



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:43 AM UTC

PDB ID : 6W3A / pdb_00006w3a
Title : Structure of unphosphorylated IRE1 in complex with G-7658
Authors : Ferri, E.; Wang, W.; Joachim, R.; Mortara, K.
Deposited on : 2020-03-09
Resolution : 2.61 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
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

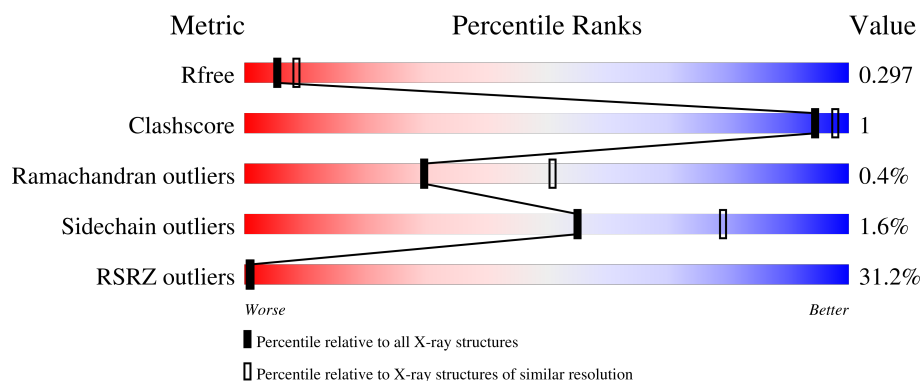
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	434	25% 80% 16%
1	B	434	28% 82% 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10953 atoms, of which 5234 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.

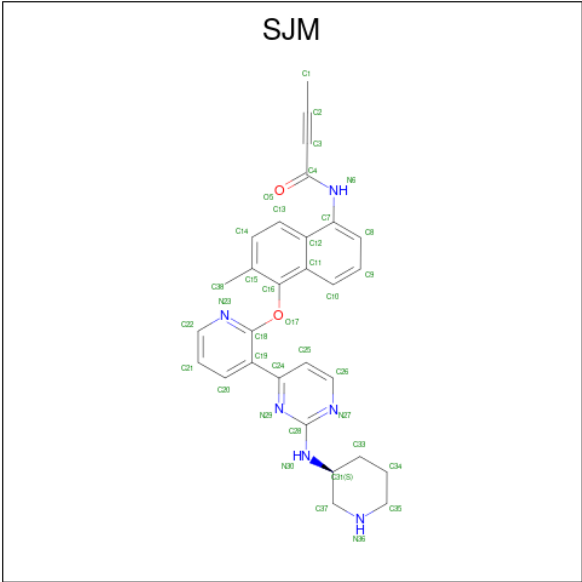
- Molecule 1 is a protein called Serine/threonine-protein kinase/endoribonuclease IRE1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	363	Total	C	H	N	O	S	0	1	0
			5417	1792	2622	486	500	17			
1	B	371	Total	C	H	N	O	S	0	0	0
			5418	1797	2610	484	510	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	978	GLY	-	expression tag	UNP O75460
A	979	ASN	-	expression tag	UNP O75460
A	980	SER	-	expression tag	UNP O75460
B	978	GLY	-	expression tag	UNP O75460
B	979	ASN	-	expression tag	UNP O75460
B	980	SER	-	expression tag	UNP O75460

- Molecule 2 is {N}-[6-methyl-5-[3-[2-[[[(3 {S})-piperidin-3-yl]amino]pyrimidin-4-yl]pyridin-2-yl]oxy-naphthalen-1-yl]but-2-ynamide (CCD ID: SJM) (formula: C₂₉H₂₈N₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			38	29	1	6	2		
2	B	1	Total	C	H	N	O	0	0
			38	29	1	6	2		

