



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:34 AM UTC

PDB ID : 5RAQ / pdb_00005raq
Title : PanDDA analysis group deposition – Crystal Structure of JMJD1B in complex with FM001577a
Authors : Snee, M.; Nowak, R.; Johansson, C.; Burgess-Brown, N.A.; Arrowsmith, C.H.; Bountra, C.; Edwards, A.M.; Oppermann, U.
Deposited on : 2020-03-16
Resolution : 1.85 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)
Xtrriage (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

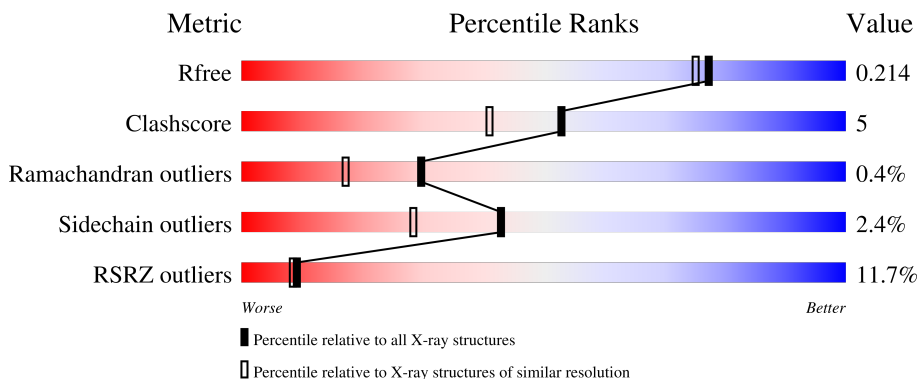
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	372	 10% 80% 10% 9%
1	B	372	 12% 82% 10% 8%

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
2	S5J	A	1801	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6301 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 Lysine-specific demethylase 3B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	340	2762	1749	482	515	16	0	4	0
1	B	344	2798	1774	492	517	15	0	2	0

There are 50 discrepancies between the modelled and reference sequences:

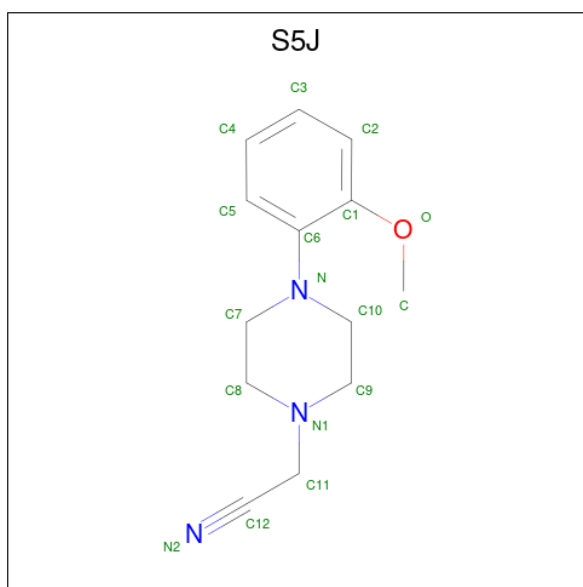
Chain	Residue	Modelled	Actual	Comment	Reference
A	1357	MET	-	initiating methionine	UNP Q7LBC6
A	1358	HIS	-	expression tag	UNP Q7LBC6
A	1359	HIS	-	expression tag	UNP Q7LBC6
A	1360	HIS	-	expression tag	UNP Q7LBC6
A	1361	HIS	-	expression tag	UNP Q7LBC6
A	1362	HIS	-	expression tag	UNP Q7LBC6
A	1363	HIS	-	expression tag	UNP Q7LBC6
A	1364	SER	-	expression tag	UNP Q7LBC6
A	1365	SER	-	expression tag	UNP Q7LBC6
A	1366	GLY	-	expression tag	UNP Q7LBC6
A	1367	VAL	-	expression tag	UNP Q7LBC6
A	1368	ASP	-	expression tag	UNP Q7LBC6
A	1369	LEU	-	expression tag	UNP Q7LBC6
A	1370	GLY	-	expression tag	UNP Q7LBC6
A	1371	THR	-	expression tag	UNP Q7LBC6
A	1372	GLU	-	expression tag	UNP Q7LBC6
A	1373	ASN	-	expression tag	UNP Q7LBC6
A	1374	LEU	-	expression tag	UNP Q7LBC6
A	1375	TYR	-	expression tag	UNP Q7LBC6
A	1376	PHE	-	expression tag	UNP Q7LBC6
A	1377	GLN	-	expression tag	UNP Q7LBC6
A	1378	SER	-	expression tag	UNP Q7LBC6
A	1379	MET	-	expression tag	UNP Q7LBC6
A	1601	GLU	GLN	conflict	UNP Q7LBC6
A	1606	HIS	GLY	conflict	UNP Q7LBC6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1357	MET	-	initiating methionine	UNP Q7LBC6
B	1358	HIS	-	expression tag	UNP Q7LBC6
B	1359	HIS	-	expression tag	UNP Q7LBC6
B	1360	HIS	-	expression tag	UNP Q7LBC6
B	1361	HIS	-	expression tag	UNP Q7LBC6
B	1362	HIS	-	expression tag	UNP Q7LBC6
B	1363	HIS	-	expression tag	UNP Q7LBC6
B	1364	SER	-	expression tag	UNP Q7LBC6
B	1365	SER	-	expression tag	UNP Q7LBC6
B	1366	GLY	-	expression tag	UNP Q7LBC6
B	1367	VAL	-	expression tag	UNP Q7LBC6
B	1368	ASP	-	expression tag	UNP Q7LBC6
B	1369	LEU	-	expression tag	UNP Q7LBC6
B	1370	GLY	-	expression tag	UNP Q7LBC6
B	1371	THR	-	expression tag	UNP Q7LBC6
B	1372	GLU	-	expression tag	UNP Q7LBC6
B	1373	ASN	-	expression tag	UNP Q7LBC6
B	1374	LEU	-	expression tag	UNP Q7LBC6
B	1375	TYR	-	expression tag	UNP Q7LBC6
B	1376	PHE	-	expression tag	UNP Q7LBC6
B	1377	GLN	-	expression tag	UNP Q7LBC6
B	1378	SER	-	expression tag	UNP Q7LBC6
B	1379	MET	-	expression tag	UNP Q7LBC6
B	1601	GLU	GLN	conflict	UNP Q7LBC6
B	1606	HIS	GLY	conflict	UNP Q7LBC6

