



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 22, 2026 – 11:29 PM UTC

PDB ID : 8BCH / pdb_00008bch
Title : Human Brr2 Helicase Region in complex with Sulfaguanidine
Authors : Vester, K.; Loll, B.; Wahl, M.C.
Deposited on : 2022-10-15
Resolution : 2.87 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

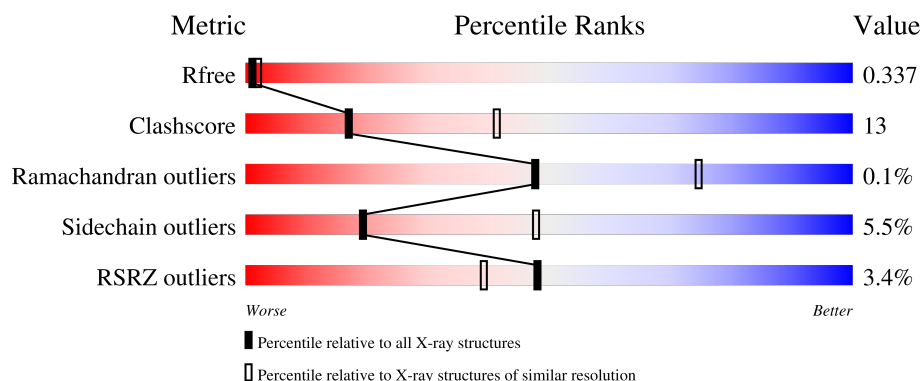
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

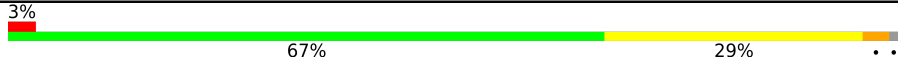
The reported resolution of this entry is 2.87 Å.

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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	B	1747	

i

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.

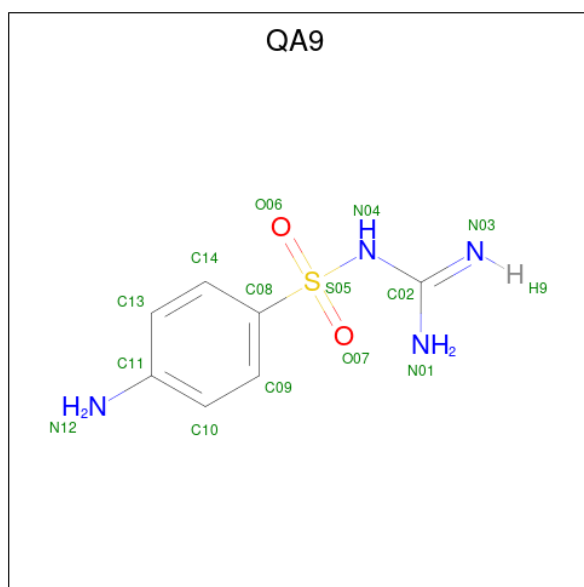
- Molecule 1 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1724	Total	C	N	O	S	0	0	0
			13859	8857	2371	2559	72			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	390	GLY	-	expression tag	UNP O75643
B	391	ALA	-	expression tag	UNP O75643
B	392	GLU	-	expression tag	UNP O75643
B	393	PHE	-	expression tag	UNP O75643

- Molecule 2 is 1-(4-aminophenyl)sulfonylguanidine (CCD ID: QA9) (formula: $\text{C}_7\text{H}_{10}\text{N}_4\text{O}_2\text{S}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			14	7	4	2	1		

