



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:29 AM UTC

PDB ID : 4P7E / pdb_00004p7e
Title : Triazolopyridine compounds as selective JAK1 inhibitors: from hit identification to GLPG0634
Authors : Menet, C.C.J.; Fletcher, S.; Van Lommen, G.; Geney, R.; Blanc, J.; Smits, K.; Jouannigot, N.; van der Aar, E.M.; Clement-Lacroix, P.; Lepescheux, L.; Galien, R.; Vayssiere, B.; Nelles, L.; Christophe, T.; Brys, R.; Uhring, M.; Ciesielski, F.; Van Rompaey, L.
Deposited on : 2014-03-27
Resolution : 2.40 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)

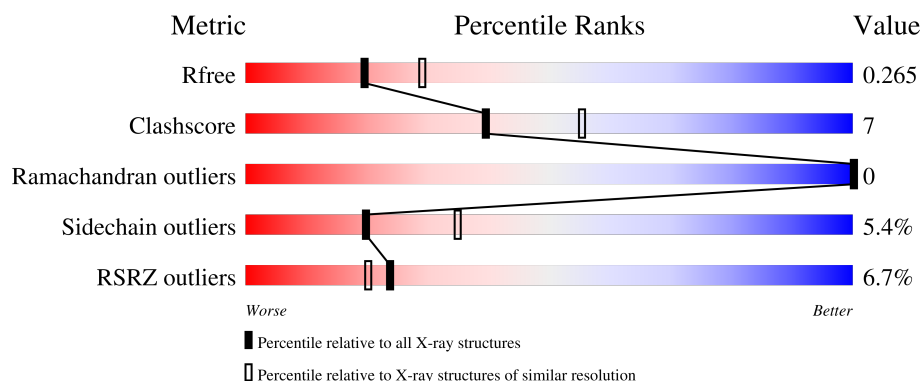
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	293	7% 81% 14% ..
1	B	293	6% 77% 18% ..

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5052 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.

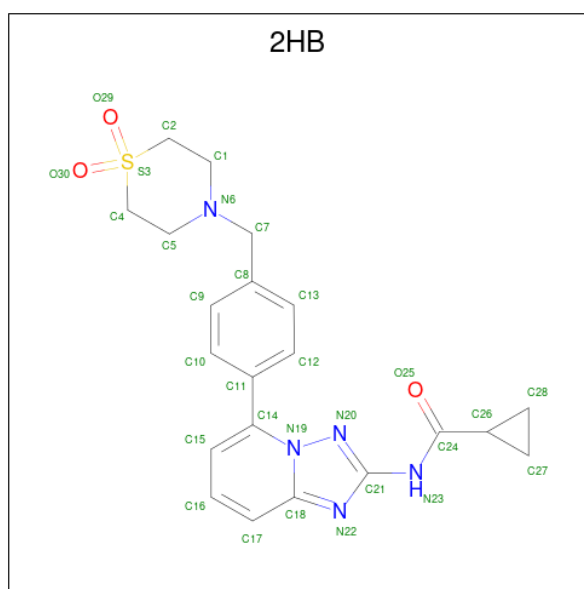
- Molecule 1 is a protein called Tyrosine-protein kinase JAK2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	P	S	0	0	0
			2348	1492	403	437	2	14			
1	B	287	Total	C	N	O	P	S	0	0	0
			2379	1511	407	445	2	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1129	GLN	ASN	engineered mutation	UNP O60674
B	1129	GLN	ASN	engineered mutation	UNP O60674

- Molecule 2 is N-(5-{4-[(1,1-dioxidothiomorpholin-4-yl)methyl]phenyl}[1,2,4]triazolo[1,5-a]pyridin-2-yl)cyclopropanecarboxamide (CCD ID: 2HB) (formula: C₂₁H₂₃N₅O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			30	21	5	3	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			30	21	5	3	1		

