



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 07:34 AM EDT

PDB ID : 6W3E / pdb_00006w3e
Title : Structure of phosphorylated IRE1 in complex with G-0701
Authors : Ferri, E.; Wang, W.; Joachim, R.; Mortara, K.
Deposited on : 2020-03-09
Resolution : 2.74 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

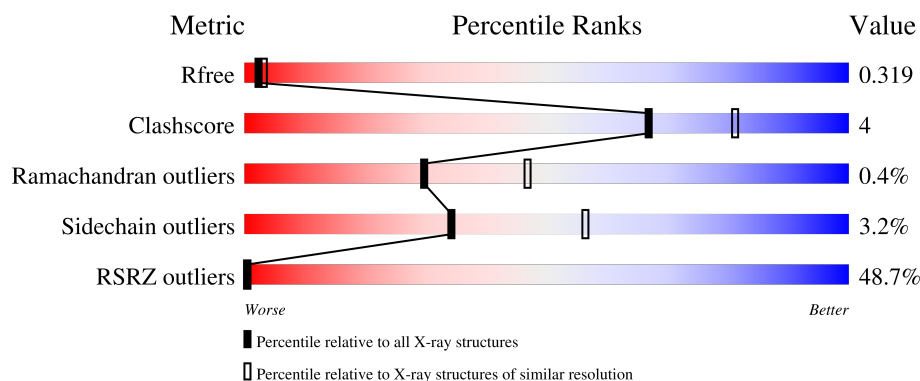
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	431	37% 77% 7% 15%
1	B	431	48% 77% 12% 10%

2 Entry composition [i](#)

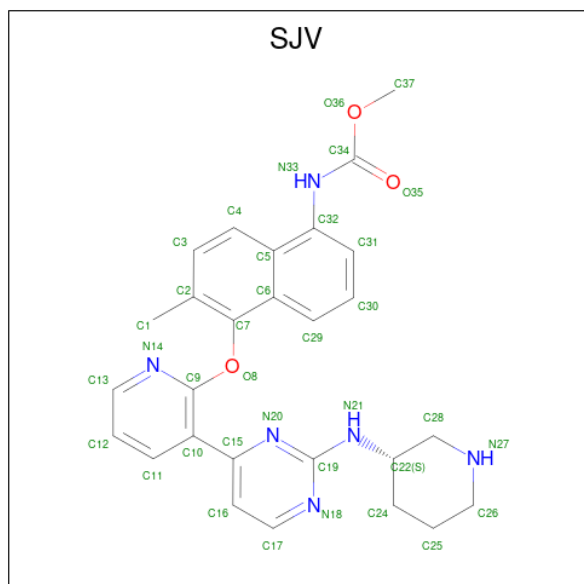
There are 2 unique types of molecules in this entry. The entry contains 11782 atoms, of which 5751 are hydrogens and 0 are deuteriums.

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	366	Total	C	H	N	O	S	0	0	0
			5686	1853	2793	504	519	17			
1	B	389	Total	C	H	N	O	P	0	0	0
			6022	1952	2956	538	556	2			

- Molecule 2 is methyl {N}-[6-methyl-5-[3-[2-[(3 {S})-piperidin-3-yl]amino]pyrimidin-4-yl]pyridin-2-yl]oxy-naphthalen-1-yl]carbamate (CCD ID: SJV) (formula: C₂₇H₂₈N₆O₃) (labeled as "Ligand of Interest" by depositor).