- Molecule 2 is 2-[4-(2-methoxyphenyl)piperazin-1-yl]ethanenitrile (CCD ID: S5J) (formula: C₁₃H₁₇N₃O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	13	3	1		
2	B	1	Total	C	N	O	0	0
			17	13	3	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Cl	0	0
			4	4		
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		
4	B	1	Total	Mn	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	369	Total	O	0	0
			369	369		

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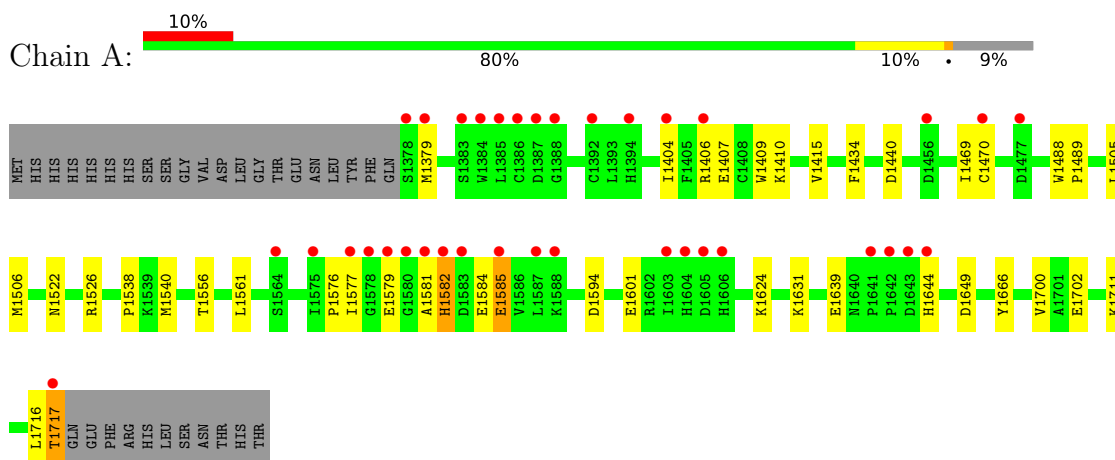
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	331	Total 331	O 331	0	0