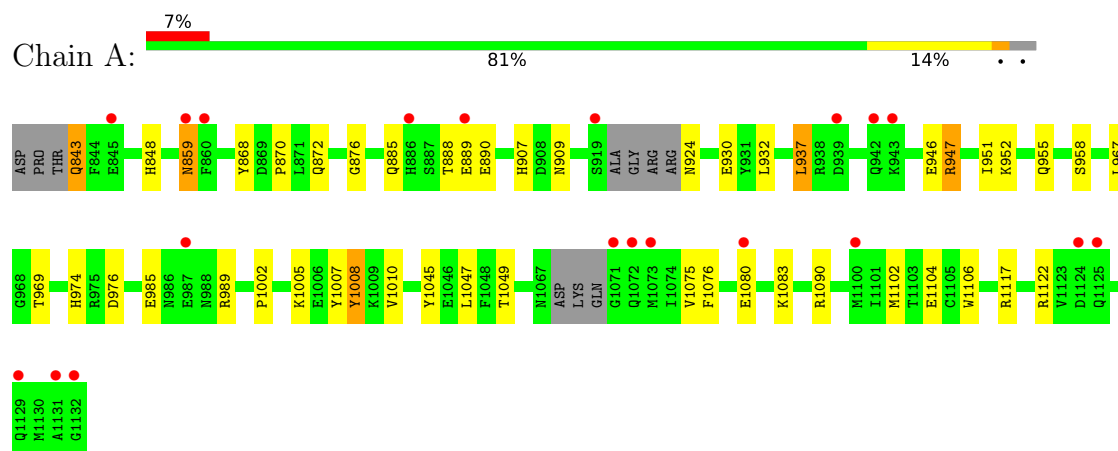
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	138	Total	O	0	0
			138	138		
3	B	127	Total	O	0	0
			127	127		

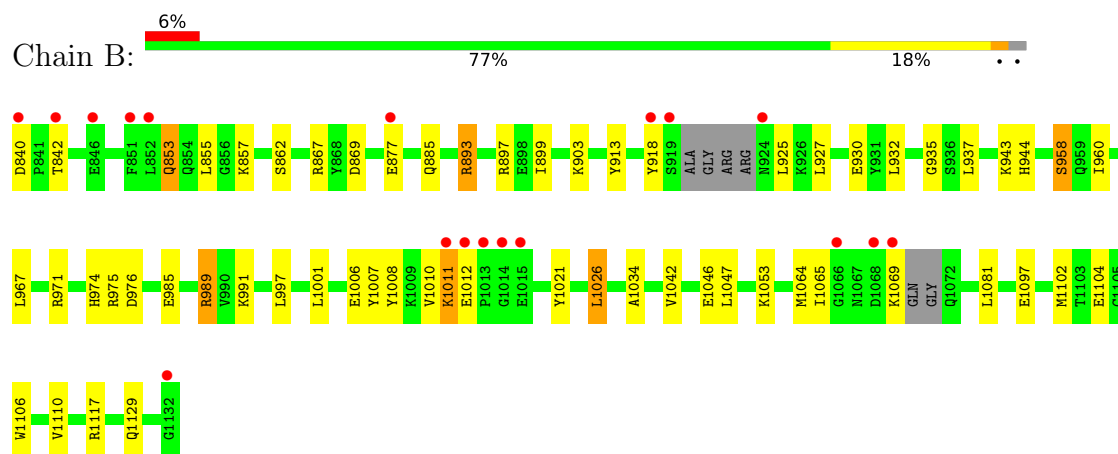
3 Residue-property plots [i](#)

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: Tyrosine-protein kinase JAK2



- Molecule 1: Tyrosine-protein kinase JAK2



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	111.39Å 111.39Å 71.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	111.39 – 2.40 111.39 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (111.39-2.40) 99.3 (111.39-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.95 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.267 0.204 , 0.265	Depositor DCC
R_{free} test set	1722 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5052	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: PTR, 2HB

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	0.61	0/2363	0.89	0/3175
1	B	0.61	0/2395	0.87	0/3220
All	All	0.61	0/4758	0.88	0/6395

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	2348	0	2319	28	0
1	B	2379	0	2345	37	0
2	A	30	0	23	1	0
2	B	30	0	23	3	0
3	A	138	0	0	3	0
3	B	127	0	0	7	0
All	All	5052	0	4710	64	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 7.

