



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 03:08 pm BST

PDB ID : 6EG2
Title : Crystal structure of human BRM in complex with compound 16
Authors : Zhu, X.; Kulathila, R.; Hu, T.; Xie, X.
Deposited on : 2018-08-17
Resolution : 2.98 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 : 2.11
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) : 2.11

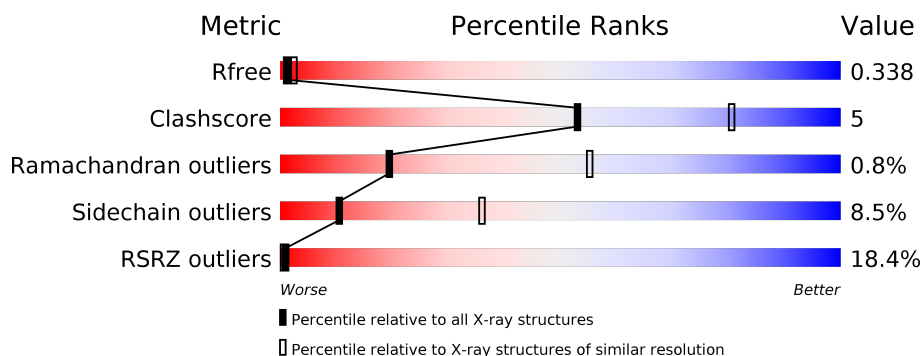
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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 on 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	621	<div> <div>18%</div> <div>78%</div> <div>20%</div> </div>

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	IPA	A	1002	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4933 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.

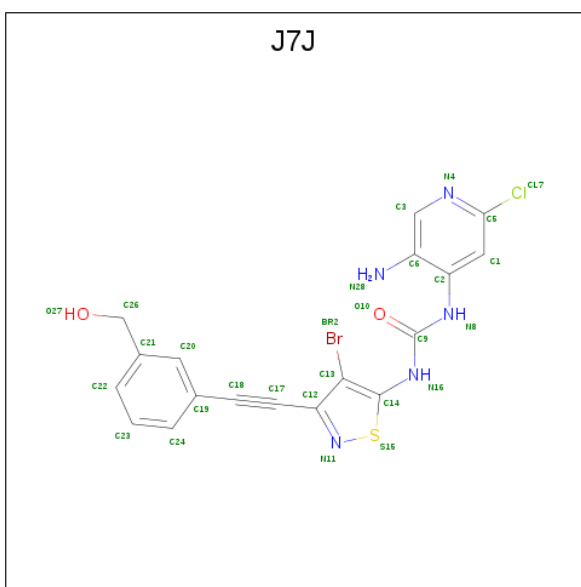
- Molecule 1 is a protein called Maltose/maltodextrin-binding periplasmic protein, Probable global transcription activator SNF2L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	619	Total	C	N	O	S	0	0	0
			4894	3163	822	894	15			

There are 9 discrepancies between the modelled and reference sequences:

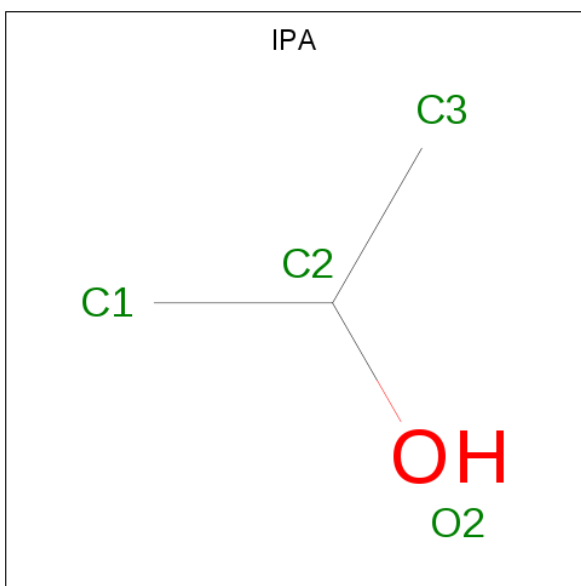
Chain	Residue	Modelled	Actual	Comment	Reference
A	416	ALA	ASP	conflict	UNP P0AEY0
A	417	ALA	LYS	conflict	UNP P0AEY0
A	506	ALA	GLU	conflict	UNP P0AEY0
A	507	ALA	ASN	conflict	UNP P0AEY0
A	573	ALA	LYS	conflict	UNP P0AEY0
A	701	ASN	-	linker	UNP P0AEY0
A	702	ALA	-	linker	UNP P0AEY0
A	703	ALA	-	linker	UNP P0AEY0
A	704	ALA	-	linker	UNP P0AEY0