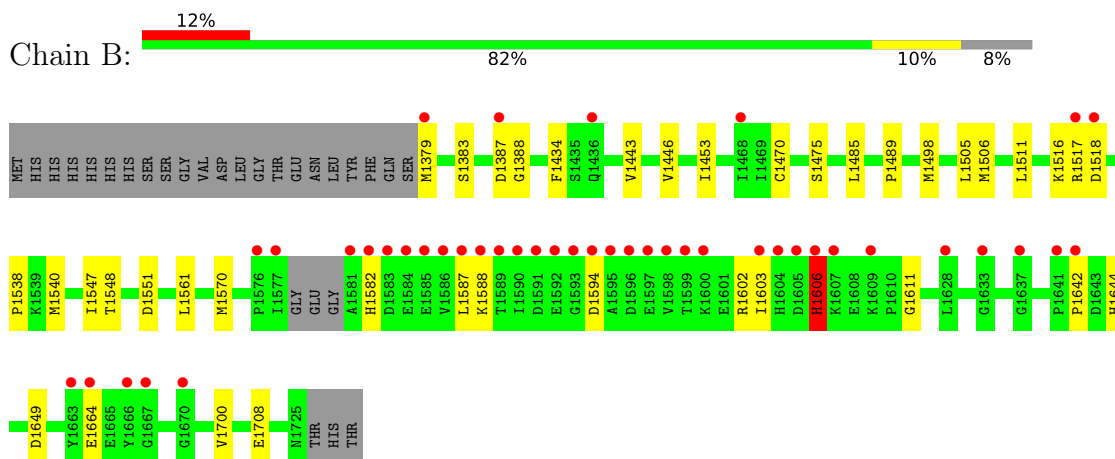
3 Residue-property plots [i](#)

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: Lysine-specific demethylase 3B



- Molecule 1: Lysine-specific demethylase 3B



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.37Å 93.72Å 93.47Å 90.00° 108.11° 90.00°	Depositor
Resolution (Å)	64.56 – 1.85 64.56 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.6 (64.56-1.85) 98.6 (64.56-1.85)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 1.86Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.181 , 0.216 (Not available) , 0.214	Depositor DCC
R_{free} test set	3975 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtrriage
Anisotropy	0.120	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.034 for h,-k,-h-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6301	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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: CL, S5J, MN

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	1.21	3/2835 (0.1%)	1.29	8/3846 (0.2%)
1	B	1.13	2/2872 (0.1%)	1.32	7/3895 (0.2%)
All	All	1.17	5/5707 (0.1%)	1.30	15/7741 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1556	THR	C-O	5.57	1.30	1.24
1	B	1547	ILE	N-CA	5.54	1.51	1.46
1	A	1409	TRP	C-O	5.54	1.30	1.24
1	B	1511	LEU	N-CA	5.12	1.50	1.46
1	A	1415	VAL	C-O	5.01	1.29	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1606	HIS	CA-CB-CG	6.58	120.38	113.80
1	A	1469	ILE	CA-C-O	-5.67	115.06	120.95
1	A	1716	LEU	CA-C-N	5.58	131.74	121.70
1	A	1716	LEU	C-N-CA	5.58	131.74	121.70
1	A	1717	THR	CA-C-O	-5.47	111.50	120.80
1	B	1642	PRO	CA-C-N	5.45	127.58	120.28
1	B	1642	PRO	C-N-CA	5.45	127.58	120.28
1	A	1576	PRO	CA-C-N	5.41	129.60	122.51
1	A	1576	PRO	C-N-CA	5.41	129.60	122.51
1	A	1582	HIS	CA-C-N	5.16	127.72	120.28
1	A	1582	HIS	C-N-CA	5.16	127.72	120.28
1	B	1606	HIS	N-CA-CB	5.16	117.86	110.06
1	B	1708	GLU	CB-CG-CD	5.04	121.17	112.60
1	B	1475	SER	CA-C-N	5.01	127.25	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	1475	SER	C-N-CA	5.01	127.25	120.38