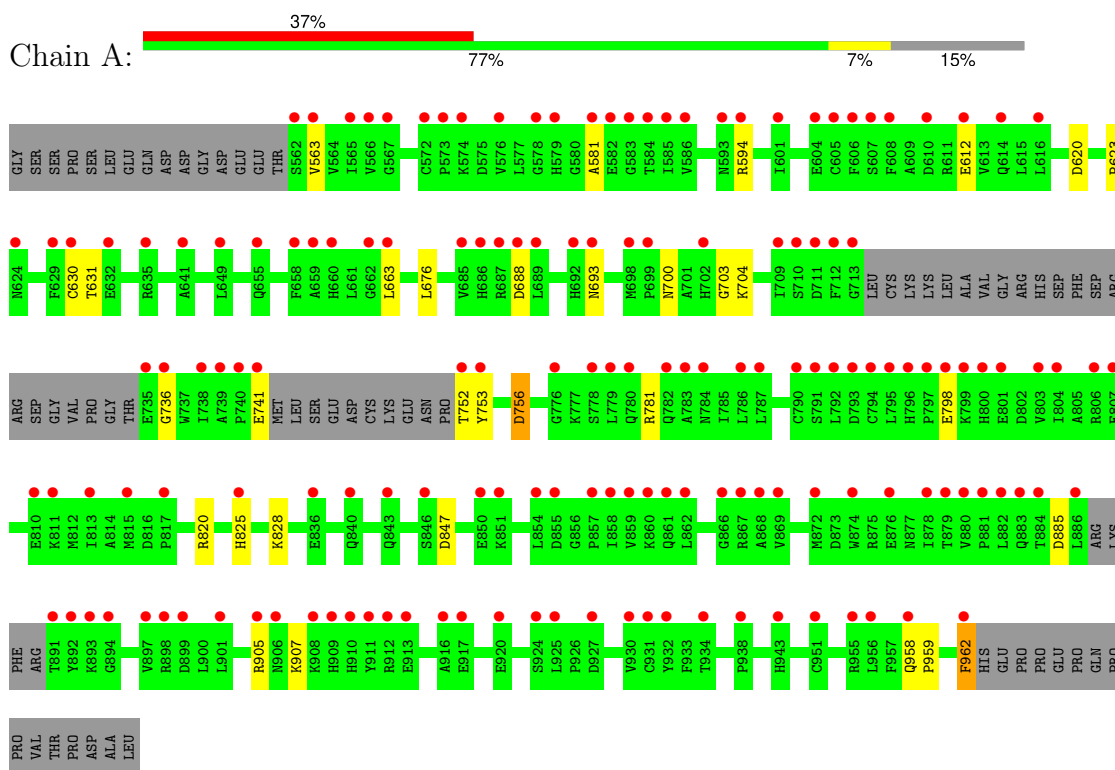


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			37	27	1	6	3		
2	B	1	Total	C	H	N	O	0	0
			37	27	1	6	3		

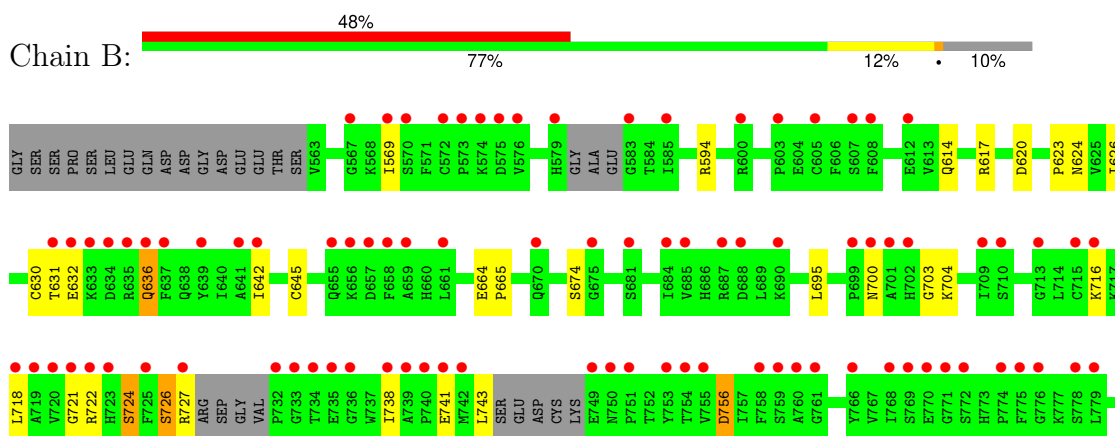
3 Residue-property plots

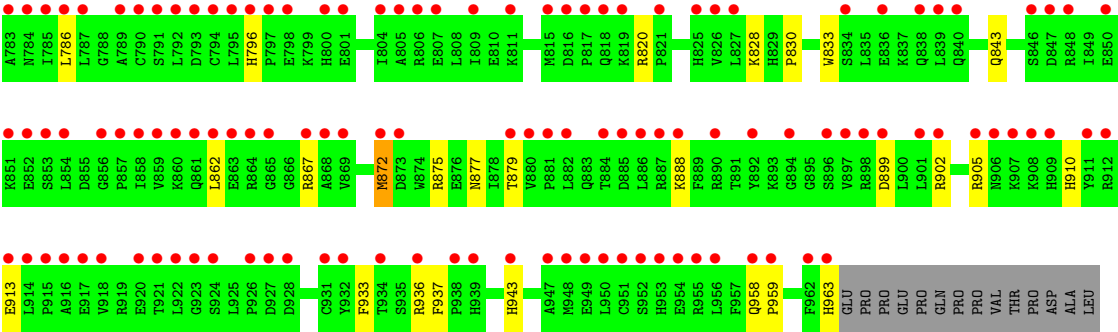
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.67Å 139.24Å 63.95Å 90.00° 114.90° 90.00°	Depositor
Resolution (Å)	55.94 – 2.74 55.94 – 2.74	Depositor EDS
% Data completeness (in resolution range)	67.4 (55.94-2.74) 67.4 (55.94-2.74)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.262 , 0.317 0.266 , 0.319	Depositor DCC
R_{free} test set	1742 reflections (6.75%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 78.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.044 for l,-k,h	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	11782	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: SEP, SJV

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	0/2964	0.72	0/4013
1	B	0.30	0/3116	0.71	0/4213
All	All	0.30	0/6080	0.72	0/8226

There are no bond length outliers.

There are no bond angle outliers.

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	2893	2793	2797	17	0
1	B	3066	2956	2956	31	0
2	A	36	1	0	0	0
2	B	36	1	0	1	0
All	All	6031	5751	5753	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 4.