- Molecule 2 is N-(5-amino-2-chloropyridin-4-yl)-N'-(4-bromo-3-{[3-(hydroxymethyl)phenyl]ethynyl}-1,2-thiazol-5-yl)urea (three-letter code: J7J) (formula: C₁₈H₁₃BrClN₅O₂S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	Br	C	Cl	N	O	S	0	0
			28	1	18	1	5	2	1		

- Molecule 3 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	3	1		
3	A	1	Total	C	O	0	0
			4	3	1		

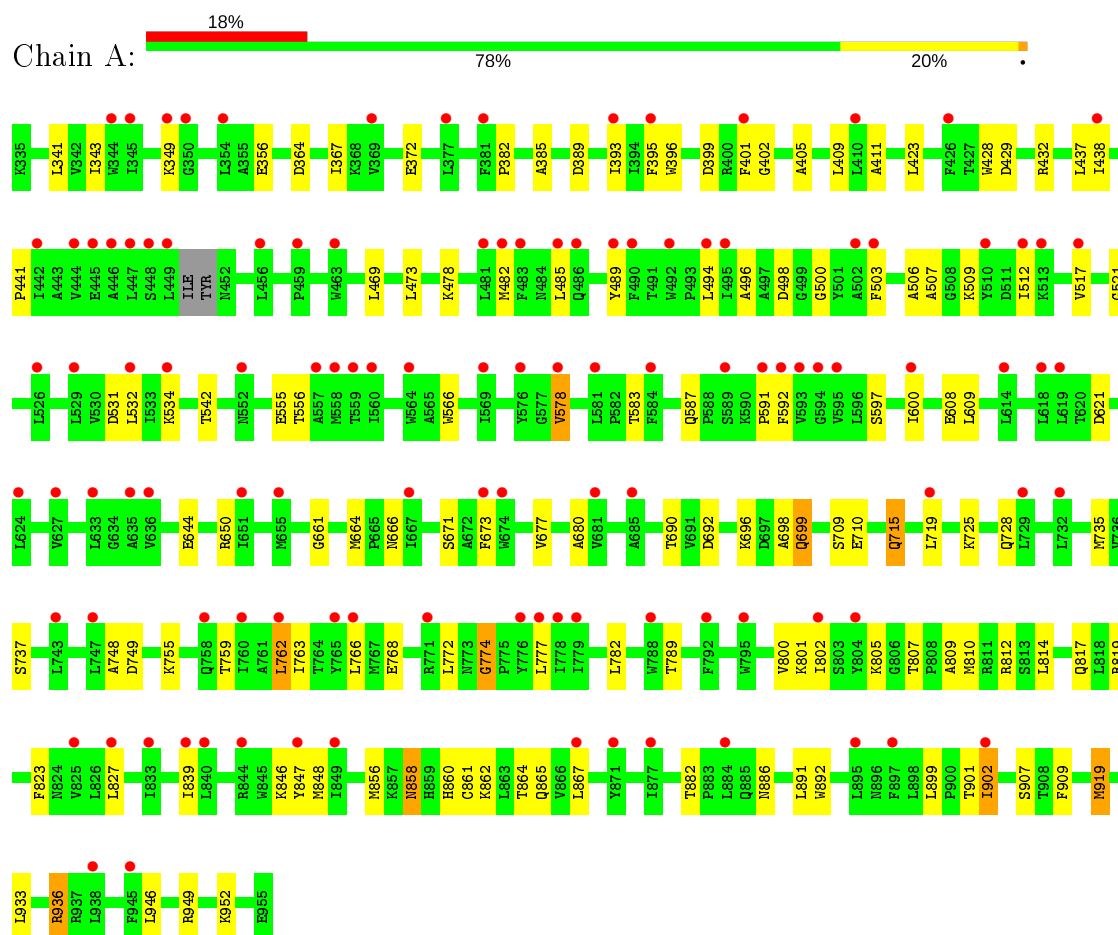
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Maltose/maltodextrin-binding periplasmic protein, Probable global transcription activator SNF2L2



