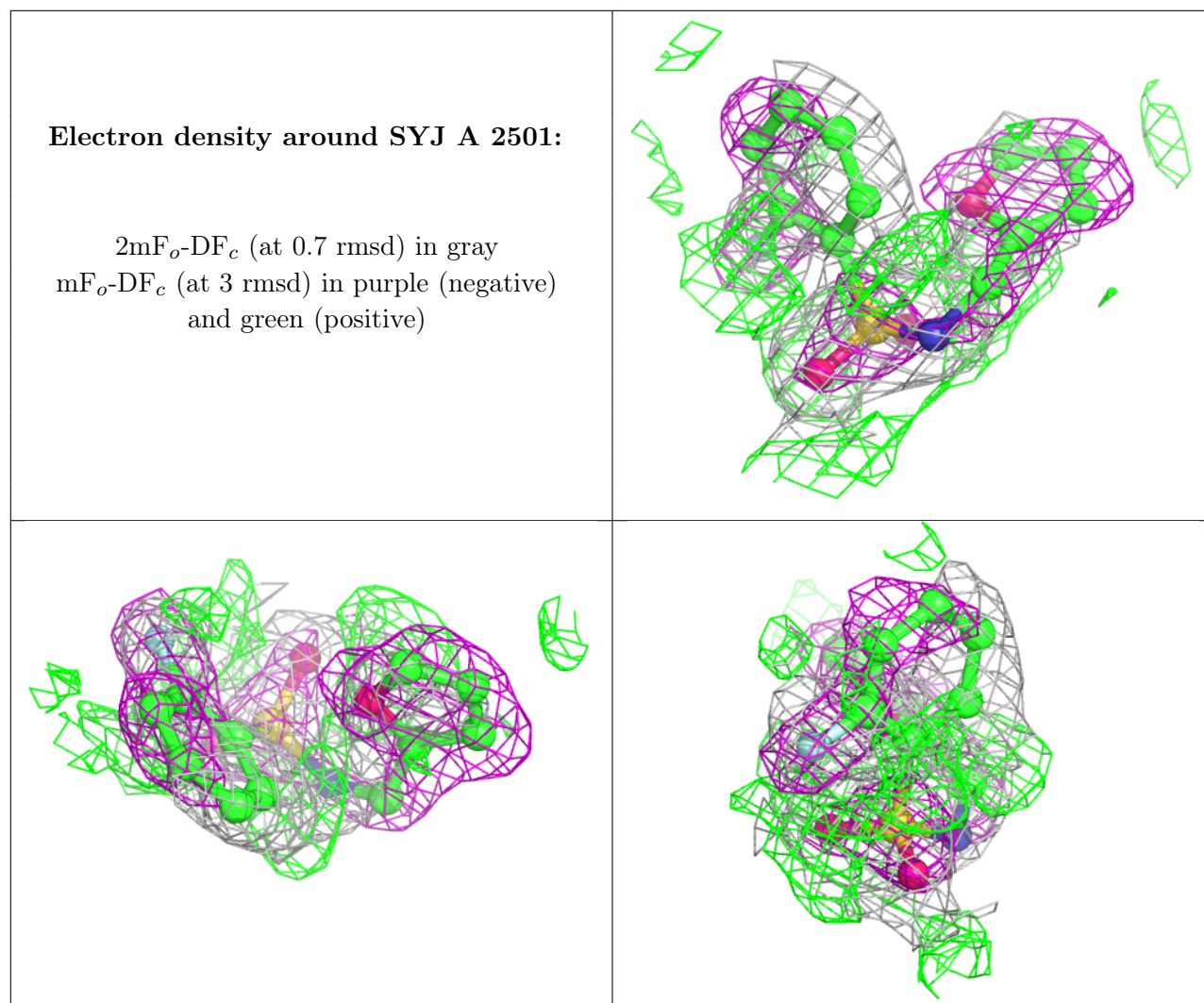
There are no monosaccharides in this entry.

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(\AA^2)	Q<0.9
3	SYJ	A	2501	17/17	0.81	0.33	20,20,20,20	17

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.