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)
1:B:700:ASN:OD1	1:B:704:LYS:N	2.18	0.76
1:B:724:SEP:O1P	1:B:724:SEP:N	2.24	0.70
1:B:741:GLU:OE1	1:B:820:ARG:NH1	2.32	0.62
1:B:899:ASP:OD1	1:B:902:ARG:NH2	2.34	0.59
1:B:910:HIS:ND1	1:B:913:GLU:OE1	2.34	0.59
1:B:933:PHE:O	1:B:937:PHE:N	2.36	0.59
1:A:700:ASN:OD1	1:A:703:GLY:N	2.38	0.56
1:A:752:THR:OG1	1:A:753:TYR:N	2.37	0.56
1:B:630:CYS:SG	1:B:631:THR:N	2.78	0.56
1:A:700:ASN:OD1	1:A:704:LYS:N	2.38	0.56
1:B:624:ASN:OD1	1:B:674:SER:OG	2.24	0.55
1:B:626:ILE:HD11	1:B:642:ILE:CG2	2.37	0.54
1:A:741:GLU:OE2	1:A:820:ARG:NH1	2.41	0.54
1:B:756:ASP:N	1:B:756:ASP:OD1	2.41	0.53
1:A:623:PRO:HG3	1:B:623:PRO:HG3	1.91	0.53
1:A:847:ASP:OD2	1:A:905:ARG:NH1	2.42	0.52
1:A:630:CYS:SG	1:A:631:THR:N	2.82	0.52
1:B:877:ASN:O	1:B:936:ARG:NH1	2.42	0.52
1:A:756:ASP:N	1:A:756:ASP:OD1	2.45	0.50
1:B:645:CYS:O	2:B:1001:SJV:N21	2.44	0.49
1:A:594:ARG:NH1	1:B:620:ASP:OD1	2.46	0.49
1:B:636:GLN:OE1	1:B:636:GLN:N	2.47	0.48
1:A:688:ASP:O	1:A:693:ASN:ND2	2.46	0.47
1:B:828:LYS:HZ2	1:B:963:HIS:C	2.22	0.47
1:B:626:ILE:HD12	1:B:695:LEU:HD12	1.98	0.46
1:A:905:ARG:HH22	1:B:905:ARG:HH22	1.63	0.46
1:A:828:LYS:HD2	1:A:962:PHE:HB3	1.98	0.45
1:A:798:GLU:N	1:A:798:GLU:OE1	2.51	0.44
1:A:620:ASP:OD2	1:B:594:ARG:NH1	2.48	0.44
1:A:885:ASP:OD1	1:A:907:LYS:NZ	2.50	0.44
1:B:830:PRO:HA	1:B:833:TRP:CG	2.51	0.44
1:B:862:LEU:O	1:B:943:HIS:NE2	2.46	0.44
1:B:626:ILE:HD12	1:B:695:LEU:CD1	2.48	0.43
1:B:614:GLN:OE1	1:B:617:ARG:NH2	2.44	0.43
1:A:736:GLY:HA2	1:A:781:ARG:HB3	2.00	0.43
1:A:958:GLN:N	1:A:959:PRO:HD2	2.34	0.43
1:B:626:ILE:HD11	1:B:642:ILE:HG21	2.00	0.43
1:B:910:HIS:HD1	1:B:913:GLU:CD	2.25	0.42
1:B:664:GLU:N	1:B:665:PRO:CD	2.83	0.41
1:B:867:ARG:O	1:B:872:MET:N	2.45	0.41
1:B:700:ASN:OD1	1:B:703:GLY:N	2.53	0.41
1:B:726:SEP:OG	1:B:727:ARG:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:LEU:HB3	1:B:786:LEU:HD21	2.03	0.41
1:B:958:GLN:N	1:B:959:PRO:HD2	2.36	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	358/431 (83%)	336 (94%)	20 (6%)	2 (1%)	21	36
1	B	379/431 (88%)	352 (93%)	26 (7%)	1 (0%)	36	54
All	All	737/862 (86%)	688 (93%)	46 (6%)	3 (0%)	30	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	581	ALA
1	B	721	GLY
1	A	563	VAL

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	305/379 (80%)	299 (98%)	6 (2%)	48	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	319/379 (84%)	305 (96%)	14 (4%)	25	45
All	All	624/758 (82%)	604 (97%)	20 (3%)	34	56

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	612	GLU
1	A	663	LEU
1	A	676	LEU
1	A	756	ASP
1	A	825	HIS
1	A	962	PHE
1	B	569	ILE
1	B	632	GLU
1	B	636	GLN
1	B	716	LYS
1	B	718	LEU
1	B	722	ARG
1	B	738	ILE
1	B	756	ASP
1	B	796	HIS
1	B	843	GLN
1	B	872	MET
1	B	875	ARG
1	B	879	THR
1	B	888	LYS

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	678	HIS
1	A	909	HIS
1	B	800	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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
1	SEP	B	724	1	8,9,10	1.62	1 (12%)	7,12,14	1.58	1 (14%)
1	SEP	B	726	1	8,9,10	1.62	1 (12%)	7,12,14	1.16	1 (14%)

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
1	SEP	B	724	1	-	2/6/8/10	-
1	SEP	B	726	1	-	1/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	724	SEP	P-O1P	3.55	1.61	1.50
1	B	726	SEP	P-O1P	3.54	1.61	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	724	SEP	OG-CB-CA	3.51	111.56	108.14
1	B	726	SEP	OG-CB-CA	2.36	110.44	108.14