All (64) 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:960:ILE:HG13	3:B:1423:HOH:O	1.50	1.11
1:B:958:SER:HB2	3:B:1302:HOH:O	1.66	0.94
1:A:1002:PRO:HG2	1:A:1005:LYS:HB2	1.69	0.74
1:A:1008:PTR:HE1	1:A:1010:VAL:HB	1.71	0.70
1:B:1117:ARG:HD3	3:B:1411:HOH:O	1.95	0.66
1:B:885:GLN:HG3	3:B:1379:HOH:O	1.99	0.62
1:A:848:HIS:HD2	1:A:872:GLN:HE21	1.46	0.61
1:B:1034:ALA:CB	1:B:1110:VAL:HG13	2.30	0.61
1:A:1008:PTR:O3P	1:A:1008:PTR:HE2	2.02	0.60
1:B:1034:ALA:HB3	1:B:1110:VAL:HG13	1.84	0.59
1:A:952:LYS:HD3	1:A:955:GLN:HE21	1.69	0.57
1:B:855:LEU:HD22	2:B:1201:2HB:H22	1.86	0.56
1:A:974:HIS:HD2	1:A:976:ASP:H	1.53	0.56
1:B:857:LYS:HG3	1:B:862:SER:HB3	1.88	0.56
1:A:1045:TYR:O	1:A:1049:THR:HG23	2.05	0.56
1:A:1090:ARG:NH2	1:B:1104:GLU:OE1	2.40	0.55
1:B:867:ARG:HG2	1:B:869:ASP:HB2	1.90	0.54
1:B:943:LYS:HG3	1:B:944:HIS:CD2	2.44	0.53
1:A:985:GLU:OE1	1:A:989:ARG:HD2	2.09	0.53
1:A:1102:MET:HE3	1:A:1106:TRP:CH2	2.45	0.52
1:B:932:LEU:HD22	1:B:985:GLU:HG3	1.91	0.52
1:B:893:ARG:HG3	1:B:897:ARG:HH21	1.76	0.51
1:A:868:TYR:O	1:A:876:GLY:HA3	2.11	0.50
1:B:840:ASP:OD1	1:B:842:THR:HG22	2.10	0.50
1:B:1102:MET:HE3	1:B:1106:TRP:CH2	2.47	0.50
1:B:1102:MET:HE3	1:B:1106:TRP:HH2	1.76	0.50
1:A:888:THR:HG22	1:A:889:GLU:H	1.77	0.49
1:A:890:GLU:HG3	3:A:1426:HOH:O	2.12	0.49
1:A:1102:MET:HE3	1:A:1106:TRP:HH2	1.78	0.49
1:B:989:ARG:HG3	1:B:989:ARG:NH1	2.28	0.48
1:A:930:GLU:O	2:A:1201:2HB:H17	2.12	0.48
1:B:935:GLY:HA2	2:B:1201:2HB:C24	2.43	0.48
1:B:903:LYS:HG3	1:B:913:TYR:CE2	2.49	0.48
1:A:947:ARG:O	1:A:947:ARG:HG2	2.13	0.48
1:A:1045:TYR:HB2	1:A:1102:MET:HE3	1.96	0.48
1:A:932:LEU:HD22	1:A:985:GLU:HG3	1.97	0.47
1:B:976:ASP:HB2	1:B:997:LEU:HD12	1.95	0.47
1:B:1065:ILE:HG13	1:B:1081:LEU:HD22	1.96	0.47
1:B:1064:MET:HG3	1:B:1081:LEU:HD21	1.96	0.47
1:B:971:ARG:NH2	1:B:1006:GLU:OE1	2.48	0.46
1:B:1011:LYS:HD3	1:B:1011:LYS:H	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:960:ILE:CG1	3:B:1423:HOH:O	2.32	0.46
1:B:989:ARG:HG3	1:B:989:ARG:HH11	1.80	0.46
1:A:1104:GLU:OE1	1:A:1122:ARG:NH1	2.46	0.46
1:B:899:ILE:HG12	1:B:927:LEU:HD13	1.98	0.46
1:B:989:ARG:CZ	3:B:1328:HOH:O	2.64	0.46
1:A:937:LEU:HD13	1:A:1047:LEU:HD21	1.99	0.44
1:A:888:THR:HG22	1:A:889:GLU:N	2.31	0.44
1:B:853:GLN:HE21	1:B:853:GLN:HB2	1.69	0.43
1:B:974:HIS:O	1:B:975:ARG:HB2	2.19	0.42
1:A:1075:VAL:HG23	3:A:1392:HOH:O	2.20	0.42
1:B:1021:TYR:HB3	1:B:1026:LEU:HD13	2.01	0.42
1:A:859:ASN:HD22	1:A:859:ASN:HA	1.59	0.42
1:A:885:GLN:OE1	1:A:885:GLN:HA	2.19	0.42
1:B:1110:VAL:HG11	3:B:1396:HOH:O	2.20	0.42
1:A:907:HIS:HE1	1:A:909:ASN:HD22	1.68	0.41
1:B:932:LEU:HD11	1:B:991:LYS:HD2	2.02	0.41
1:A:1076:PHE:O	1:A:1080:GLU:HG2	2.21	0.41
1:B:937:LEU:HD21	1:B:1047:LEU:HD21	2.01	0.41
1:A:843:GLN:N	3:A:1314:HOH:O	2.54	0.41
1:B:1042:VAL:O	1:B:1046:GLU:HG3	2.21	0.41
1:B:930:GLU:O	2:B:1201:2HB:H17	2.21	0.40
1:B:975:ARG:NH2	1:B:1010:VAL:HG21	2.36	0.40
1:A:848:HIS:CG	1:A:870:PRO:HA	2.57	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	275/293 (94%)	264 (96%)	11 (4%)	0	100	100
1	B	279/293 (95%)	269 (96%)	10 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	554/586 (94%)	533 (96%)	21 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	257/265 (97%)	245 (95%)	12 (5%)	23	41
1	B	261/265 (98%)	245 (94%)	16 (6%)	17	30
All	All	518/530 (98%)	490 (95%)	28 (5%)	20	35