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	2762	0	2646	28	0
1	B	2798	0	2685	27	0
2	A	17	0	0	0	0
2	B	17	0	0	0	0
3	A	4	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	369	0	0	16	0
5	B	331	0	0	6	0
All	All	6301	0	5331	55	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 (55) 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:1470:CYS:O	5:A:1901:HOH:O	1.60	1.19
1:B:1470:CYS:SG	5:B:2219:HOH:O	2.36	0.84
1:A:1406[A]:ARG:NH2	5:A:1904:HOH:O	2.10	0.84
1:A:1506:MET:HE2	1:A:1538:PRO:HD3	1.67	0.75
1:B:1489:PRO:HG2	1:B:1498:MET:HE2	1.68	0.75
1:B:1644:HIS:NE2	1:B:1649:ASP:OD2	2.21	0.73
1:B:1516:LYS:HE3	5:B:1928:HOH:O	1.88	0.73
1:A:1601:GLU:OE1	5:A:1903:HOH:O	2.05	0.73
1:B:1517[B]:ARG:CG	1:B:1517[B]:ARG:HH11	2.03	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1602:ARG:O	1:B:1606:HIS:O	2.08	0.70
1:B:1517[B]:ARG:HH11	1:B:1517[B]:ARG:HG3	1.60	0.66
1:B:1517[B]:ARG:HG3	1:B:1517[B]:ARG:NH1	2.12	0.64
1:B:1518:ASP:HB3	5:B:2133:HOH:O	1.99	0.63
1:A:1711:LYS:CB	5:A:2088:HOH:O	2.47	0.62
1:A:1522:ASN:O	1:A:1526:ARG:NH1	2.33	0.61
1:A:1505:LEU:HD22	1:A:1700:VAL:HG11	1.82	0.61
1:B:1518:ASP:OD1	5:B:1901:HOH:O	2.16	0.58
1:B:1506:MET:CE	1:B:1538:PRO:HG3	2.34	0.57
1:A:1582:HIS:CE1	5:A:1934:HOH:O	2.57	0.57
1:A:1639:GLU:O	5:A:1905:HOH:O	2.18	0.57
1:A:1585:GLU:H	1:A:1585:GLU:CD	2.12	0.56
1:B:1664[B]:GLU:HA	1:B:1664[B]:GLU:OE1	2.06	0.55
1:A:1406[A]:ARG:NH1	5:A:1915:HOH:O	2.39	0.55
1:A:1440:ASP:HB2	5:A:2038:HOH:O	2.06	0.54
1:B:1388:GLY:N	5:B:1904:HOH:O	2.29	0.54
1:B:1505:LEU:HD22	1:B:1700:VAL:HG11	1.90	0.53
1:A:1631:LYS:HE2	1:A:1666:TYR:OH	2.10	0.51
1:B:1517[B]:ARG:HH11	1:B:1517[B]:ARG:CB	2.23	0.51
1:B:1561:LEU:C	1:B:1561:LEU:HD12	2.37	0.50
1:B:1606:HIS:H	1:B:1606:HIS:CD2	2.29	0.50
1:B:1434:PHE:CZ	1:B:1540:MET:HE1	2.47	0.50
1:A:1649:ASP:CB	5:A:2053:HOH:O	2.60	0.49
1:A:1505:LEU:HD22	1:A:1700:VAL:CG1	2.41	0.49
1:B:1517[B]:ARG:HH11	1:B:1517[B]:ARG:HB2	1.77	0.48
1:A:1506:MET:HE1	1:A:1702:GLU:CD	2.40	0.47
1:A:1561:LEU:C	1:A:1561:LEU:HD12	2.40	0.47
1:A:1582:HIS:O	1:A:1582:HIS:CG	2.68	0.46
1:B:1506:MET:HE2	1:B:1538:PRO:HG3	1.96	0.46
1:A:1649:ASP:HB3	5:A:2053:HOH:O	2.16	0.46
1:B:1446:VAL:HG22	1:B:1453:ILE:HD13	1.98	0.45
1:B:1548:THR:O	1:B:1551:ASP:HB2	2.16	0.45
1:A:1407:GLU:CG	5:A:2204:HOH:O	2.64	0.44
1:B:1443:VAL:HG21	1:B:1485:LEU:HD11	1.98	0.44
1:A:1624:LYS:NZ	5:A:1902:HOH:O	1.84	0.44
1:A:1407:GLU:HG3	5:A:2204:HOH:O	2.17	0.44
1:A:1379[A]:MET:CE	5:A:2100:HOH:O	2.65	0.44
1:B:1606:HIS:H	1:B:1606:HIS:HD2	1.65	0.43
1:A:1582:HIS:HE1	5:A:1934:HOH:O	1.97	0.43
1:B:1379:MET:N	5:B:1913:HOH:O	2.50	0.43
1:B:1506:MET:HE3	1:B:1538:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1407:GLU:O	1:A:1410:LYS:HG2	2.19	0.41
1:B:1570:MET:HE3	1:B:1611:GLY:HA3	2.03	0.41
1:A:1488:TRP:HA	1:A:1489:PRO:C	2.44	0.41
1:A:1649:ASP:CG	5:A:2053:HOH:O	2.63	0.41
1:A:1434:PHE:CZ	1:A:1540:MET:HE1	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	342/372 (92%)	333 (97%)	7 (2%)	2 (1%)	21	10
1	B	342/372 (92%)	335 (98%)	6 (2%)	1 (0%)	36	25
All	All	684/744 (92%)	668 (98%)	13 (2%)	3 (0%)	30	17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1581	ALA
1	B	1594	ASP
1	A	1594	ASP

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	298/331 (90%)	291 (98%)	7 (2%)	44	30
1	B	302/331 (91%)	295 (98%)	7 (2%)	44	30
All	All	600/662 (91%)	586 (98%)	14 (2%)	43	30

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1404	ILE
1	A	1577	ILE
1	A	1579	GLU
1	A	1584	GLU
1	A	1585	GLU
1	A	1644	HIS
1	A	1717	THR
1	B	1383	SER
1	B	1387	ASP
1	B	1582	HIS
1	B	1587	LEU
1	B	1588	LYS
1	B	1603	ILE
1	B	1606	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1640	ASN
1	A	1648	HIS
1	A	1650	GLN
1	B	1413	GLN
1	B	1508	ASN
1	B	1606	HIS
1	B	1640	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 for Mogul analysis.