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	724	SEP	C-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
1	B	726	SEP	N-CA-CB-OG
1	B	724	SEP	CA-CB-OG-P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	724	SEP	1	0
1	B	726	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	SJV	B	1001	-	38,40,40	0.80	1 (2%)	50,55,55	2.33	13 (26%)
2	SJV	A	1001	-	38,40,40	0.79	1 (2%)	50,55,55	2.25	10 (20%)

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	SJV	B	1001	-	-	4/18/26/26	0/5/5/5
2	SJV	A	1001	-	-	0/18/26/26	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	SJV	C19-N21	3.56	1.38	1.34
2	A	1001	SJV	C19-N21	3.37	1.38	1.34

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	SJV	O36-C34-N33	7.89	119.40	109.19
2	A	1001	SJV	O36-C34-N33	7.39	118.75	109.19
2	B	1001	SJV	C17-N18-C19	6.60	120.93	115.42
2	A	1001	SJV	C17-N18-C19	6.52	120.87	115.42
2	A	1001	SJV	C15-N20-C19	5.22	120.83	116.81
2	B	1001	SJV	C15-N20-C19	5.05	120.70	116.81
2	B	1001	SJV	C7-O8-C9	4.77	121.80	116.84
2	A	1001	SJV	N18-C19-N20	-4.73	121.85	126.42
2	B	1001	SJV	N18-C19-N20	-4.71	121.86	126.42
2	A	1001	SJV	C7-O8-C9	4.30	121.31	116.84
2	B	1001	SJV	O36-C34-O35	-3.98	118.83	124.62
2	A	1001	SJV	C16-C17-N18	-3.92	119.16	123.97
2	B	1001	SJV	C16-C17-N18	-3.92	119.17	123.97
2	A	1001	SJV	O36-C34-O35	-3.80	119.09	124.62
2	B	1001	SJV	C16-C15-N20	-2.93	118.11	121.97
2	A	1001	SJV	C16-C15-N20	-2.81	118.26	121.97
2	B	1001	SJV	C2-C7-C6	-2.66	119.25	122.44
2	A	1001	SJV	C19-N21-C22	-2.53	120.39	124.32
2	A	1001	SJV	C2-C7-C6	-2.38	119.59	122.44
2	B	1001	SJV	N21-C19-N20	2.33	120.74	117.09
2	B	1001	SJV	C17-C16-C15	2.09	119.22	117.20
2	B	1001	SJV	O35-C34-N33	-2.05	121.77	126.12
2	B	1001	SJV	C3-C2-C7	2.02	120.97	117.75

There are no chirality outliers.

All (4) torsion outliers are listed below:

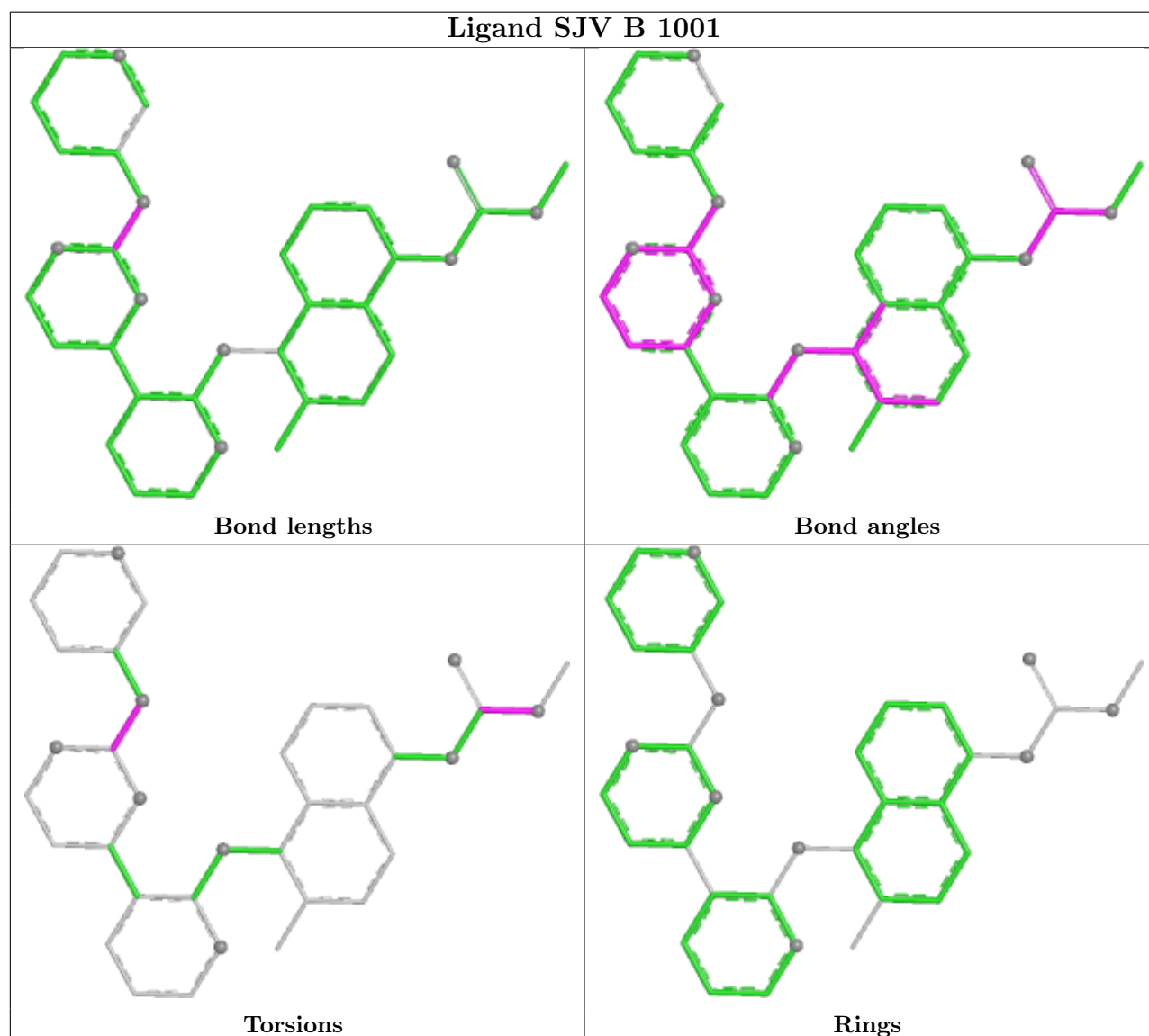
Mol	Chain	Res	Type	Atoms
2	B	1001	SJV	N33-C34-O36-C37
2	B	1001	SJV	O35-C34-O36-C37
2	B	1001	SJV	N18-C19-N21-C22
2	B	1001	SJV	N20-C19-N21-C22

