



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:00 AM UTC

PDB ID : 2DXU / pdb_00002dxu
Title : Crystal Structure Of Biotin Protein Ligase From Pyrococcus Horikoshii Complexed with Biotinyl-5'-AMP, Mutation R48A
Authors : Bagautdinov, B.; Taketa, M.; Matsuura, Y.; Kunishima, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2006-08-30
Resolution : 1.28 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

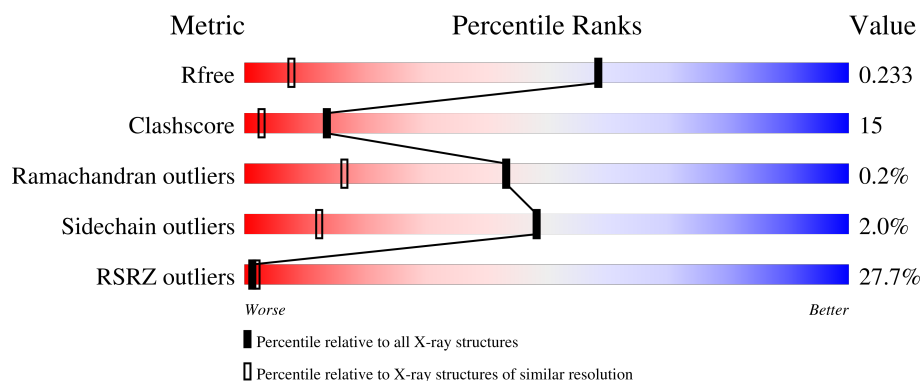
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.28 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	2836 (1.30-1.26)
Clashscore	190562	2911 (1.30-1.26)
Ramachandran outliers	187476	2841 (1.30-1.26)
Sidechain outliers	187428	2840 (1.30-1.26)
RSRZ outliers	180081	2832 (1.30-1.26)

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	235	25% 74% 23% .
1	B	235	28% 73% 20% 6%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4146 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.

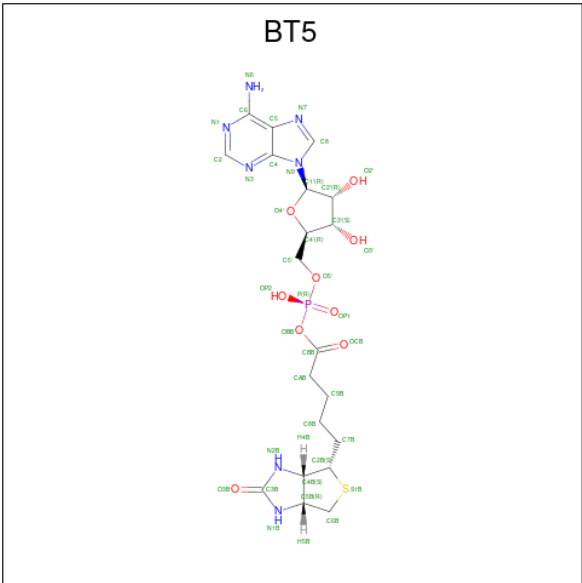
- Molecule 1 is a protein called biotin--[acetyl-CoA-carboxylase] ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1807	1168	304	330	5			
1	B	221	Total	C	N	O	S	0	0	0
			1723	1112	291	315	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	ALA	ARG	engineered mutation	UNP O57883
B	48	ALA	ARG	engineered mutation	UNP O57883

- Molecule 2 is BIOTINYL-5-AMP (CCD ID: BT5) (formula: C₂₀H₂₈N₇O₉PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	S	0	0
			38	20	7	9	1	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	S	0	0
			38	20	7	9	1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	276	Total	O	0	0
			276	276		
3	B	264	Total	O	0	0
			264	264		

i

- Molecule 1: biotin--[acetyl-CoA-carboxylase] ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	38.24Å 82.85Å 72.35Å 90.00° 101.37° 90.00°	Depositor
Resolution (Å)	37.49 – 1.28 37.49 – 1.28	Depositor EDS
% Data completeness (in resolution range)	97.0 (37.49-1.28) 96.9 (37.49-1.28)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.41 (at 1.28Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.233 0.223 , 0.233	Depositor DCC
R_{free} test set	5518 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	12.1	Xtriage
Anisotropy	0.644	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4146	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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: BT5

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	0.42	0/1834	0.90	4/2473 (0.2%)
1	B	0.40	0/1748	0.87	3/2358 (0.1%)
All	All	0.41	0/3582	0.88	7/4831 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	GLY	N-CA-C	-8.02	101.00	112.55
1	B	49	LEU	CA-C-N	-5.96	113.05	122.95
1	B	49	LEU	C-N-CA	-5.96	113.05	122.95
1	A	28	THR	N-CA-C	5.71	117.58	111.36
1	A	135	LYS	N-CA-C	-5.37	102.93	110.50
1	A	17	GLN	N-CA-C	-5.13	105.76	111.36
1	A	99	ILE	N-CA-C	5.11	115.94	108.58

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	1807	0	1904	60	0
1	B	1723	0	1819	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	76	0	50	0	0
3	A	276	0	0	12	0
3	B	264	0	0	17	0
All	All	4146	0	3773	108	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 15.