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	136.79 Å 136.79 Å 120.69 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.73 – 2.98 96.73 – 2.98	Depositor EDS
% Data completeness (in resolution range)	97.5 (96.73-2.98) 97.7 (96.73-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.96 Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.251 , 0.304 0.264 , 0.338	Depositor DCC
R_{free} test set	1155 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	91.5	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 82.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4933	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: J7J, IPA

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	0.50	0/5011	0.71	0/6800

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 [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	4894	0	4947	53	0
2	A	28	0	0	1	0
3	A	8	0	16	0	0
4	A	3	0	0	0	0
All	All	4933	0	4963	53	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (53) 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:496:ALA:HA	1:A:500:GLY:O	1.85	0.77
1:A:725:LYS:H	1:A:728:GLN:HE21	1.37	0.73
1:A:498:ASP:HB3	1:A:521:GLY:HA2	1.73	0.70
1:A:367:ILE:HG21	1:A:609:LEU:HD21	1.73	0.69
1:A:899:LEU:HB3	1:A:902:ILE:HD12	1.82	0.60
1:A:735:MET:HB3	1:A:762:LEU:HD13	1.86	0.56
1:A:503:PHE:HD1	1:A:512:ILE:HA	1.72	0.55
1:A:891:LEU:HG	2:A:1001:J7J:CL7	2.45	0.54
1:A:772:LEU:HD11	1:A:846:LYS:HB3	1.90	0.54
1:A:583:THR:HA	1:A:587:GLN:O	2.08	0.53
1:A:680:ALA:HB2	1:A:698:ALA:HB2	1.91	0.53
1:A:396:TRP:HB3	1:A:401:PHE:CE1	2.44	0.52
1:A:715:GLN:HB2	1:A:719:LEU:HD23	1.91	0.52
1:A:861:CYS:HA	1:A:864:THR:HG22	1.92	0.52
1:A:506:ALA:HB3	1:A:509:LYS:O	2.09	0.52
1:A:809:ALA:HA	1:A:812:ARG:HD2	1.92	0.52
1:A:759:THR:HG22	1:A:763:ILE:HD11	1.92	0.51
1:A:578:VAL:HG22	1:A:650:ARG:HA	1.92	0.51
1:A:411:ALA:HB3	1:A:600:ILE:HG13	1.93	0.50
1:A:865:GLN:HE22	1:A:907:SER:HA	1.77	0.50
1:A:396:TRP:HB3	1:A:401:PHE:HE1	1.76	0.49
1:A:748:ALA:HB3	1:A:946:LEU:HD21	1.94	0.49
1:A:800:VAL:HG23	1:A:823:PHE:HA	1.95	0.49
1:A:485:LEU:HD12	1:A:542:THR:HB	1.95	0.49
1:A:591:PRO:HD2	1:A:661:GLY:HA3	1.94	0.48
1:A:566:TRP:CH2	1:A:650:ARG:HB3	2.48	0.48
1:A:774:GLY:HA3	1:A:846:LYS:HG3	1.96	0.48
1:A:777:LEU:HD23	1:A:848:MET:HE2	1.96	0.48
1:A:489:TYR:HE1	1:A:592:PHE:HB2	1.78	0.48
1:A:531:ASP:HA	1:A:534:LYS:HE2	1.96	0.47
1:A:402:GLY:HA3	1:A:666:ASN:HB2	1.94	0.47
1:A:673:PHE:O	1:A:677:VAL:HG23	2.14	0.47
1:A:933:LEU:HA	1:A:936:ARG:HB2	1.96	0.47
1:A:802:ILE:HG23	1:A:814:LEU:HD22	1.97	0.46
1:A:860:HIS:CE1	1:A:862:LYS:HG3	2.51	0.46
1:A:858:ASN:HD22	1:A:858:ASN:H	1.64	0.45
1:A:503:PHE:CD1	1:A:512:ILE:HA	2.52	0.45
1:A:807:THR:OG1	1:A:810:MET:HG3	2.16	0.45
1:A:749:ASP:HB2	1:A:755:LYS:HD2	1.99	0.45
1:A:385:ALA:HB1	1:A:409:LEU:HB3	1.98	0.45
1:A:382:PRO:HA	1:A:409:LEU:HD13	2.00	0.44
1:A:395:PHE:HA	1:A:597:SER:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:ASP:O	1:A:696:LYS:HB2	2.17	0.43
1:A:423:LEU:HD12	1:A:428:TRP:CZ2	2.54	0.43
1:A:343:ILE:HG12	1:A:393:ILE:HB	2.00	0.42
1:A:341:LEU:HG	1:A:609:LEU:HD23	2.00	0.42
1:A:478:LYS:HD2	1:A:555:GLU:HA	2.01	0.42
1:A:517:VAL:HB	1:A:699:GLN:HB2	2.01	0.41
1:A:405:ALA:HB2	1:A:438:ILE:HD13	2.01	0.41
1:A:482:MET:HB2	1:A:556:THR:HG21	2.02	0.41
1:A:429:ASP:HA	1:A:432:ARG:NH2	2.36	0.41
1:A:892:TRP:CG	1:A:909:PHE:HB3	2.55	0.41
1:A:428:TRP:CZ3	1:A:441:PRO:HD3	2.56	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	615/621 (99%)	554 (90%)	56 (9%)	5 (1%)	19	55