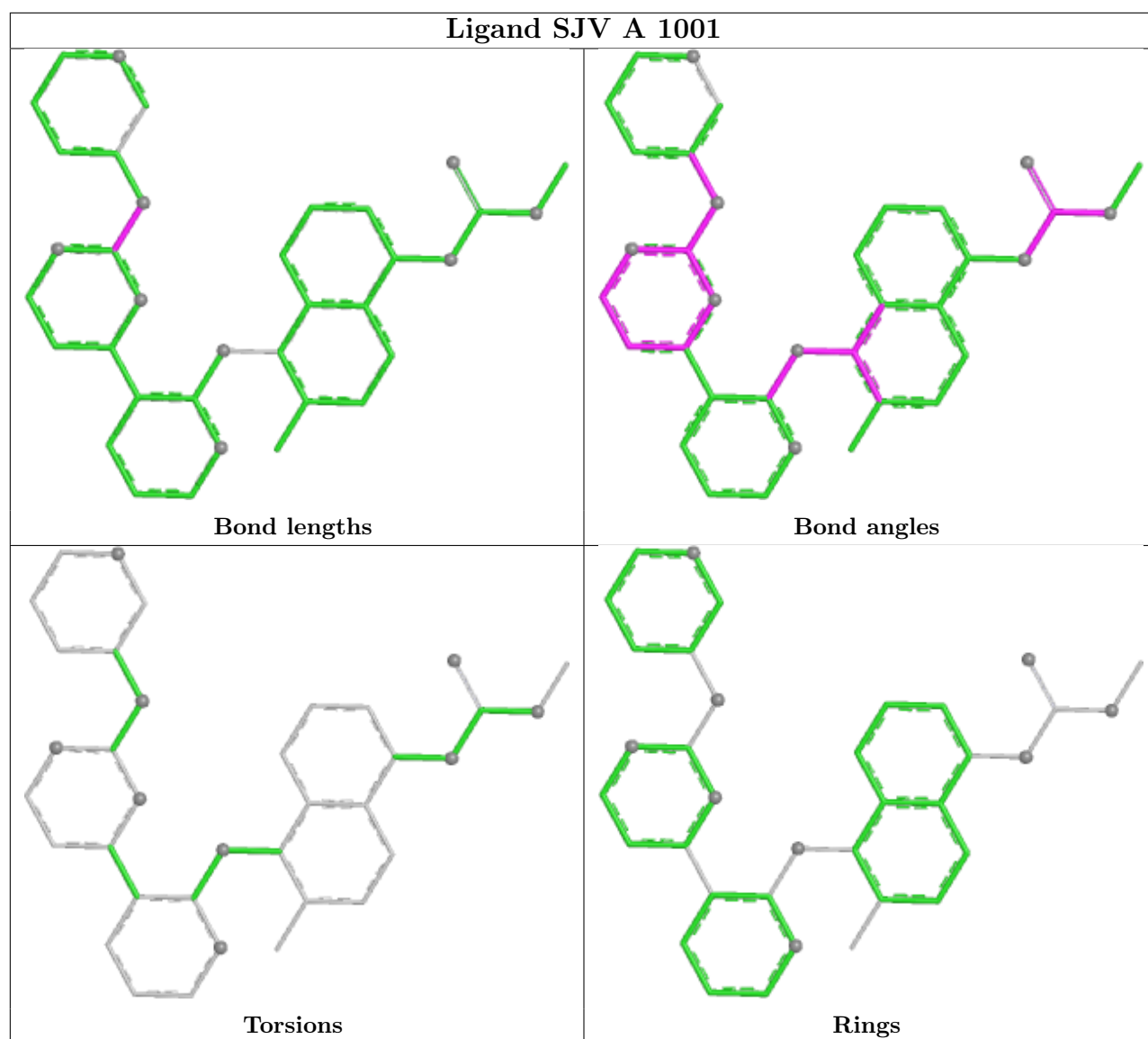
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	SJV	1	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	366/431 (84%)	1.87	158 (43%)  	39, 80, 113, 147	0
1	B	387/431 (89%)	2.24	209 (54%)  	39, 89, 126, 161	0
All	All	753/862 (87%)	2.06	367 (48%)  	39, 84, 124, 161	0