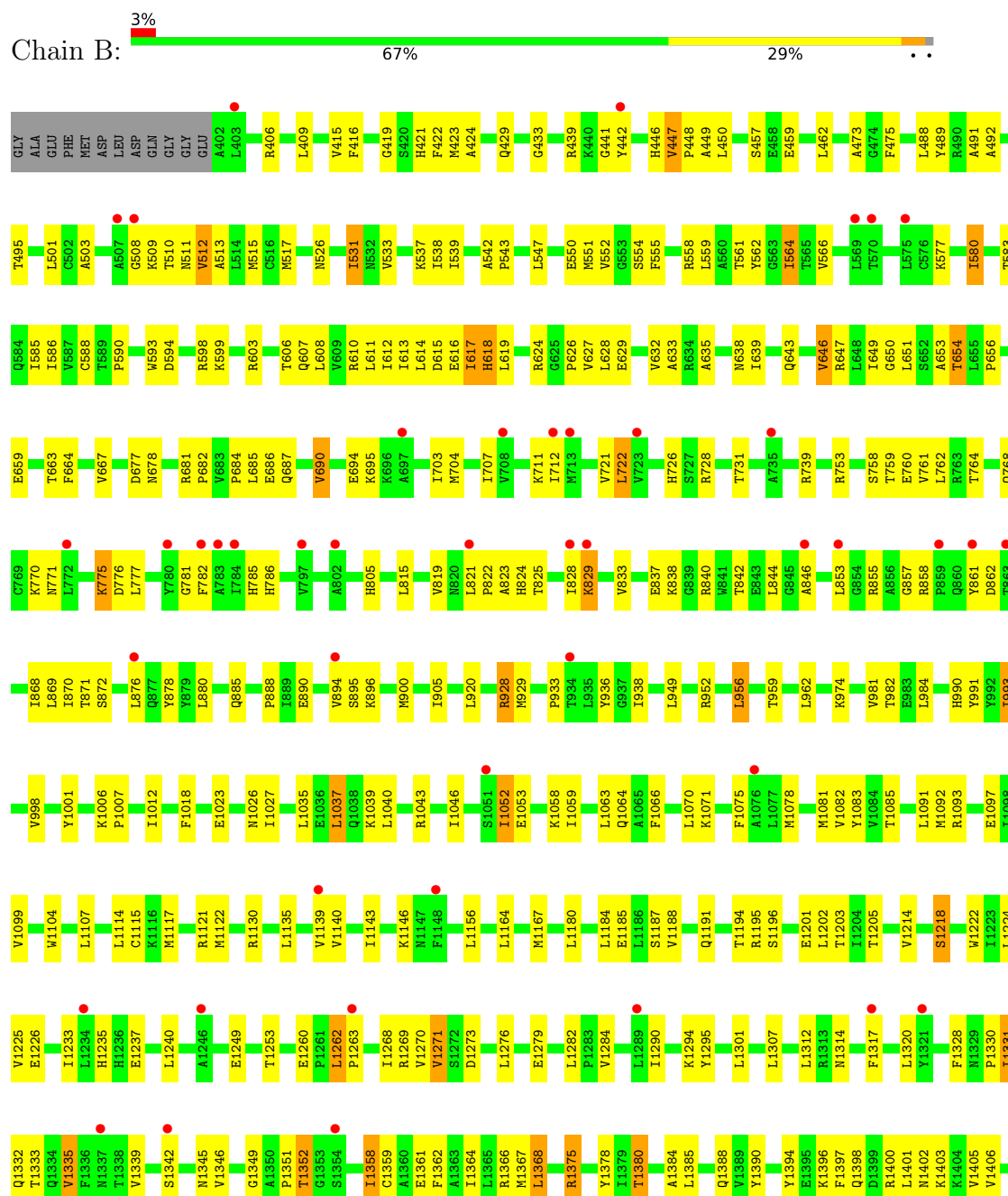
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	11	Total	O	0	0
			11	11		

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: U5 small nuclear ribonucleoprotein 200 kDa helicase