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	507	ALA
1	A	919	MET
1	A	902	ILE
1	A	774	GLY
1	A	715	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	515/517 (100%)	471 (92%)	44 (8%)	10	36

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	349	LYS
1	A	356	GLU
1	A	364	ASP
1	A	372	GLU
1	A	389	ASP
1	A	399	ASP
1	A	437	LEU
1	A	469	LEU
1	A	473	LEU
1	A	494	LEU
1	A	532	LEU
1	A	578	VAL
1	A	608	GLU
1	A	621	ASP
1	A	644	GLU
1	A	664	MET
1	A	671	SER
1	A	690	THR
1	A	699	GLN
1	A	709	SER
1	A	710	GLU
1	A	737	SER
1	A	762	LEU
1	A	766	LEU
1	A	768	GLU
1	A	782	LEU
1	A	789	THR
1	A	801	LYS
1	A	805	LYS
1	A	817	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	819	ARG
1	A	827	LEU
1	A	839	ILE
1	A	847	TYR
1	A	856	MET
1	A	858	ASN
1	A	867	LEU
1	A	882	THR
1	A	886	ASN
1	A	901	THR
1	A	919	MET
1	A	936	ARG
1	A	949	ARG
1	A	952	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	HIS
1	A	728	GLN
1	A	740	ASN
1	A	824	ASN
1	A	858	ASN
1	A	865	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

3 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	J7J	A	1001	-	25,30,30	1.06	2 (8%)	29,41,41	2.21	7 (24%)
3	IPA	A	1003	-	3,3,3	0.54	0	3,3,3	0.26	0
3	IPA	A	1002	-	3,3,3	0.52	0	3,3,3	0.21	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
2	J7J	A	1001	-	-	0/10/15/15	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	J7J	C12-C13	3.43	1.46	1.39
2	A	1001	J7J	C12-N11	-2.31	1.26	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	J7J	C12-N11-S15	5.62	113.03	104.84
2	A	1001	J7J	N16-C9-N8	4.74	120.76	112.49
2	A	1001	J7J	BR2-C13-C12	-4.48	119.55	126.81
2	A	1001	J7J	C1-C5-N4	-4.11	121.86	125.60
2	A	1001	J7J	C3-N4-C5	4.10	121.58	116.35
2	A	1001	J7J	O10-C9-N8	-3.31	118.03	123.62
2	A	1001	J7J	C19-C20-C21	-2.07	118.19	120.29

There are no chirality outliers.