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	843	GLN
1	A	859	ASN
1	A	924	ASN
1	A	937	LEU
1	A	946	GLU
1	A	947	ARG
1	A	951	ILE
1	A	958	SER
1	A	967	LEU
1	A	969	THR
1	A	1083	LYS
1	A	1117	ARG
1	B	853	GLN
1	B	877	GLU
1	B	893	ARG
1	B	918	TYR
1	B	925	LEU
1	B	958	SER
1	B	967	LEU
1	B	989	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1001	LEU
1	B	1011	LYS
1	B	1012	GLU
1	B	1026	LEU
1	B	1053	LYS
1	B	1069	LYS
1	B	1097	GLU
1	B	1129	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	848	HIS
1	A	853	GLN
1	A	859	ASN
1	A	872	GLN
1	A	909	ASN
1	A	944	HIS
1	A	950	HIS
1	A	955	GLN
1	A	974	HIS
1	A	988	ASN
1	A	1072	GLN
1	B	853	GLN
1	B	854	GLN
1	B	891	HIS
1	B	909	ASN
1	B	924	ASN
1	B	944	HIS
1	B	955	GLN
1	B	1111	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	PTR	B	1007	1	15,16,17	2.00	1 (6%)	17,22,24	0.75	1 (5%)
1	PTR	B	1008	1	15,16,17	1.96	1 (6%)	17,22,24	0.82	0
1	PTR	A	1008	1	15,16,17	2.02	1 (6%)	17,22,24	0.96	1 (5%)
1	PTR	A	1007	1	15,16,17	2.03	1 (6%)	17,22,24	0.69	1 (5%)

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	PTR	B	1007	1	-	2/10/11/13	0/1/1/1
1	PTR	B	1008	1	-	1/10/11/13	0/1/1/1
1	PTR	A	1008	1	-	1/10/11/13	0/1/1/1
1	PTR	A	1007	1	-	0/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1007	PTR	OH-CZ	-7.35	1.24	1.40
1	A	1007	PTR	OH-CZ	-7.27	1.24	1.40
1	A	1008	PTR	OH-CZ	-7.22	1.24	1.40
1	B	1008	PTR	OH-CZ	-7.05	1.24	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1007	PTR	O3P-P-OH	2.67	113.20	105.32
1	A	1007	PTR	O2P-P-OH	2.54	112.84	105.32
1	A	1008	PTR	OH-CZ-CE2	2.04	125.35	119.22

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1008	PTR	CZ-OH-P-O3P
1	B	1007	PTR	CZ-OH-P-O2P
1	B	1008	PTR	CZ-OH-P-O3P
1	B	1007	PTR	CZ-OH-P-O1P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1008	PTR	2	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	2HB	A	1201	-	34,34,34	1.53	6 (17%)	46,50,50	1.78	13 (28%)
2	2HB	B	1201	-	34,34,34	1.54	4 (11%)	46,50,50	1.75	14 (30%)