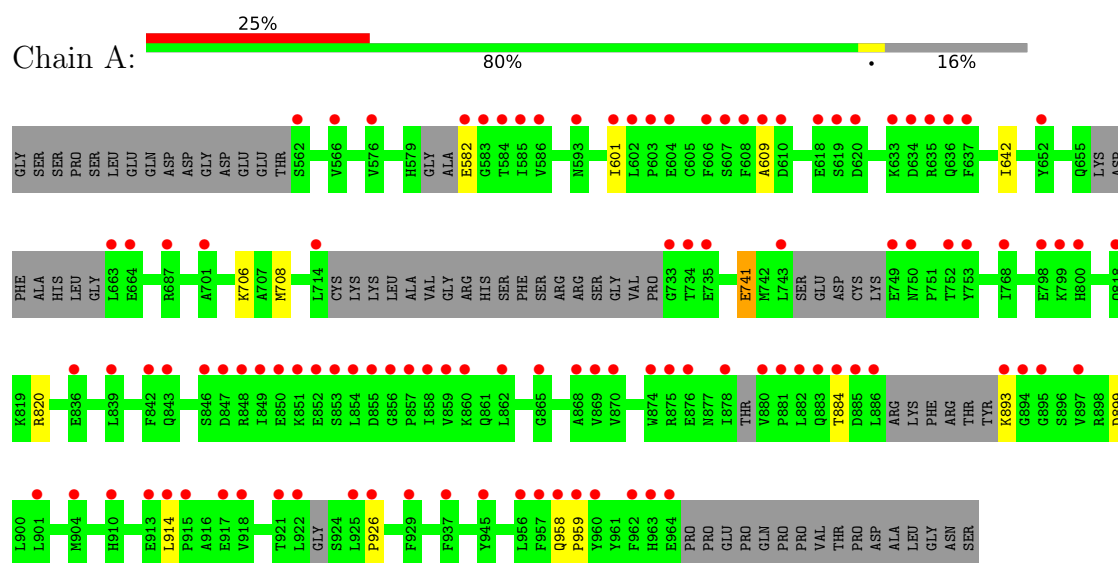
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	23	Total	O	0	0
			23	23		

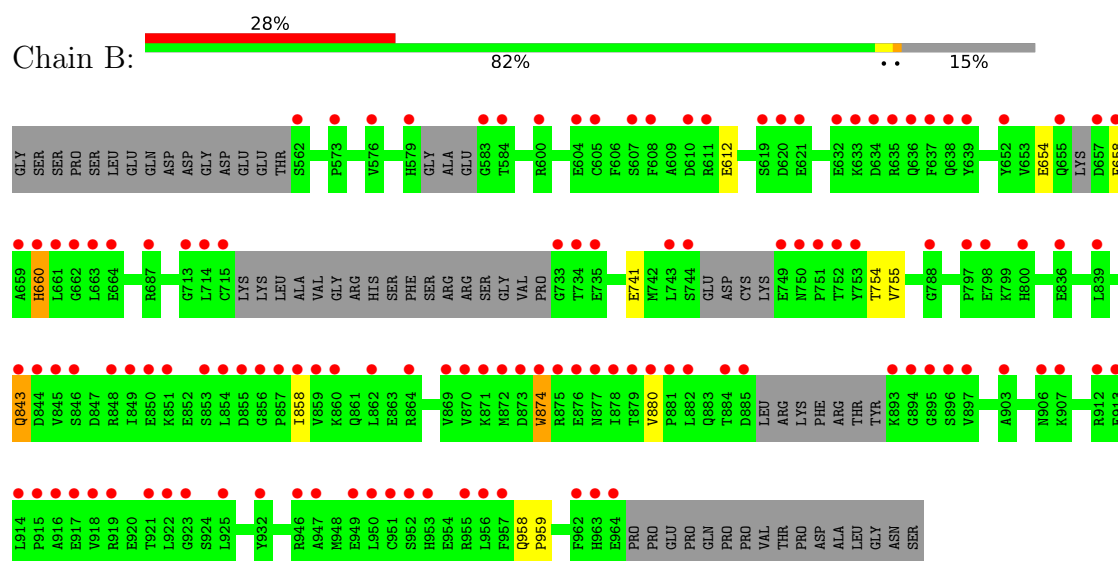
3 Residue-property plots

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: Serine/threonine-protein kinase/endoribonuclease IRE1



- Molecule 1: Serine/threonine-protein kinase/endoribonuclease IRE1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.11Å 82.39Å 164.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.12 – 2.61 58.12 – 2.61	Depositor EDS
% Data completeness (in resolution range)	77.4 (58.12-2.61) 77.4 (58.12-2.61)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.247 , 0.290 0.254 , 0.297	Depositor DCC
R_{free} test set	1332 reflections (4.08%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 71.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10953	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3916e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SJM

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	0.29	0/2864	0.61	0/3884
1	B	0.29	0/2873	0.63	1/3902 (0.0%)
All	All	0.29	0/5737	0.62	1/7786 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	880	VAL	CB-CA-C	-5.86	108.14	113.70

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	2795	2622	2621	7	0
1	B	2808	2610	2609	5	0
2	A	37	1	0	1	0
2	B	37	1	0	2	0
3	A	19	0	0	2	0
3	B	23	0	0	0	0
All	All	5719	5234	5230	14	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 1.