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	S5J	B	1801	-	18,18,18	2.01	4 (22%)	23,23,23	3.18	8 (34%)
2	S5J	A	1801	-	18,18,18	2.29	5 (27%)	23,23,23	2.79	8 (34%)

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	S5J	B	1801	-	-	2/8/19/19	0/2/2/2
2	S5J	A	1801	-	-	8/8/19/19	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1801	S5J	C11-N1	6.98	1.54	1.46
2	B	1801	S5J	C11-N1	6.03	1.53	1.46
2	A	1801	S5J	C6-C1	3.20	1.45	1.40
2	A	1801	S5J	C8-N1	2.95	1.54	1.46
2	A	1801	S5J	C9-N1	2.88	1.54	1.46
2	B	1801	S5J	C6-N	2.78	1.47	1.41
2	B	1801	S5J	C8-N1	2.46	1.53	1.46
2	A	1801	S5J	C11-C12	-2.32	1.44	1.47
2	B	1801	S5J	C9-N1	2.29	1.53	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1801	S5J	C11-C12-N2	-9.74	164.40	177.91
2	B	1801	S5J	C12-C11-N1	-8.51	104.36	113.98
2	A	1801	S5J	C5-C6-N	-6.38	112.42	122.42
2	A	1801	S5J	C1-C6-N	6.22	129.32	119.14
2	A	1801	S5J	C-O-C1	5.06	124.94	117.51
2	A	1801	S5J	O-C1-C6	4.61	121.77	116.04
2	A	1801	S5J	C11-C12-N2	-4.33	171.91	177.91
2	B	1801	S5J	O-C1-C6	-3.41	111.81	116.04
2	A	1801	S5J	O-C1-C2	-3.03	119.19	124.30
2	B	1801	S5J	C9-C10-N	2.92	116.92	110.78
2	B	1801	S5J	C11-N1-C8	-2.67	108.72	111.68
2	B	1801	S5J	C8-C7-N	2.66	116.39	110.78
2	A	1801	S5J	C7-C8-N1	-2.64	105.33	110.65
2	B	1801	S5J	C1-C6-N	2.44	123.14	119.14
2	B	1801	S5J	C5-C6-N	-2.27	118.86	122.42
2	A	1801	S5J	C9-C10-N	2.13	115.27	110.78

There are no chirality outliers.

All (10) torsion outliers are listed below:

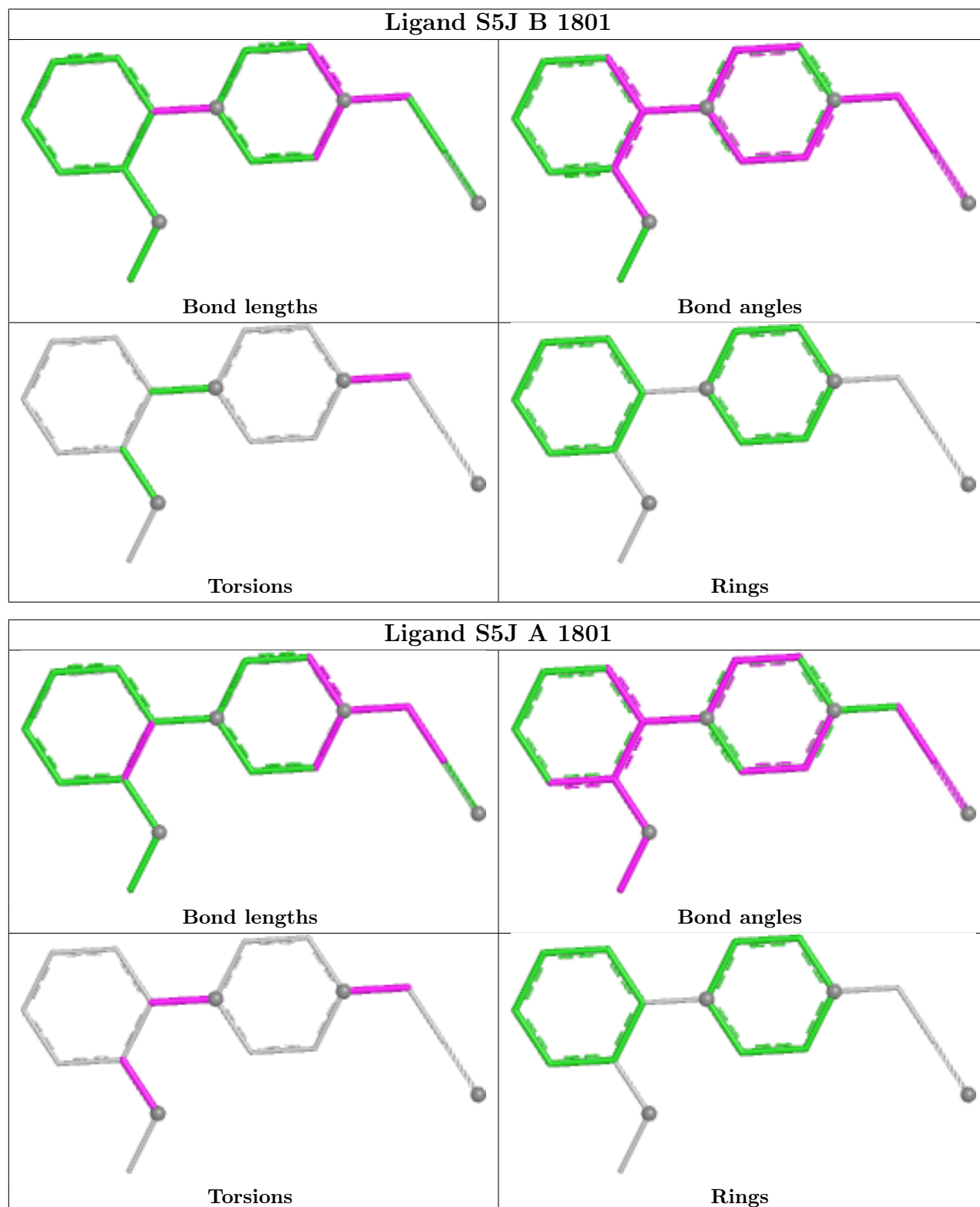
Mol	Chain	Res	Type	Atoms
2	A	1801	S5J	C12-C11-N1-C8
2	A	1801	S5J	C12-C11-N1-C9
2	B	1801	S5J	C12-C11-N1-C8
2	B	1801	S5J	C12-C11-N1-C9
2	A	1801	S5J	C2-C1-O-C
2	A	1801	S5J	C6-C1-O-C
2	A	1801	S5J	C1-C6-N-C7
2	A	1801	S5J	C1-C6-N-C10
2	A	1801	S5J	C5-C6-N-C7
2	A	1801	S5J	C5-C6-N-C10

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	340/372 (91%)	0.75	36 (10%) 11 11	6, 31, 66, 110	12 (3%)
1	B	344/372 (92%)	0.71	44 (12%) 7 7	9, 34, 66, 103	31 (9%)
All	All	684/744 (91%)	0.73	80 (11%) 9 8	6, 32, 66, 110	43 (6%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1384	TRP	17.9
1	A	1385	LEU	16.7
1	A	1386	CYS	15.4
1	A	1379[A]	MET	15.0
1	A	1383	SER	13.5
1	A	1392	CYS	13.3
1	A	1388	GLY	13.3
1	A	1588[A]	LYS	12.4
1	A	1394	HIS	12.4
1	A	1387	ASP	11.7
1	A	1564[A]	SER	11.2
1	A	1406[A]	ARG	10.2
1	A	1577	ILE	10.0
1	B	1581	ALA	9.8
1	B	1517[A]	ARG	9.0
1	B	1583	ASP	8.6
1	B	1664[A]	GLU	8.1
1	B	1582	HIS	8.0
1	B	1586	VAL	6.8
1	B	1577	ILE	6.2
1	B	1606	HIS	5.4
1	B	1587	LEU	5.0
1	B	1595	ALA	4.9
1	B	1585	GLU	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	1603	ILE	4.7
1	A	1581	ALA	4.6
1	B	1590	ILE	4.6
1	A	1582	HIS	4.3
1	A	1470	CYS	4.3
1	B	1598	VAL	4.1
1	A	1717	THR	4.1
1	A	1606	HIS	4.0
1	B	1591	ASP	3.8
1	B	1609	LYS	3.7
1	B	1596	ASP	3.7
1	A	1578	GLY	3.7
1	B	1599	THR	3.5
1	B	1593	GLY	3.5
1	B	1667	GLY	3.4
1	B	1589	THR	3.3
1	B	1588	LYS	3.2
1	A	1378	SER	3.1
1	A	1605	ASP	3.1
1	B	1518	ASP	3.0
1	B	1584	GLU	3.0
1	B	1600	LYS	2.9
1	B	1576	PRO	2.8
1	B	1597	GLU	2.8
1	B	1642	PRO	2.8
1	B	1637	GLY	2.7
1	A	1641	PRO	2.7
1	B	1604	HIS	2.6
1	B	1436	GLN	2.6
1	A	1603	ILE	2.6
1	B	1594	ASP	2.6
1	B	1663	TYR	2.6
1	A	1642	PRO	2.6
1	B	1605	ASP	2.6
1	B	1666	TYR	2.5
1	A	1579	GLU	2.5
1	B	1641	PRO	2.5
1	B	1387	ASP	2.5
1	A	1575	ILE	2.4
1	A	1644	HIS	2.4
1	B	1607	LYS	2.4
1	B	1592	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1604	HIS	2.4
1	A	1580	GLY	2.4
1	A	1583	ASP	2.3
1	A	1456	ASP	2.3
1	A	1585	GLU	2.2
1	B	1670	GLY	2.2
1	B	1633	GLY	2.2
1	A	1477	ASP	2.2
1	A	1404	ILE	2.1
1	B	1628	LEU	2.1
1	A	1643	ASP	2.1
1	B	1379	MET	2.1
1	A	1587	LEU	2.1
1	B	1468	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