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	2HB	A	1201	-	-	0/16/30/30	0/5/5/5
2	2HB	B	1201	-	-	2/16/30/30	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	2HB	C11-C14	-5.00	1.40	1.48
2	A	1201	2HB	C11-C14	-4.85	1.40	1.48
2	B	1201	2HB	C18-N19	-3.02	1.35	1.39
2	A	1201	2HB	C18-N19	-2.86	1.35	1.39
2	A	1201	2HB	C21-N23	2.78	1.42	1.38
2	B	1201	2HB	C21-N23	2.64	1.42	1.38
2	B	1201	2HB	N19-N20	-2.31	1.34	1.38
2	A	1201	2HB	N19-N20	-2.20	1.34	1.38
2	A	1201	2HB	C21-N20	2.03	1.35	1.33
2	A	1201	2HB	C15-C14	2.01	1.41	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	2HB	C1-N6-C5	4.42	118.36	108.84
2	A	1201	2HB	N20-C21-N22	-4.38	110.83	116.67
2	B	1201	2HB	N20-C21-N22	-4.24	111.02	116.67
2	B	1201	2HB	C1-N6-C5	4.09	117.64	108.84
2	B	1201	2HB	C24-N23-C21	-3.45	121.47	127.40
2	A	1201	2HB	C7-N6-C5	3.40	118.38	111.07
2	B	1201	2HB	C7-N6-C5	3.38	118.35	111.07
2	A	1201	2HB	C24-N23-C21	-3.24	121.82	127.40
2	A	1201	2HB	C4-S3-C2	-3.21	96.14	101.11
2	A	1201	2HB	O29-S3-O30	3.19	120.54	117.89
2	B	1201	2HB	O29-S3-O30	3.08	120.45	117.89
2	B	1201	2HB	C4-S3-C2	-3.07	96.37	101.11
2	A	1201	2HB	C17-C18-N19	2.90	123.34	117.76
2	A	1201	2HB	C26-C24-N23	2.86	118.16	114.18
2	B	1201	2HB	C28-C26-C24	-2.77	114.53	117.24
2	B	1201	2HB	C17-C18-N19	2.66	122.89	117.76
2	B	1201	2HB	C15-C14-N19	2.52	118.21	115.22
2	A	1201	2HB	C7-N6-C1	2.31	116.04	111.07
2	A	1201	2HB	C14-N19-N20	2.22	129.59	125.77
2	B	1201	2HB	C27-C26-C24	2.20	119.39	117.24
2	A	1201	2HB	C16-C17-C18	-2.17	116.80	119.60
2	B	1201	2HB	C7-N6-C1	2.15	115.69	111.07
2	B	1201	2HB	C26-C24-N23	2.14	117.16	114.18
2	B	1201	2HB	C16-C17-C18	-2.13	116.85	119.60
2	B	1201	2HB	C2-C1-N6	-2.12	110.43	114.12
2	A	1201	2HB	C15-C14-N19	2.08	117.69	115.22
2	A	1201	2HB	C18-N19-N20	-2.02	109.08	111.96

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1201	2HB	N23-C24-C26-C28
2	B	1201	2HB	O25-C24-C26-C28

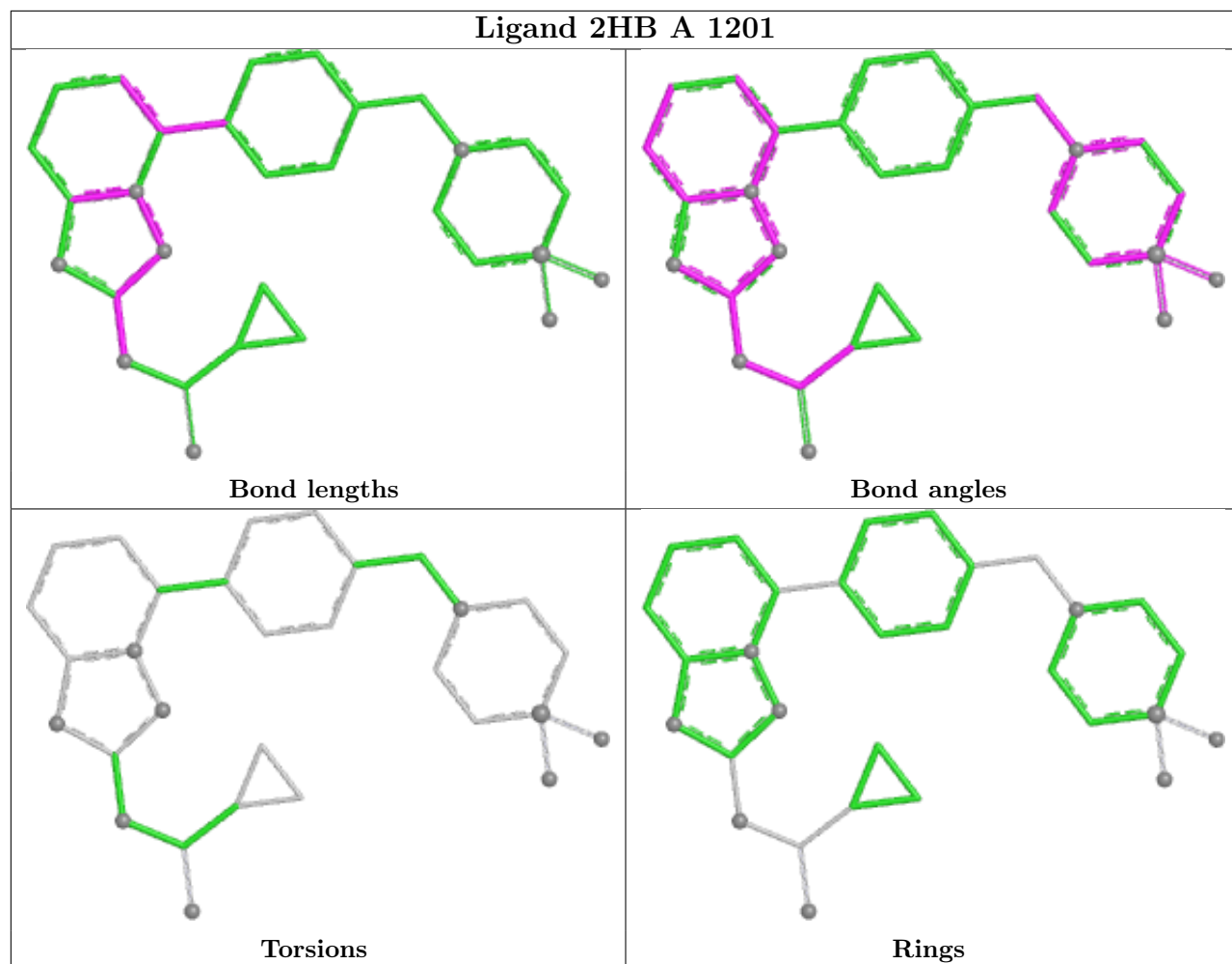
There are no ring outliers.