All (14) 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:893:LYS:N	1:A:899:ASP:OD2	2.32	0.62
1:A:582:GLU:N	3:A:1101:HOH:O	2.39	0.56
1:B:612:GLU:OE2	2:B:1001:SJM:N6	2.41	0.54
1:A:706:LYS:NZ	1:A:708:MET:SD	2.85	0.50
1:B:843:GLN:OE1	1:B:843:GLN:N	2.44	0.49
1:A:884:THR:N	3:A:1102:HOH:O	2.45	0.49
1:A:958:GLN:N	1:A:959:PRO:HD2	2.32	0.45
1:B:874:TRP:CD1	1:B:874:TRP:C	2.96	0.44
1:A:741:GLU:OE2	1:A:820:ARG:NH2	2.46	0.44
1:B:958:GLN:N	1:B:959:PRO:CD	2.82	0.43
1:B:658:PHE:O	1:B:660:HIS:N	2.52	0.42
1:A:601:ILE:CD1	1:A:609:ALA:HB2	2.50	0.42
2:B:1001:SJM:C18	2:B:1001:SJM:C38	2.98	0.42
2:A:1001:SJM:C18	2:A:1001:SJM:C38	2.98	0.41

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	348/434 (80%)	324 (93%)	23 (7%)	1 (0%)	36	58
1	B	359/434 (83%)	342 (95%)	15 (4%)	2 (1%)	21	42
All	All	707/868 (82%)	666 (94%)	38 (5%)	3 (0%)	30	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	926	PRO
1	B	654	GLU
1	B	660	HIS

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	282/384 (73%)	279 (99%)	3 (1%)	65	84
1	B	279/384 (73%)	273 (98%)	6 (2%)	45	72
All	All	561/768 (73%)	552 (98%)	9 (2%)	55	79

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	642	ILE
1	A	741	GLU
1	A	914	LEU
1	B	741	GLU
1	B	754	THR
1	B	755	VAL
1	B	843	GLN
1	B	858	ILE
1	B	874	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	683	ASN
1	A	877	ASN
1	A	939	HIS
1	A	953	HIS
1	B	939	HIS

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 ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SJM	A	1001	-	37,41,41	0.83	1 (2%)	48,56,56	2.26	12 (25%)
2	SJM	B	1001	-	37,41,41	0.82	1 (2%)	48,56,56	2.28	12 (25%)

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
2	SJM	A	1001	-	-	5/16/27/27	0/5/5/5
2	SJM	B	1001	-	-	5/16/27/27	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	SJM	C28-N30	3.65	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	SJM	C28-N30	3.50	1.38	1.34

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	SJM	C16-O17-C18	7.85	125.01	116.84
2	A	1001	SJM	C16-O17-C18	6.93	124.05	116.84
2	A	1001	SJM	C26-N27-C28	6.69	121.01	115.42
2	B	1001	SJM	C26-N27-C28	6.42	120.78	115.42
2	A	1001	SJM	C24-N29-C28	5.44	121.00	116.81
2	B	1001	SJM	C24-N29-C28	5.42	120.98	116.81
2	A	1001	SJM	N27-C28-N29	-4.80	121.78	126.42
2	B	1001	SJM	N27-C28-N29	-4.62	121.95	126.42
2	A	1001	SJM	C25-C26-N27	-4.20	118.83	123.97
2	B	1001	SJM	C25-C26-N27	-4.03	119.03	123.97
2	A	1001	SJM	C25-C24-N29	-3.21	117.74	121.97
2	B	1001	SJM	C25-C24-N29	-3.09	117.90	121.97
2	B	1001	SJM	C12-C7-N6	2.98	123.33	118.35
2	A	1001	SJM	C12-C7-N6	2.81	123.03	118.35
2	A	1001	SJM	O17-C16-C15	2.61	123.94	118.32
2	A	1001	SJM	C15-C16-C11	-2.59	119.33	122.44
2	A	1001	SJM	C26-C25-C24	2.53	119.64	117.20
2	B	1001	SJM	O17-C16-C15	2.51	123.73	118.32
2	B	1001	SJM	C15-C16-C11	-2.50	119.45	122.44
2	B	1001	SJM	C28-N30-C31	-2.50	120.44	124.32
2	B	1001	SJM	C26-C25-C24	2.23	119.35	117.20
2	B	1001	SJM	C8-C7-N6	-2.07	117.71	123.50
2	A	1001	SJM	C8-C7-N6	-2.07	117.71	123.50
2	A	1001	SJM	C28-N30-C31	-2.06	121.12	124.32