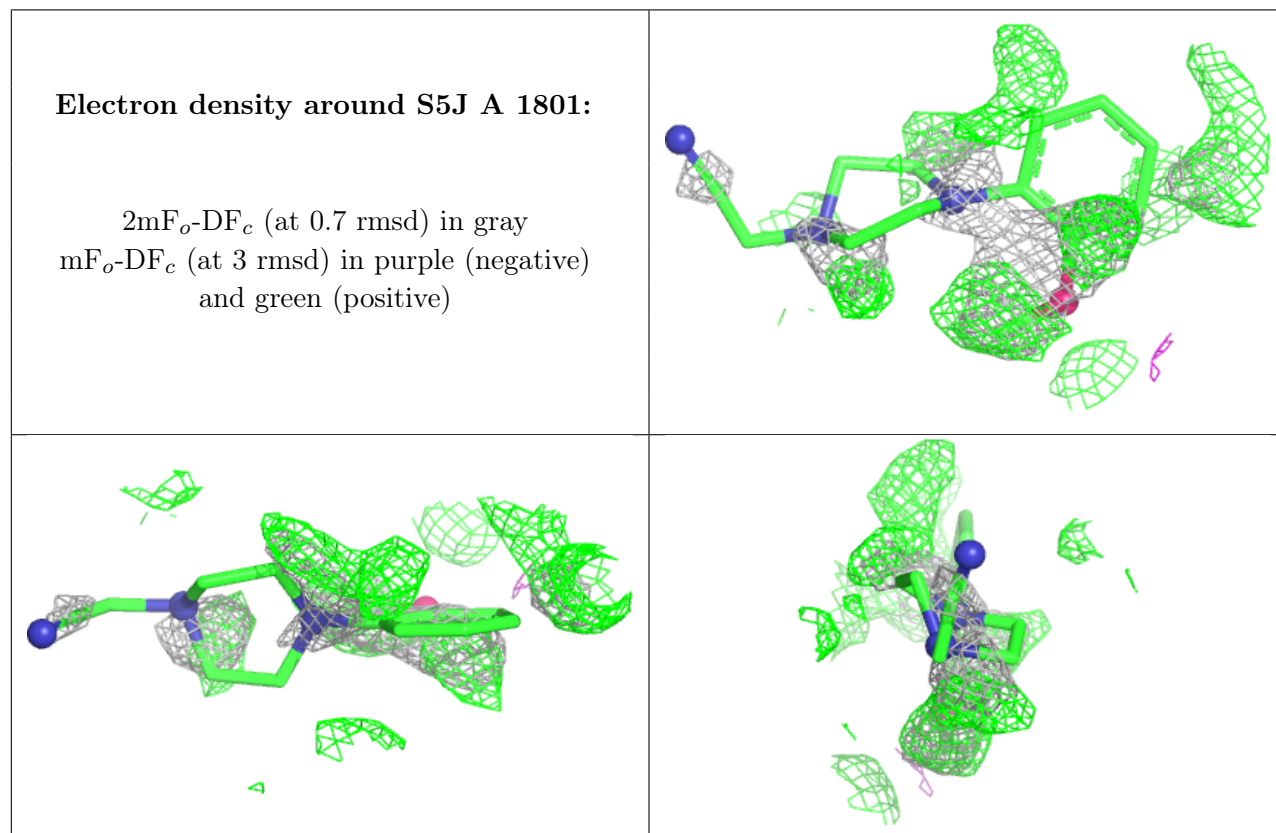
There are no oligosaccharides in this entry.