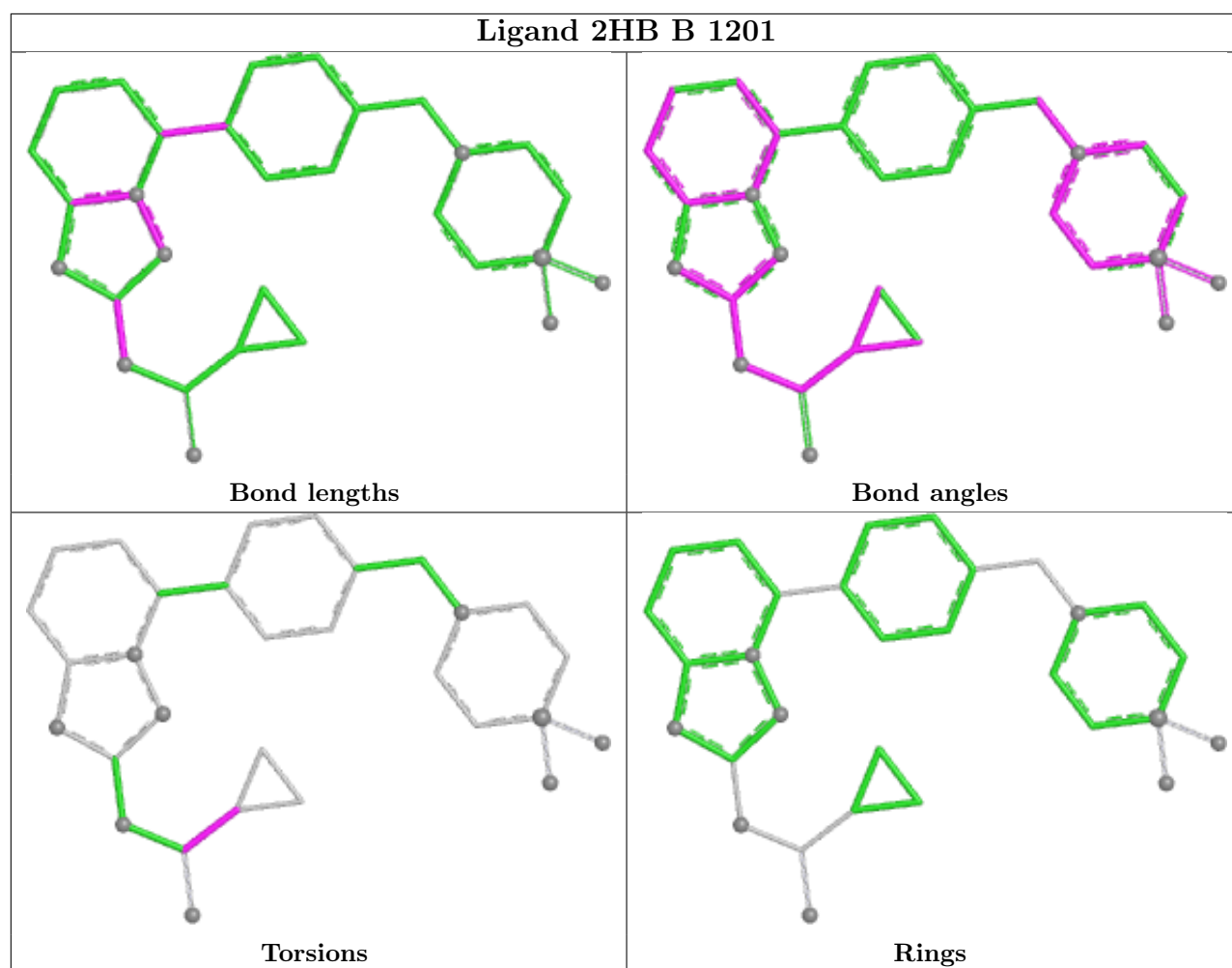
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	2HB	1	0
2	B	1201	2HB	3	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.