LYS	L1419	V1546	L1631	M1732	L1845	V1982	
GLU	I1424	H1553	I1641	H1733	L1845	V1982	
ALA	I1425	S1554	Q1642	D1734	I1849	I1985	
THR	P1555	K1556	V1645	H1735	Y1855	N1994	
ASP	L1435	K1557	R1648	V1741	Y1855	N1994	
SER	R1442	P1558	S1649	I1745	P1859	L1997	
ASP	F1451	V1559	L1650	D1750	H1863	T2000	
ASP	V1452	I1560	M1654	A1751	L1879	Q2003	
	V1453	R1566	N1655	V1752	N1880	I2004	
	V1456	K1567	V1656	V1753	N1881	I2004	
	H1457	T1568	A1657	V1754	P1882	V2007	
	L1458	T1569	A1658	L1755	P1887	F2010	
	I1459	D1575	H1659	Y1761	P1887	F2010	
	L1467	I1576	V1661	R1763	K1890	S2020	
	E1468	L1577	I1662	P1768	T1891	V2023	
	V1469	C1580	I1663	M1769	L1899	V2024	
	I1470		M1664		S1900	D2025	
	I1481	Q1585	T1666	L1773	R1901	Q2040	
	E1482	Q1587	K1672	Q1774	L1904	Q2040	
	R1483	R1588		G1775		R2043	
	I1487	E1594	D1678	H1780	I1915	R2043	
	A1489	K1595	Y1679	L1781	I1915	V2051	
	L1490	I1598	D1683	L1785	I1920	I2052	
	S1493	P1599	Q1686	T1792	R1921	L2055	
	L1494	Y1600	M1687	L1796	L1923	L2055	
	S1495	L1601	V1688		L1930	R2060	
		E1602	G1689			W2064	
	V1500	K1603	R1693	K1800	A1942		
		L1604	P1694	C1801	L1945	V2067	
		S1607	L1695	I1802	A1946	I2068	
		T1608	Q1696	E1805	V1949	L2084	
	S1510	L1609	D1697	D1806	T1950	Q2085	
	T1511	K1610				Q2086	
	F1512	E1611	R1701	L1813	M1953		
	H1515	T1612	C1702	N1814		L2092	
	P1516	L1613	V1703	L1815	Y1959		
	N1517	L1614	I1704	G1816		P2097	
		N1615		M1817	L1963		
		G1616	S1709	Y1822		H2102	
		V1617	K1710		F1966	Y2107	
			F1713	M1825	T1967		
		L1620	F1714	Y1826	S1968	S2110	
		H1621	K1715		E1969	D2111	
		E1622		I1829	H1970	A2112	
			E1720	E1830	I1971	Y2113	
		S1625	P1721	L1831		M2114	
					C1974		
		E1628	E1725	K1841	V1979	D2125	
		R1629		V1942		VAL	
		R1630					

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.29Å 149.53Å 141.49Å 90.00° 120.32° 90.00°	Depositor
Resolution (Å)	47.20 – 2.87 47.20 – 2.87	Depositor EDS
% Data completeness (in resolution range)	93.2 (47.20-2.87) 93.4 (47.20-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.281 , 0.337 0.281 , 0.337	Depositor DCC
R_{free} test set	2013 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å ²)	82.8	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 98.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for k,h,-1/2*h-1/2*k-l 0.000 for -k,-h,-1/2*h+1/2*k-l 0.001 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13884	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: QA9

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	B	0.15	0/14153	0.35	1/19177 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	441	GLY	CA-C-O	-5.77	116.58	122.59

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	B	13859	0	14001	354	0
2	B	14	0	0	0	0
3	B	11	0	0	0	0
All	All	13884	0	14001	354	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 13.

The worst 5 of 354 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:415:VAL:HG21	1:B:895:SER:HB3	1.69	0.75
1:B:406:ARG:NH2	1:B:974:LYS:O	2.19	0.74
1:B:1950:THR:HG22	1:B:2060:ARG:HH12	1.52	0.74
1:B:1526:HIS:HB2	1:B:1703:VAL:HG12	1.69	0.74
1:B:1710:LYS:O	1:B:1713:PHE:HB3	1.88	0.73

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	B	1722/1747 (99%)	1625 (94%)	96 (6%)	1 (0%)	48	74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1713	PHE

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	B	1542/1560 (99%)	1457 (94%)	85 (6%)	19	48

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1487	ILE
1	B	1813	LEU
1	B	1490	LEU
1	B	1617	VAL
1	B	1863	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1615	ASN
1	B	1898	HIS
1	B	2074	ASN
1	B	951	GLN
1	B	978	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](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	QA9	B	2201	-	14,14,14	2.11	5 (35%)	17,20,20	4.45	4 (23%)