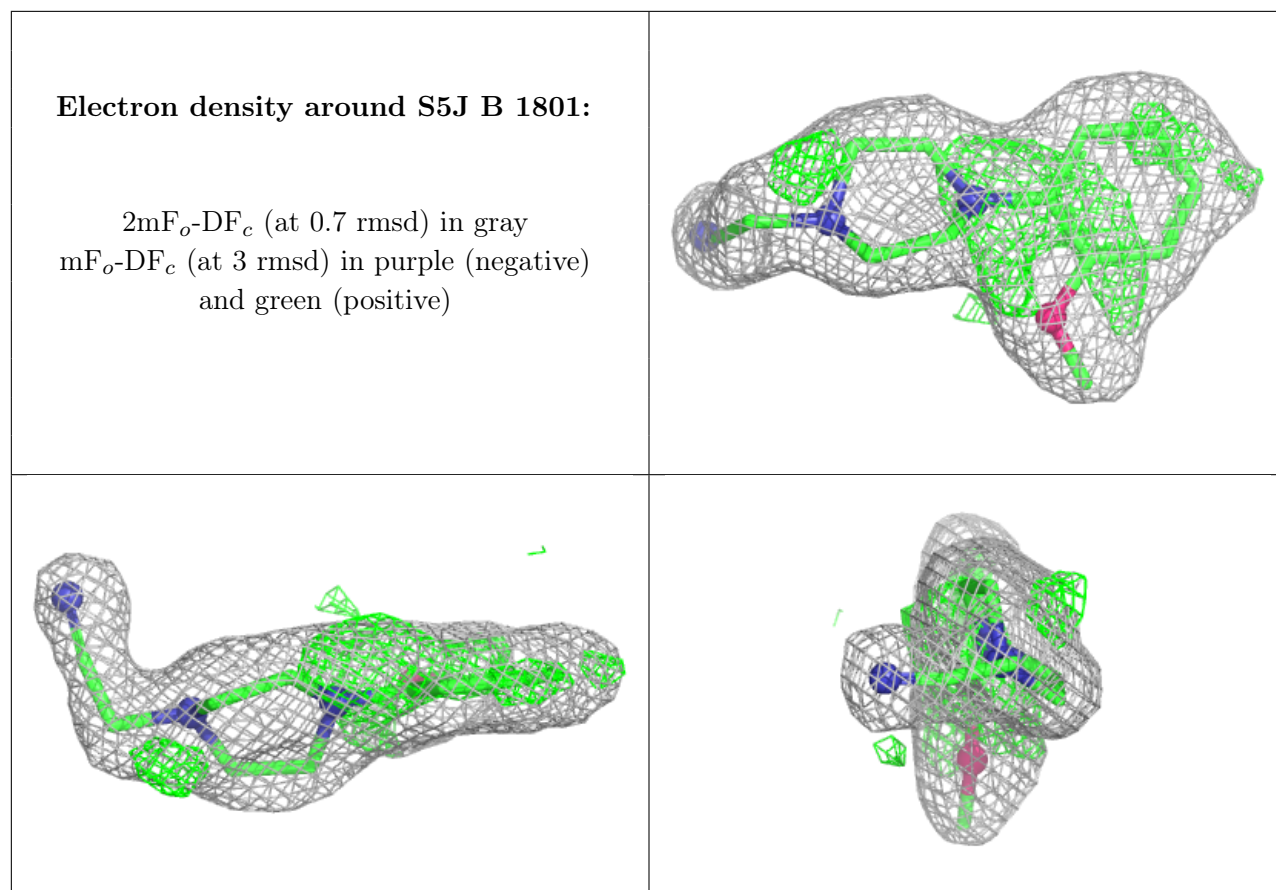
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	S5J	A	1801	17/17	0.72	0.60	46,52,55,55	17
2	S5J	B	1801	17/17	0.91	0.16	29,33,41,43	17
3	CL	A	1805	1/1	0.92	0.11	57,57,57,57	0
4	MN	A	1806	1/1	0.94	0.07	63,63,63,63	0
4	MN	B	1803	1/1	0.97	0.04	45,45,45,45	0
3	CL	A	1804	1/1	0.98	0.10	42,42,42,42	0
3	CL	A	1803	1/1	0.98	0.05	41,41,41,41	0
3	CL	A	1802	1/1	0.99	0.02	27,27,27,27	0
3	CL	B	1802	1/1	0.99	0.07	44,44,44,44	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.