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	SJM	C15-C16-O17-C18
2	B	1001	SJM	C15-C16-O17-C18
2	A	1001	SJM	C19-C18-O17-C16
2	B	1001	SJM	C19-C18-O17-C16
2	A	1001	SJM	C8-C7-N6-C4
2	B	1001	SJM	C8-C7-N6-C4
2	A	1001	SJM	C20-C19-C24-C25
2	B	1001	SJM	C20-C19-C24-C25

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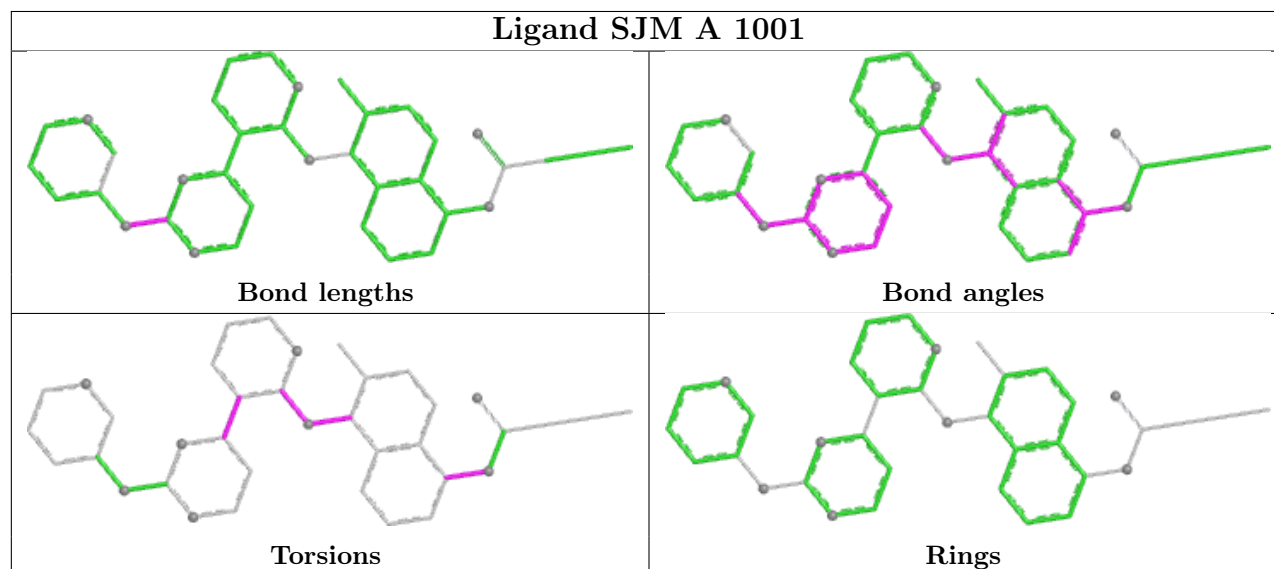
Mol	Chain	Res	Type	Atoms
2	A	1001	SJM	C20-C19-C24-N29
2	B	1001	SJM	C20-C19-C24-N29