All (367) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	713	GLY	7.4
1	B	861	GLN	6.5
1	B	727	ARG	6.4
1	B	740	PRO	6.1
1	B	779	LEU	5.9
1	A	891	THR	5.8
1	A	735	GLU	5.8
1	B	954	GLU	5.7
1	B	739	ALA	5.5
1	B	579	HIS	5.5
1	B	953	HIS	5.3
1	B	787	LEU	5.2
1	B	850	GLU	5.1
1	B	886	LEU	4.9
1	B	817	PRO	4.9
1	B	636	GLN	4.9
1	B	721	GLY	4.8
1	A	815	MET	4.8
1	B	725	PHE	4.8
1	A	584	THR	4.7
1	A	906	ASN	4.7
1	B	702	HIS	4.7
1	A	797	PRO	4.7
1	A	798	GLU	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	759	SER	4.7
1	A	608	PHE	4.6
1	B	947	ALA	4.5
1	A	793	ASP	4.5
1	B	575	ASP	4.5
1	B	719	ALA	4.4
1	A	794	CYS	4.4
1	B	567	GLY	4.4
1	B	749	GLU	4.4
1	A	711	ASP	4.4
1	B	892	TYR	4.4
1	B	963	HIS	4.3
1	A	573	PRO	4.3
1	B	952	SER	4.3
1	B	770	GLU	4.3
1	B	771	GLY	4.3
1	B	905	ARG	4.2
1	B	789	ALA	4.2
1	A	778	SER	4.2
1	B	872	MET	4.2
1	B	951	CYS	4.2
1	B	723	HIS	4.1
1	B	931	CYS	4.1
1	A	894	GLY	4.1
1	A	783	ALA	4.1
1	A	880	VAL	4.1
1	A	630	CYS	4.0
1	A	563	VAL	4.0
1	B	896	SER	4.0
1	B	793	ASP	4.0
1	B	734	THR	3.9
1	A	688	ASP	3.9
1	A	807	GLU	3.9
1	B	769	SER	3.9
1	B	637	PHE	3.9
1	A	738	ILE	3.8
1	B	608	PHE	3.8
1	B	778	SER	3.8
1	A	898	ARG	3.8
1	B	657	ASP	3.8
1	B	852	GLU	3.8
1	B	573	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	732	PRO	3.8
1	B	859	VAL	3.7
1	B	938	PRO	3.7
1	B	718	LEU	3.7
1	A	632	GLU	3.7
1	A	799	LYS	3.7
1	B	853	SER	3.7
1	A	686	HIS	3.7
1	B	709	ILE	3.7
1	A	581	ALA	3.7
1	B	801	GLU	3.6
1	B	795	LEU	3.6
1	B	858	ILE	3.6
1	B	687	ARG	3.6
1	A	881	PRO	3.6
1	B	962	PHE	3.6
1	B	685	VAL	3.6
1	B	834	SER	3.6
1	B	847	ASP	3.6
1	B	736	GLY	3.6
1	B	635	ARG	3.5
1	B	720	VAL	3.5
1	A	813	ILE	3.5
1	A	662	GLY	3.5
1	B	761	GLY	3.5
1	B	846	SER	3.5
1	A	858	ILE	3.5
1	A	893	LYS	3.5
1	B	922	LEU	3.5
1	A	943	HIS	3.5
1	B	836	GLU	3.4
1	B	864	ARG	3.4
1	B	912	ARG	3.4
1	B	700	ASN	3.4
1	B	818	GLN	3.4
1	B	914	LEU	3.4
1	B	800	HIS	3.4
1	A	958	GLN	3.4
1	B	786	LEU	3.4
1	B	825	HIS	3.4
1	B	755	VAL	3.4
1	A	872	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	772	SER	3.3
1	A	582	GLU	3.3
1	A	567	GLY	3.3
1	A	687	ARG	3.3
1	A	740	PRO	3.3
1	B	797	PRO	3.3
1	B	807	GLU	3.3
1	B	902	ARG	3.3
1	A	753	TYR	3.3
1	A	692	HIS	3.3
1	A	606	PHE	3.3
1	B	924	SER	3.3
1	A	803	VAL	3.3
1	A	867	ARG	3.3
1	B	716	LYS	3.3
1	B	908	LYS	3.3
1	A	660	HIS	3.2
1	B	574	LYS	3.2
1	A	659	ALA	3.2
1	B	758	PHE	3.2
1	A	951	CYS	3.2
1	B	863	GLU	3.2
1	B	733	GLY	3.2
1	B	932	TYR	3.2
1	B	742	MET	3.2
1	A	857	PRO	3.2
1	B	655	GLN	3.2
1	B	860	LYS	3.1
1	B	754	THR	3.1
1	A	804	ILE	3.1
1	A	712	PHE	3.1
1	B	750	ASN	3.1
1	B	917	GLU	3.1
1	B	670	GLN	3.1
1	A	607	SER	3.1
1	A	897	VAL	3.1
1	B	688	ASP	3.1
1	A	879	THR	3.1
1	A	578	GLY	3.1
1	B	701	ALA	3.1
1	A	791	SER	3.1
1	A	779	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	906	ASN	3.1
1	A	614	GLN	3.1
1	B	939	HIS	3.0
1	A	806	ARG	3.0
1	A	843	GLN	3.0
1	B	633	LYS	3.0
1	B	738	ILE	3.0
1	B	865	GLY	3.0
1	A	859	VAL	3.0
1	A	574	LYS	3.0
1	A	860	LYS	3.0
1	A	585	ILE	3.0
1	A	562	SER	3.0
1	B	888	LYS	3.0
1	B	868	ALA	3.0
1	A	810	GLU	2.9
1	B	796	HIS	2.9
1	B	857	PRO	2.9
1	A	924	SER	2.9
1	B	607	SER	2.9
1	A	782	GLN	2.9
1	A	709	ILE	2.9
1	A	930	VAL	2.9
1	A	862	LEU	2.9
1	A	801	GLU	2.9
1	B	815	MET	2.9
1	B	911	TYR	2.9
1	A	868	ALA	2.9
1	A	699	PRO	2.9
1	B	585	ILE	2.9
1	B	583	GLY	2.9
1	B	839	LEU	2.9
1	A	796	HIS	2.9
1	A	836	GLU	2.8
1	B	681	SER	2.8
1	A	565	ILE	2.8
1	A	604	GLU	2.8
1	A	876	GLU	2.8
1	A	840	GLN	2.8