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	QA9	B	2201	-	-	4/9/11/11	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2201	QA9	C02-N04	4.42	1.46	1.36
2	B	2201	QA9	C02-N01	3.26	1.46	1.34
2	B	2201	QA9	S05-N04	2.93	1.71	1.64
2	B	2201	QA9	C08-S05	2.51	1.80	1.76
2	B	2201	QA9	O07-S05	2.51	1.46	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2201	QA9	O07-S05-O06	-16.85	99.06	119.52
2	B	2201	QA9	C08-S05-N04	4.52	113.28	106.06
2	B	2201	QA9	O07-S05-N04	3.46	116.67	106.77
2	B	2201	QA9	O06-S05-C08	2.89	111.62	107.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

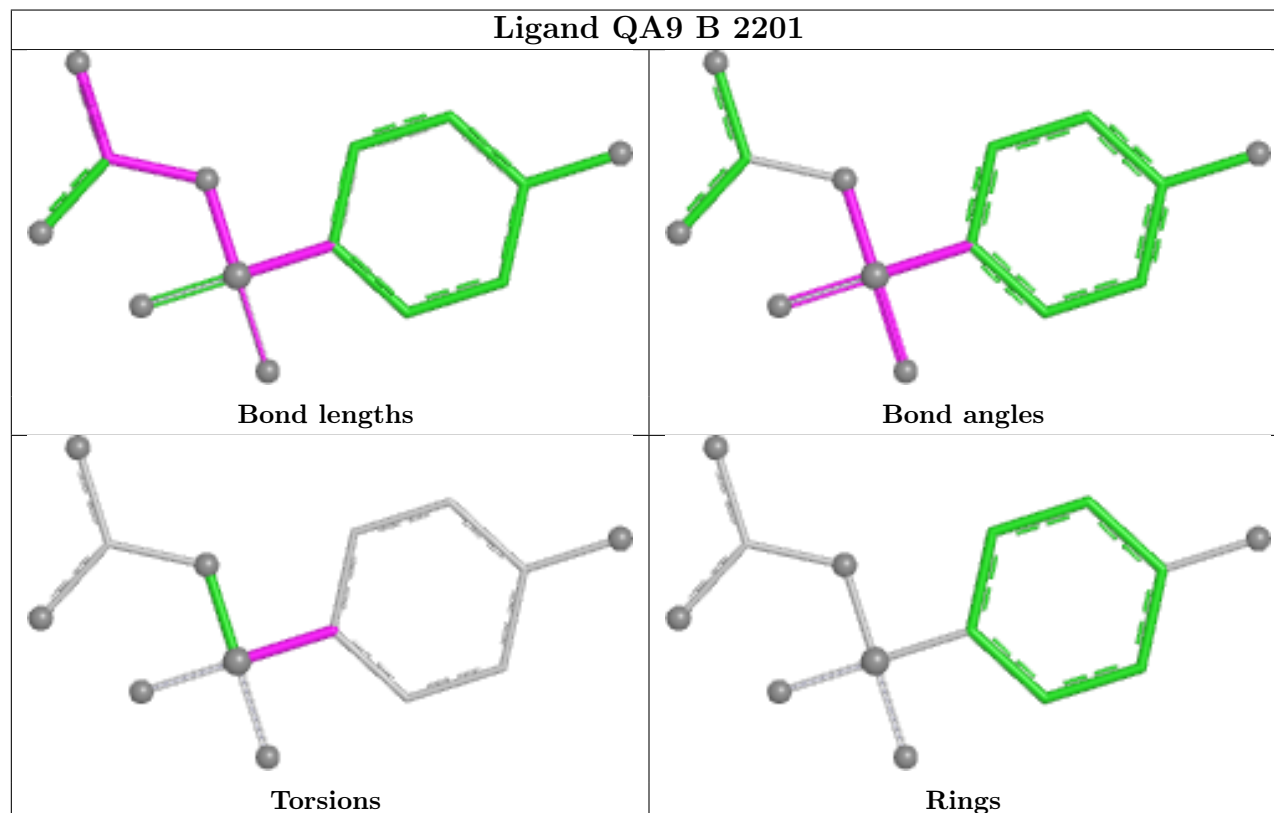
Mol	Chain	Res	Type	Atoms
2	B	2201	QA9	C14-C08-S05-O06
2	B	2201	QA9	C09-C08-S05-O06
2	B	2201	QA9	C14-C08-S05-N04
2	B	2201	QA9	C09-C08-S05-N04

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	B	1724/1747 (98%)	0.49	58 (3%) 48 39	52, 112, 198, 330	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1985	ILE	4.6
1	B	1761	TYR	3.8
1	B	829	LYS	3.7
1	B	782	PHE	3.5
1	B	853	LEU	3.2

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.