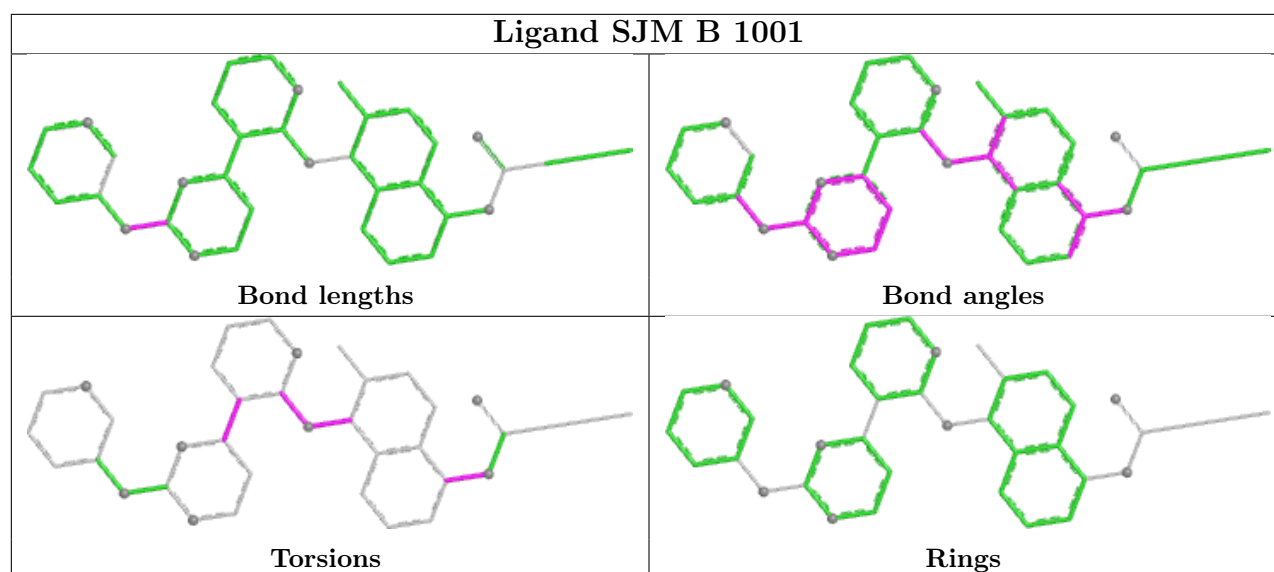
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	SJM	1	0
2	B	1001	SJM	2	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

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	363/434 (83%)	1.37	107 (29%)  	15, 61, 137, 274	1 (0%)
1	B	371/434 (85%)	1.64	122 (32%)  	16, 63, 167, 323	0
All	All	734/868 (84%)	1.51	229 (31%)  	15, 62, 155, 323	1 (0%)