Ligand 2HB A 1201





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	281/293 (95%)	0.40	20 (7%)	22 18	18, 32, 56, 68	0
1	B	285/293 (97%)	0.55	18 (6%)	26 22	21, 36, 58, 67	0
All	All	566/586 (96%)	0.48	38 (6%)	24 20	18, 35, 58, 68	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1013	PRO	5.7
1	A	1132	GLY	5.3
1	A	1071	GLY	4.6
1	B	924	ASN	3.7
1	B	1012	GLU	3.7
1	B	1014	GLY	3.1
1	A	1073	MET	3.0
1	A	1131	ALA	3.0
1	A	1072	GLN	2.9
1	A	919	SER	2.7
1	B	842	THR	2.7
1	A	1124	ASP	2.7
1	B	851	PHE	2.7
1	B	1068	ASP	2.6
1	B	1011	LYS	2.6
1	B	918	TYR	2.6
1	A	1125	GLN	2.6
1	B	1132	GLY	2.5
1	A	845	GLU	2.5
1	B	1066	GLY	2.5
1	A	939	ASP	2.5
1	A	1080	GLU	2.5
1	A	987	GLU	2.4
1	B	1069	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	942	GLN	2.3
1	B	852	LEU	2.3
1	B	840	ASP	2.3
1	B	919	SER	2.2
1	B	846	GLU	2.2
1	A	886	HIS	2.2
1	A	889	GLU	2.2
1	A	1129	GLN	2.2
1	A	1100	MET	2.1
1	A	859	ASN	2.1
1	B	877	GLU	2.1
1	A	943	LYS	2.1
1	B	1015	GLU	2.0
1	A	860	PHE	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($\text{\AA}^2$)	Q<0.9
1	PTR	A	1007	16/17	0.86	0.14	41,45,55,55	0
1	PTR	B	1008	16/17	0.86	0.16	56,60,63,64	0
1	PTR	A	1008	16/17	0.89	0.13	40,45,51,51	0
1	PTR	B	1007	16/17	0.92	0.13	55,56,59,59	0

6.3 Carbohydrates [i](#)

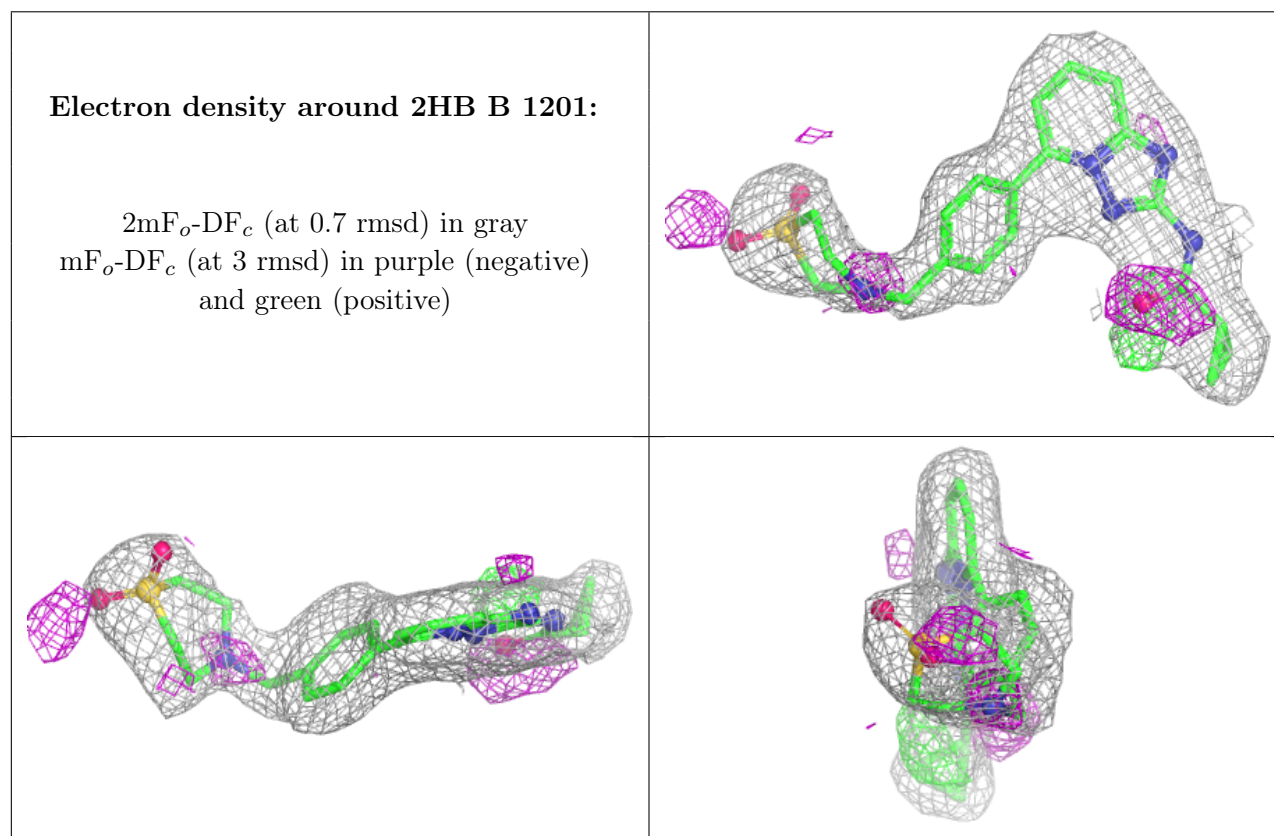
There are no oligosaccharides in this entry.