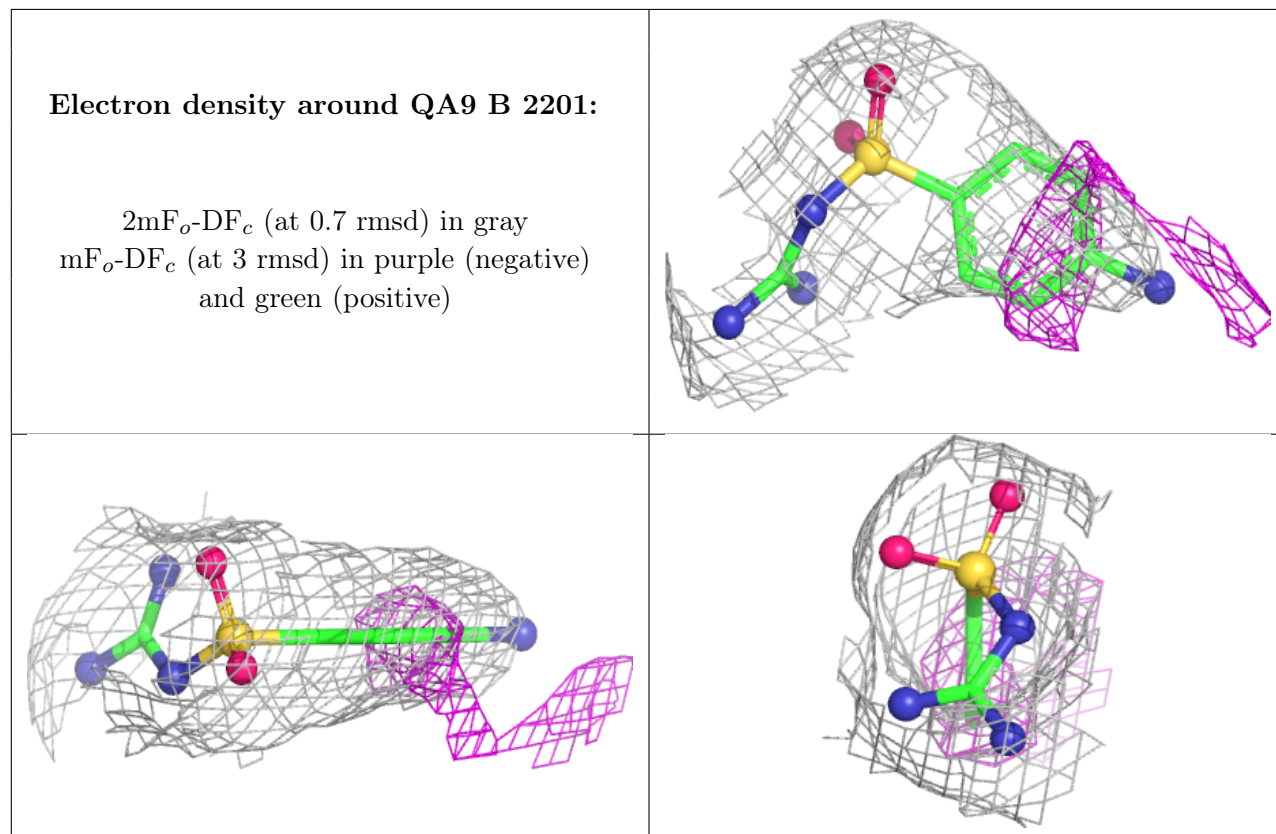
6.4 Ligands [i](#)

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	QA9	B	2201	14/14	0.88	0.11	50,57,66,94	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.