All (229) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	657	ASP	12.2
1	B	658	PHE	9.1
1	B	661	LEU	9.0
1	B	659	ALA	8.7
1	A	853	SER	7.9
1	A	855	ASP	7.7
1	B	858	ILE	7.7
1	A	854	LEU	7.0
1	B	882	LEU	6.3
1	A	857	PRO	6.3
1	B	636	GLN	6.3
1	A	852	GLU	6.3
1	A	851	LYS	6.2
1	A	849	ILE	6.2
1	B	637	PHE	6.1
1	B	660	HIS	6.1
1	B	843	GLN	6.1
1	B	634	ASP	6.0
1	B	877	ASN	6.0
1	B	854	LEU	6.0
1	B	878	ILE	5.8
1	A	858	ILE	5.8
1	B	744	SER	5.8
1	B	881	PRO	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	619	SER	5.7
1	A	882	LEU	5.5
1	B	855	ASP	5.4
1	A	886	LEU	5.4
1	A	850	GLU	5.3
1	A	753[A]	TYR	5.2
1	B	879	THR	5.1
1	B	876	GLU	5.1
1	B	875	ARG	5.0
1	A	856	GLY	5.0
1	B	652	TYR	5.0
1	B	880	VAL	4.9
1	A	904	MET	4.9
1	B	633	LYS	4.9
1	A	883	GLN	4.9
1	B	849	ILE	4.8
1	B	964	GLU	4.8
1	B	638	GLN	4.8
1	B	956	LEU	4.8
1	B	885	ASP	4.8
1	B	872	MET	4.7
1	B	845	VAL	4.7
1	B	850	GLU	4.6
1	B	893	LYS	4.6
1	A	884	THR	4.6
1	A	637	PHE	4.6
1	A	917	GLU	4.5
1	A	848	ARG	4.5
1	B	635	ARG	4.4
1	B	912	ARG	4.4
1	A	957	PHE	4.4
1	A	964	GLU	4.4
1	B	913	GLU	4.4
1	A	619	SER	4.4
1	B	662	GLY	4.4
1	B	715	CYS	4.4
1	A	634	ASP	4.3
1	B	620	ASP	4.2
1	A	874	TRP	4.0
1	A	859	VAL	4.0
1	A	750	ASN	4.0
1	B	751	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	895	GLY	3.9
1	A	885	ASP	3.9
1	B	749	GLU	3.8
1	A	743	LEU	3.8
1	A	652	TYR	3.8
1	B	752	THR	3.8
1	B	871	LYS	3.7
1	A	881	PRO	3.7
1	A	922	LEU	3.7
1	B	733	GLY	3.7
1	B	860	LYS	3.7
1	A	918	VAL	3.7
1	B	862	LEU	3.7
1	B	655	GLN	3.7
1	A	607	SER	3.6
1	B	846	SER	3.6
1	B	844	ASP	3.6
1	A	663	LEU	3.6
1	B	663	LEU	3.6
1	A	584	THR	3.6
1	A	733	GLY	3.5
1	B	857	PRO	3.5
1	B	562	SER	3.5
1	B	963	HIS	3.5
1	B	921	THR	3.5
1	B	874	TRP	3.5
1	A	901	LEU	3.5
1	B	955	ARG	3.5
1	A	959	PRO	3.4
1	A	620	ASP	3.4
1	A	963	HIS	3.4
1	A	958	GLN	3.4
1	B	914	LEU	3.4
1	A	870	VAL	3.4
1	A	734	THR	3.3
1	A	913	GLU	3.3
1	A	925	LEU	3.3
1	B	714	LEU	3.3
1	B	853	SER	3.3
1	B	915	PRO	3.2
1	B	950	LEU	3.2
1	B	607	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	800	HIS	3.2
1	B	788	GLY	3.2
1	B	907	LYS	3.2
1	A	608	PHE	3.2
1	B	608	PHE	3.2
1	B	859	VAL	3.2
1	A	960	TYR	3.1
1	B	753	TYR	3.1
1	B	664	GLU	3.1
1	A	862	LEU	3.0
1	A	582	GLU	3.0
1	B	579	HIS	3.0
1	A	860	LYS	3.0
1	A	839	LEU	3.0
1	B	917	GLU	3.0
1	A	799	LYS	3.0
1	B	839	LEU	3.0
1	B	851	LYS	3.0
1	B	922	LEU	2.9
1	B	621	GLU	2.9
1	B	576	VAL	2.9
1	B	639	TYR	2.9
1	B	916	ALA	2.9
1	B	957	PHE	2.9
1	A	562	SER	2.9
1	B	952	SER	2.9
1	A	880	VAL	2.9
1	A	602	LEU	2.9
1	A	749	GLU	2.8
1	B	735	GLU	2.8
1	A	636	GLN	2.8
1	A	893	LYS	2.8
1	A	914	LEU	2.8
1	A	915	PRO	2.8
1	B	870	VAL	2.8
1	A	603	PRO	2.7
1	B	584	THR	2.7
1	B	906	ASN	2.7
1	A	846	SER	2.7
1	B	894	GLY	2.7
1	A	929	PHE	2.7
1	B	884	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	956	LEU	2.7
1	A	937	PHE	2.7
1	B	919	ARG	2.6
1	A	735	GLU	2.6
1	B	583	GLY	2.6
1	B	734	THR	2.6
1	A	714	LEU	2.6
1	B	605	CYS	2.6
1	B	632	GLU	2.6
1	B	798	GLU	2.6
1	A	962	PHE	2.6
1	B	897	VAL	2.6
1	A	847	ASP	2.6
1	B	873	ASP	2.6
1	A	664	GLU	2.6
1	A	635	ARG	2.5
1	A	576	VAL	2.5
1	A	868	ALA	2.5
1	B	903	ALA	2.5
1	B	848	ARG	2.5
1	B	750	ASN	2.5
1	A	610	ASP	2.5
1	A	618	GLU	2.5
1	B	946	ARG	2.5
1	B	797	PRO	2.5
1	A	843	GLN	2.5
1	A	604	GLU	2.4
1	B	918	VAL	2.4
1	A	585	ILE	2.4
1	A	601	ILE	2.4
1	A	633	LYS	2.4
1	A	566	VAL	2.4
1	B	600	ARG	2.4
1	B	953	HIS	2.4
1	A	818	GLN	2.4
1	A	583	GLY	2.4
1	A	945	TYR	2.3
1	B	611	ARG	2.3
1	A	869	VAL	2.3
1	B	962	PHE	2.3
1	B	951	CYS	2.3
1	B	836	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	896	SER	2.3
1	B	743	LEU	2.3
1	B	949	GLU	2.3
1	A	926	PRO	2.3
1	A	606	PHE	2.3
1	A	701	ALA	2.2
1	B	687	ARG	2.2
1	A	768	ILE	2.2
1	B	800	HIS	2.2
1	A	842	PHE	2.2
1	A	878	ILE	2.2
1	B	947	ALA	2.2
1	A	752	THR	2.2
1	A	836	GLU	2.2
1	A	876	GLU	2.1
1	B	925	LEU	2.1
1	B	932	TYR	2.1
1	A	894	GLY	2.1
1	A	910	HIS	2.1
1	A	897	VAL	2.1
1	A	875	ARG	2.1
1	B	573	PRO	2.1
1	A	865	GLY	2.1
1	B	923	GLY	2.1
1	B	869	VAL	2.1
1	A	687	ARG	2.0
1	A	609	ALA	2.0
1	A	895	GLY	2.0
1	B	713	GLY	2.0
1	B	864	ARG	2.0
1	A	798	GLU	2.0
1	B	604	GLU	2.0
1	B	610	ASP	2.0
1	A	921	THR	2.0
1	A	593	ASN	2.0
1	B	856	GLY	2.0
1	A	586	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