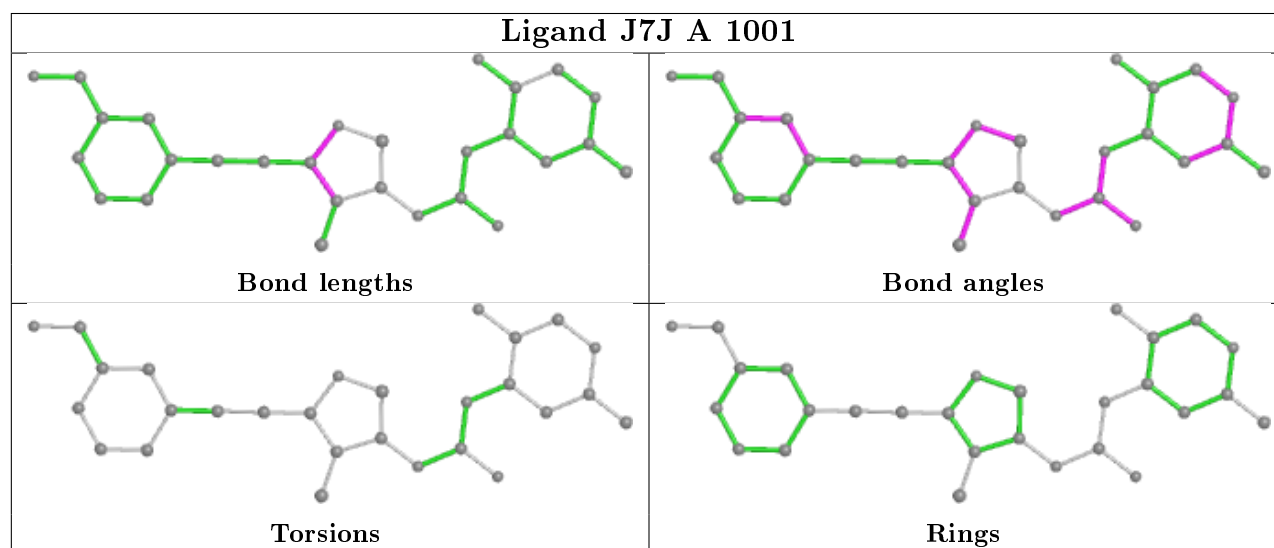
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	J7J	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	619/621 (99%)	0.98	114 (18%) 1 0	50, 101, 144, 162	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	447	LEU	7.7
1	A	446	ALA	6.4
1	A	529	LEU	5.8
1	A	619	LEU	5.1
1	A	560	ILE	5.0
1	A	448	SER	5.0
1	A	589	SER	5.0
1	A	581	LEU	4.9
1	A	395	PHE	4.7
1	A	552	ASN	4.6
1	A	494	LEU	4.6
1	A	593	VAL	4.6
1	A	847	TYR	4.4
1	A	485	LEU	4.3
1	A	578	VAL	4.2
1	A	489	TYR	4.2
1	A	674	TRP	4.1
1	A	482	MET	4.1
1	A	840	LEU	3.9
1	A	345	ILE	3.9
1	A	490	PHE	3.9
1	A	673	PHE	3.8
1	A	381	PHE	3.8
1	A	788	TRP	3.7
1	A	442	ILE	3.7
1	A	776	TYR	3.6
1	A	778	ILE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	758	GLN	3.5
1	A	685	ALA	3.5
1	A	681	VAL	3.4
1	A	463	TRP	3.4
1	A	833	ILE	3.3
1	A	719	LEU	3.3
1	A	557	ALA	3.3
1	A	377	LEU	3.3
1	A	559	THR	3.2
1	A	495	ILE	3.2
1	A	592	PHE	3.2
1	A	456	LEU	3.2
1	A	526	LEU	3.1
1	A	827	LEU	3.1
1	A	483	PHE	3.1
1	A	792	PHE	3.0
1	A	897	PHE	3.0
1	A	401	PHE	3.0
1	A	503	PHE	3.0
1	A	760	ILE	2.9
1	A	354	LEU	2.9
1	A	777	LEU	2.9
1	A	584	PHE	2.9
1	A	779	ILE	2.9
1	A	871	TYR	2.9
1	A	633	LEU	2.9
1	A	802	ILE	2.8
1	A	624	LEU	2.8
1	A	534	LYS	2.8
1	A	564	TRP	2.8
1	A	771	ARG	2.8
1	A	349	LYS	2.7
1	A	600	ILE	2.7
1	A	595	VAL	2.7
1	A	618	LEU	2.7
1	A	350	GLY	2.7
1	A	614	LEU	2.7
1	A	502	ALA	2.7
1	A	438	ILE	2.6
1	A	825	VAL	2.6
1	A	945	PHE	2.6
1	A	627	VAL	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	594	GLY	2.5
1	A	636	VAL	2.5
1	A	369	VAL	2.5
1	A	762	LEU	2.5
1	A	839	ILE	2.5
1	A	747	LEU	2.5
1	A	804	TYR	2.5
1	A	510	TYR	2.5
1	A	444	VAL	2.5
1	A	532	LEU	2.5
1	A	844	ARG	2.4
1	A	445	GLU	2.4
1	A	729	LEU	2.4
1	A	877	ILE	2.4
1	A	344	TRP	2.4
1	A	576	TYR	2.4
1	A	732	LEU	2.4
1	A	481	LEU	2.4
1	A	884	LEU	2.4
1	A	635	ALA	2.4
1	A	449	LEU	2.3
1	A	849	ILE	2.3
1	A	867	LEU	2.3
1	A	902	ILE	2.3
1	A	393	ILE	2.3
1	A	410	LEU	2.3
1	A	895	LEU	2.3
1	A	743	LEU	2.2
1	A	492	TRP	2.2
1	A	938	LEU	2.2
1	A	512	ILE	2.2
1	A	558	MET	2.1
1	A	667	ILE	2.1
1	A	591	PRO	2.1
1	A	517	VAL	2.1
1	A	651	ILE	2.1
1	A	569	ILE	2.1
1	A	655	MET	2.1
1	A	513	LYS	2.1
1	A	426	PHE	2.1
1	A	766	LEU	2.1
1	A	459	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	795	TRP	2.0
1	A	765	TYR	2.0
1	A	486	GLN	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](#)