1	A	649	LEU	2.8
1	A	931	CYS	2.8
1	B	659	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	698	MET	2.8
1	B	907	LYS	2.8
1	B	894	GLY	2.8
1	B	898	ARG	2.8
1	B	955	ARG	2.8
1	B	798	GLU	2.8
1	B	791	SER	2.7
1	B	950	LEU	2.7
1	A	800	HIS	2.7
1	B	867	ARG	2.7
1	B	572	CYS	2.7
1	B	768	ILE	2.7
1	A	912	ARG	2.7
1	A	927	ASP	2.7
1	B	923	GLY	2.7
1	A	884	THR	2.7
1	B	885	ASP	2.7
1	A	883	GLN	2.7
1	A	850	GLU	2.7
1	B	735	GLU	2.7
1	A	869	VAL	2.7
1	B	775	PHE	2.7
1	B	921	THR	2.7
1	B	603	PRO	2.7
1	B	854	LEU	2.6
1	B	862	LEU	2.6
1	B	909	HIS	2.6
1	B	851	LYS	2.6
1	B	928	ASP	2.6
1	A	956	LEU	2.6
1	A	572	CYS	2.6
1	B	790	CYS	2.6
1	B	656	LYS	2.6
1	B	913	GLU	2.6
1	A	855	ASP	2.6
1	B	792	LEU	2.6
1	A	702	HIS	2.6
1	A	908	LYS	2.6
1	A	917	GLU	2.6
1	A	583	GLY	2.6
1	B	713	GLY	2.6
1	A	566	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	915	PRO	2.6
1	A	878	ILE	2.6
1	A	905	ARG	2.6
1	A	710	SER	2.5
1	A	874	TRP	2.5
1	B	827	LEU	2.5
1	B	936	ARG	2.5
1	B	879	THR	2.5
1	B	899	ASP	2.5
1	B	569	ILE	2.5
1	A	920	GLU	2.5
1	B	753	TYR	2.5
1	A	776	GLY	2.5
1	B	776	GLY	2.5
1	B	880	VAL	2.5
1	B	760	ALA	2.5
1	A	624	ASN	2.5
1	B	819	LYS	2.5
1	A	579	HIS	2.5
1	B	774	PRO	2.5
1	A	962	PHE	2.5
1	B	804	ILE	2.5
1	B	856	GLY	2.5
1	B	641	ALA	2.5
1	A	594	ARG	2.4
1	A	693	ASN	2.4
1	B	848	ARG	2.4
1	A	689	LEU	2.4
1	B	766	TYR	2.4
1	A	629	PHE	2.4
1	A	916	ALA	2.4
1	A	635	ARG	2.4
1	A	792	LEU	2.4
1	A	811	LYS	2.4
1	A	780	GLN	2.4
1	B	710	SER	2.4
1	B	642	ILE	2.4
1	B	884	THR	2.4
1	B	612	GLU	2.4
1	B	949	GLU	2.4
1	B	887	ARG	2.4
1	B	805	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	663	LEU	2.3
1	B	901	LEU	2.3
1	A	899	ASP	2.3
1	B	715	CYS	2.3
1	B	959	PRO	2.3
1	A	655	GLN	2.3
1	A	685	VAL	2.3
1	A	886	LEU	2.3
1	B	684	ILE	2.3
1	A	752	THR	2.3
1	A	576	VAL	2.3
1	A	741	GLU	2.3
1	B	890	ARG	2.3
1	B	576	VAL	2.3
1	B	916	ALA	2.3
1	A	910	HIS	2.3
1	B	806	ARG	2.3
1	B	821	PRO	2.3
1	B	794	CYS	2.2
1	B	784	ASN	2.2
1	B	873	ASP	2.2
1	A	795	LEU	2.2
1	B	897	VAL	2.2
1	B	956	LEU	2.2
1	A	825	HIS	2.2
1	A	851	LYS	2.2
1	B	658	PHE	2.2
1	A	909	HIS	2.2
1	B	783	ALA	2.2
1	A	605	CYS	2.2
1	A	790	CYS	2.2
1	B	600	ARG	2.2
1	B	675	GLY	2.2
1	A	911	TYR	2.2
1	B	570	SER	2.2
1	A	913	GLU	2.2
1	B	631	THR	2.2
1	A	955	ARG	2.2
1	B	605	CYS	2.2
1	A	784	ASN	2.2
1	A	892	TYR	2.2
1	B	639	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	925	LEU	2.2
1	B	809	ILE	2.2
1	B	918	VAL	2.2
1	B	741	GLU	2.1
1	B	722	ARG	2.1
1	B	926	PRO	2.1
1	A	932	TYR	2.1
1	B	838	GLN	2.1
1	A	616	LEU	2.1
1	A	882	LEU	2.1
1	A	601	ILE	2.1
1	A	658	PHE	2.1
1	B	920	GLU	2.1
1	A	938	PRO	2.1
1	B	811	LYS	2.1
1	A	901	LEU	2.1
1	A	586	VAL	2.1
1	A	641	ALA	2.1
1	B	632	GLU	2.1
1	B	690	LYS	2.1
1	B	699	PRO	2.1
1	B	881	PRO	2.1
1	B	948	MET	2.1
1	A	593	ASN	2.1
1	B	826	VAL	2.1
1	B	869	VAL	2.1
1	A	610	ASP	2.1
1	A	934	THR	2.1
1	B	934	THR	2.1
1	B	840	GLN	2.1
1	B	958	GLN	2.1
1	A	786	LEU	2.1
1	B	882	LEU	2.1
1	A	736	GLY	2.1
1	B	816	ASP	2.0
1	B	927	ASP	2.0
1	A	612	GLU	2.0
1	A	846	SER	2.0
1	B	751	PRO	2.0
1	A	787	LEU	2.0
1	A	861	GLN	2.0
1	B	661	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	943	HIS	2.0
1	A	866	GLY	2.0
1	A	739	ALA	2.0
1	B	634	ASP	2.0
1	A	817	PRO	2.0
1	A	854	LEU	2.0
1	B	785	ILE	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SEP	B	726	10/11	0.61	0.20	81,128,158,242	0
1	SEP	B	724	10/11	0.64	0.19	92,143,171,171	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