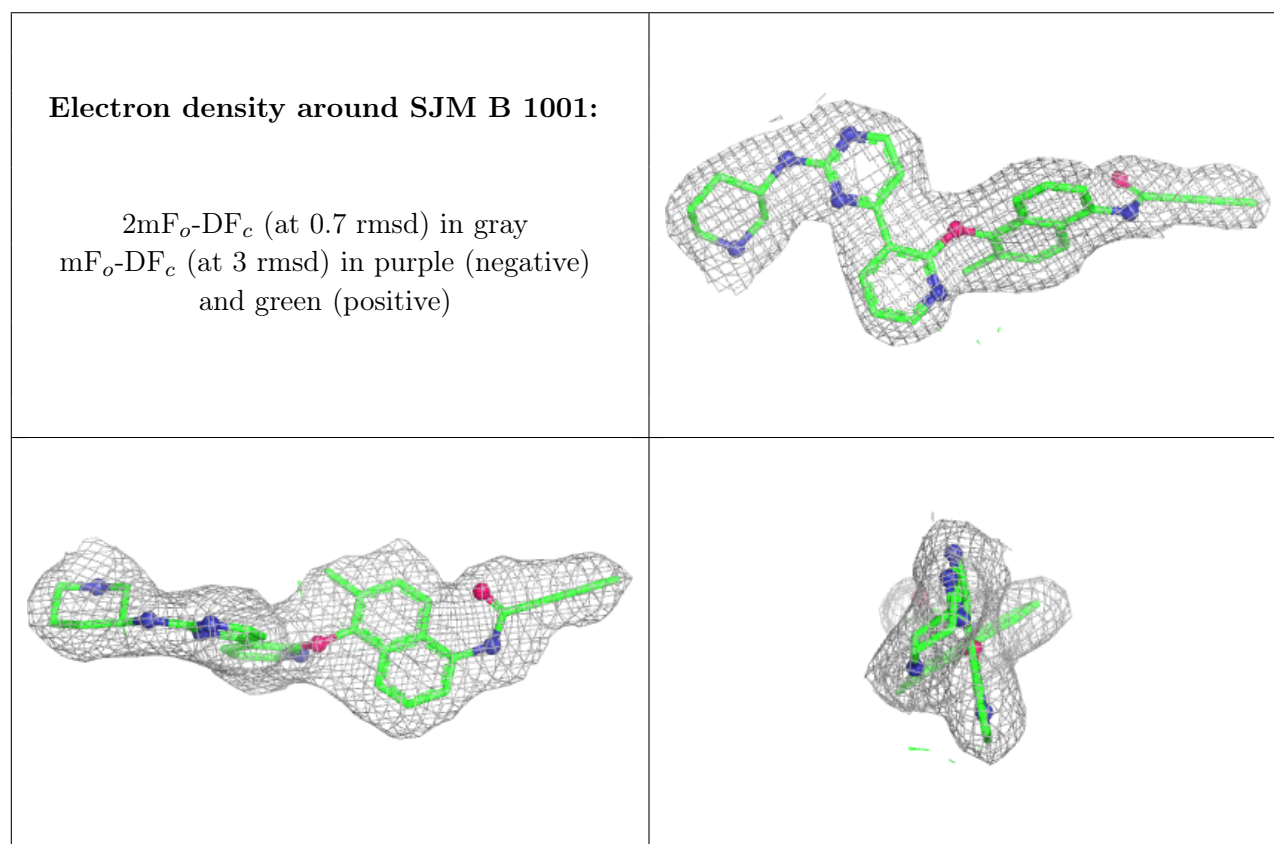
There are no oligosaccharides in this entry.