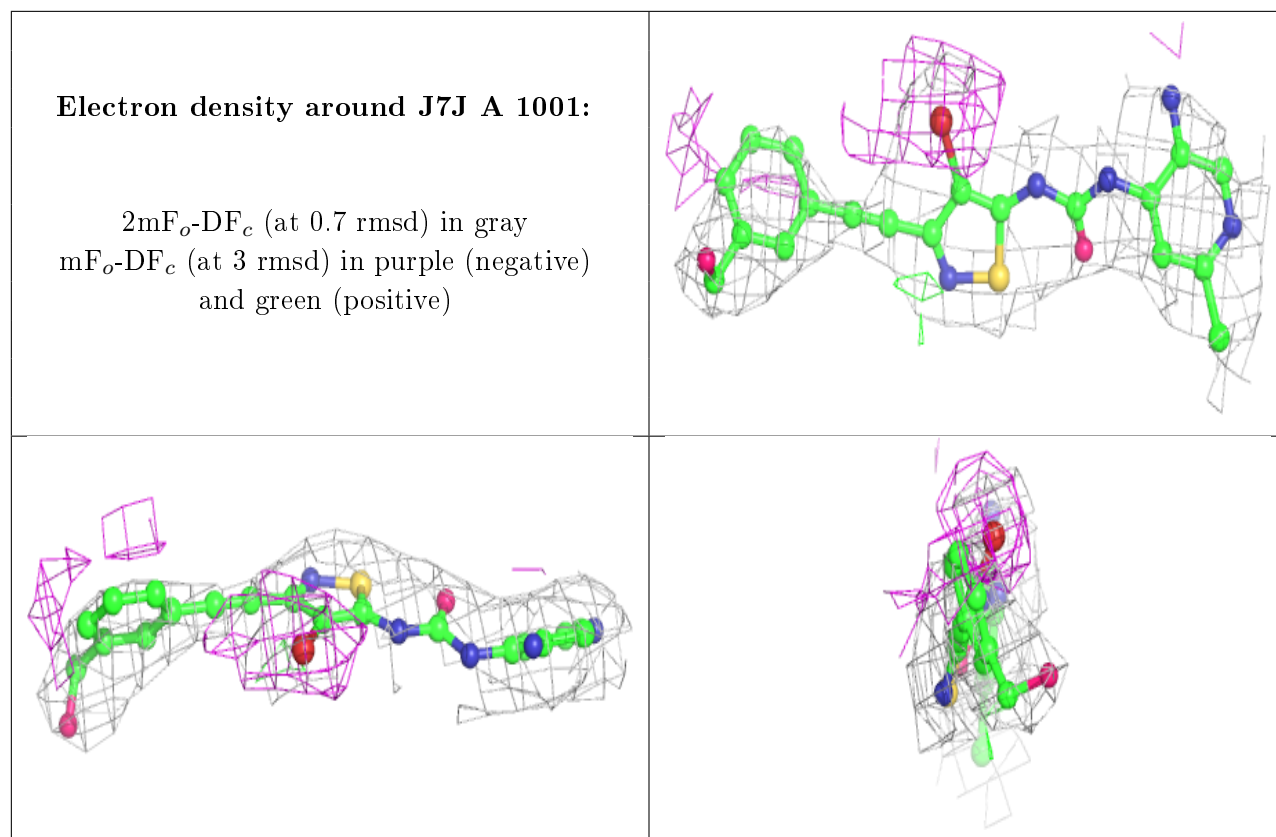
There are no carbohydrates in this entry.

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
3	IPA	A	1002	4/4	0.78	0.41	109,111,112,112	0
3	IPA	A	1003	4/4	0.86	0.17	108,109,109,109	0
2	J7J	A	1001	28/28	0.91	0.30	87,95,106,117	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.