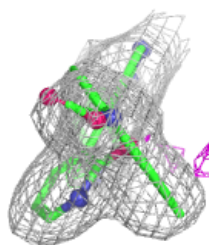
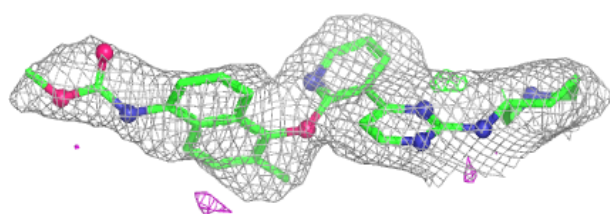
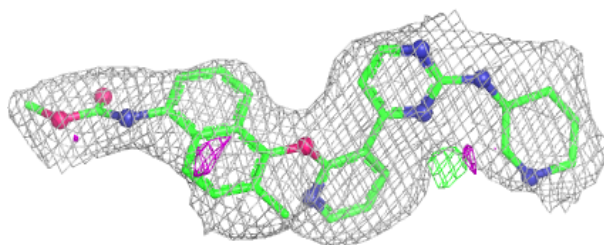
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SJV	A	1001	36/36	0.92	0.15	39,51,77,78	0
2	SJV	B	1001	36/36	0.92	0.15	44,58,104,108	0

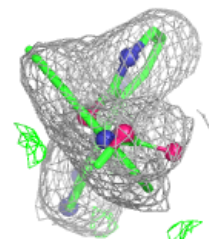
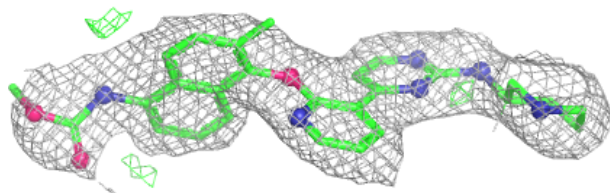
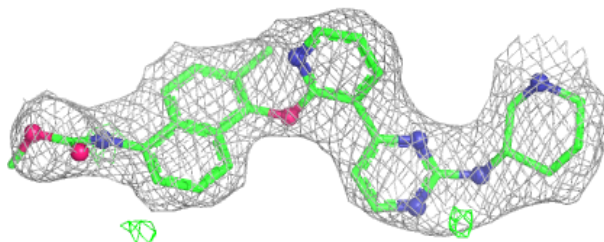
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SJV A 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around SJV B 1001:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.