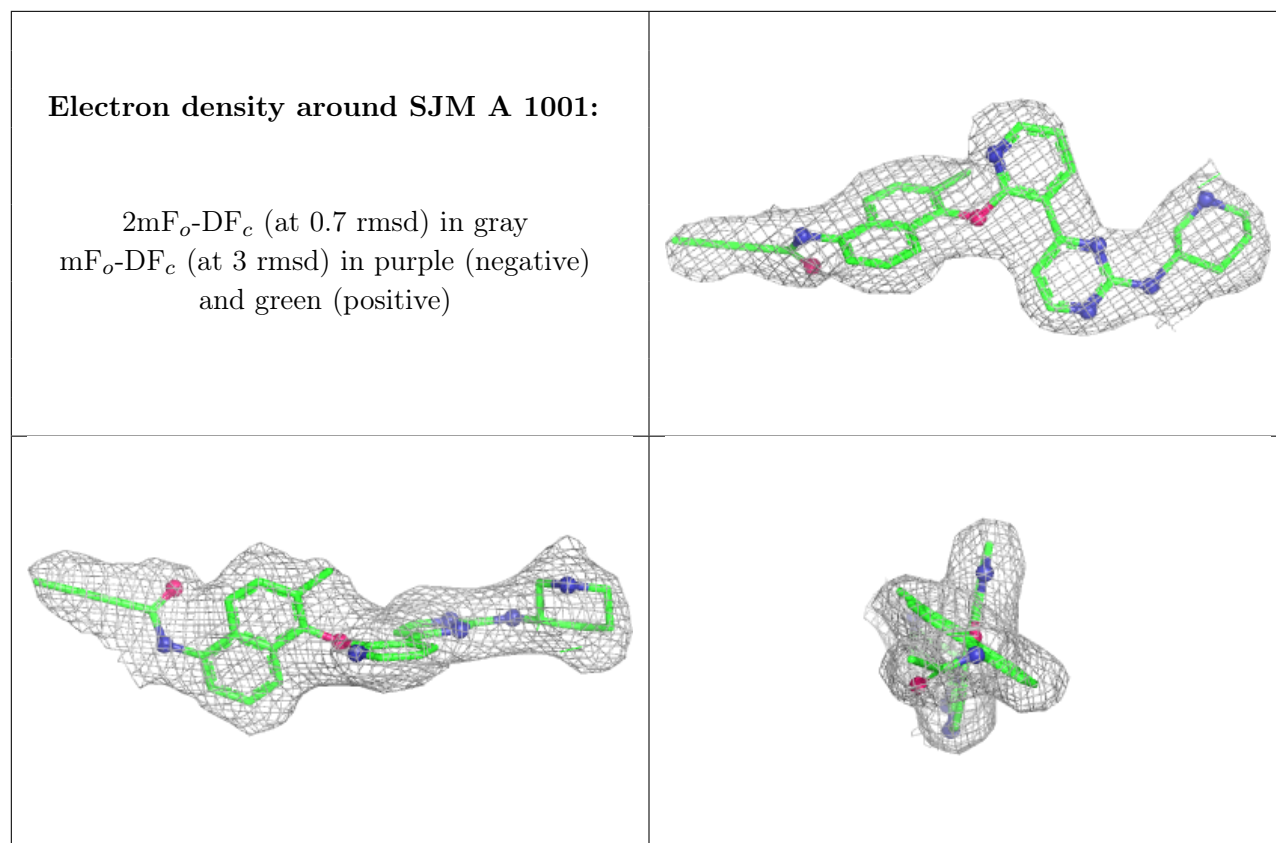
6.4 Ligands [i](#)

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
2	SJM	B	1001	37/37	0.94	0.08	15,25,41,43	0
2	SJM	A	1001	37/37	0.95	0.09	16,29,50,60	0

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.