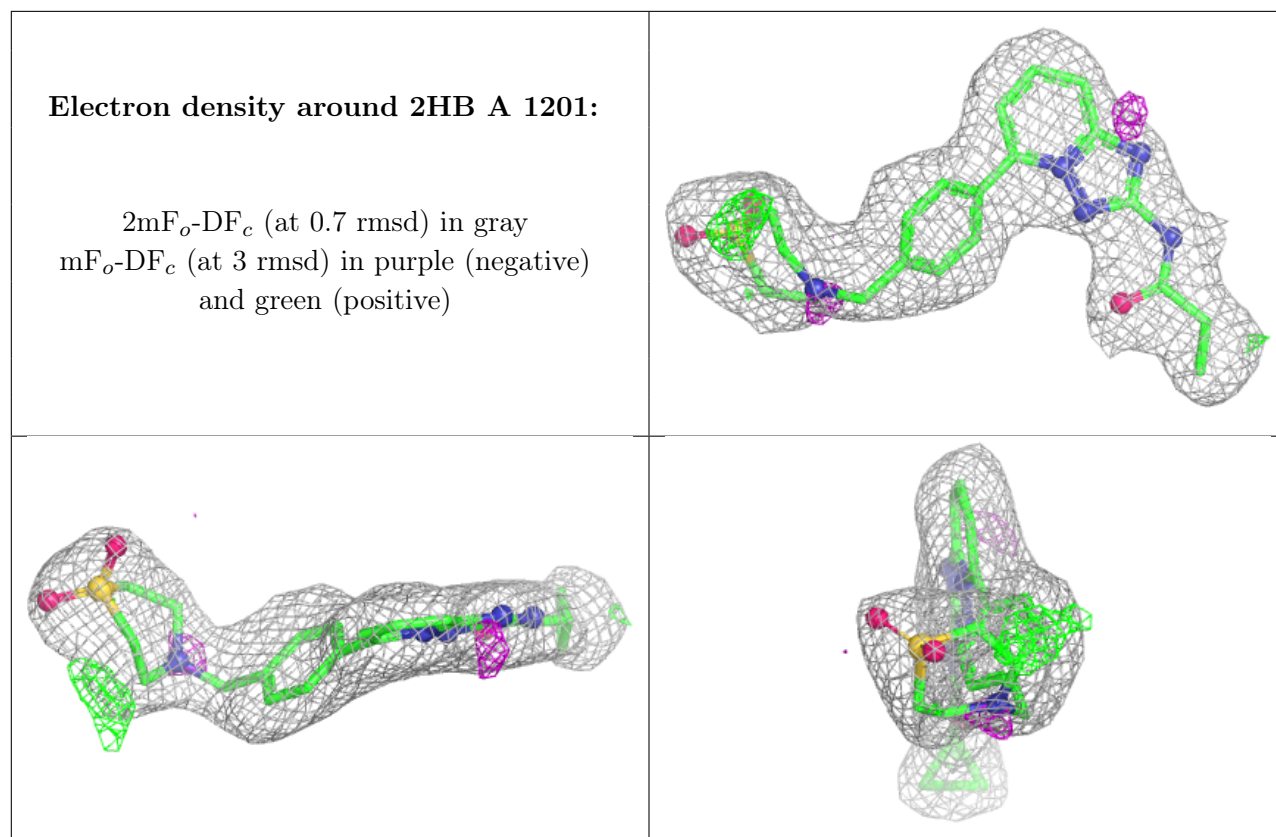
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
2	2HB	B	1201	30/30	0.90	0.12	19,24,44,45	0
2	2HB	A	1201	30/30	0.92	0.11	17,23,41,44	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.