All (108) 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:101:TRP:O	1:A:232:LEU:HD21	1.79	0.81
1:A:180:ASN:HA	1:A:183:ARG:NH1	2.01	0.74
1:A:233:ARG:NH1	1:A:233:ARG:HA	2.04	0.72
1:B:123:LYS:HB2	3:B:2523:HOH:O	1.91	0.69
1:B:147:LEU:HD13	3:B:2477:HOH:O	1.93	0.67
1:A:119:GLY:C	1:A:120:LYS:HD2	2.20	0.67
1:A:233:ARG:HA	1:A:233:ARG:CZ	2.25	0.66
1:A:200:PHE:HE1	1:A:215:ILE:HG21	1.61	0.65
1:B:69:LYS:HE2	3:B:2500:HOH:O	1.98	0.64
1:B:186:MET:HE1	1:B:207:ILE:HG23	1.80	0.64
1:A:54:GLU:CD	1:A:137:PRO:HB3	2.23	0.64
1:B:209:ASP:HB3	3:B:2559:HOH:O	1.96	0.64
1:B:122:ASP:N	3:B:2554:HOH:O	2.31	0.63
1:A:186:MET:HG3	1:A:188:LEU:HG	1.80	0.63
1:A:200:PHE:HE1	1:A:215:ILE:HD13	1.63	0.63
1:A:200:PHE:CE1	1:A:215:ILE:HD13	2.34	0.63
1:B:69:LYS:H	1:B:69:LYS:CD	2.14	0.61
1:B:215:ILE:HG13	3:B:2496:HOH:O	2.01	0.61
1:A:212:ARG:HD3	1:A:226:ILE:HD11	1.82	0.61
1:A:180:ASN:CG	1:A:183:ARG:HH12	2.09	0.60
1:A:203:ILE:HD13	3:A:345:HOH:O	2.00	0.60
1:B:225:VAL:HG21	3:B:2496:HOH:O	2.01	0.60
1:A:18:GLU:OE2	1:A:41:LYS:HE3	2.01	0.60
1:B:186:MET:HE3	1:B:188:LEU:HD11	1.84	0.59
1:A:226:ILE:HG23	3:A:441:HOH:O	2.03	0.59
1:A:54:GLU:OE2	1:A:137:PRO:HB3	2.03	0.58
1:A:100:LYS:HE3	1:A:233:ARG:HH12	1.69	0.58
1:A:66:LEU:C	1:A:68:PRO:HD3	2.29	0.57
1:A:91:LYS:HG3	3:A:370:HOH:O	2.04	0.56
1:A:183:ARG:NE	3:A:429:HOH:O	2.27	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ILE:HD12	1:A:203:ILE:N	2.21	0.56
1:A:183:ARG:HD3	1:A:206:ASP:OD1	2.05	0.56
1:A:212:ARG:HG2	1:A:226:ILE:HD13	1.88	0.56
1:A:183:ARG:NH2	3:A:449:HOH:O	2.38	0.55
1:B:69:LYS:H	1:B:69:LYS:HD2	1.71	0.55
1:B:75:LEU:HD22	1:B:124:ILE:HD11	1.87	0.55
1:A:135:LYS:HB3	1:A:135:LYS:NZ	2.21	0.55
1:B:67:SER:O	1:B:69:LYS:HE3	2.06	0.55
1:A:232:LEU:HD12	3:A:422:HOH:O	2.05	0.55
1:B:76:PRO:HA	3:B:2447:HOH:O	2.06	0.54
1:A:67:SER:N	1:A:68:PRO:HD3	2.22	0.54
1:A:120:LYS:HD2	1:A:120:LYS:N	2.23	0.54
1:A:200:PHE:CE1	1:A:215:ILE:HG21	2.42	0.54
1:A:71:PRO:HD2	1:A:74:ASP:OD2	2.09	0.53
1:A:101:TRP:HE3	1:A:232:LEU:CD2	2.21	0.53
1:B:203:ILE:N	1:B:203:ILE:CD1	2.71	0.53
1:A:49:LEU:HD11	1:A:229:ASP:OD1	2.09	0.52
1:A:183:ARG:NH2	3:A:429:HOH:O	2.42	0.52
1:A:183:ARG:HG2	1:A:207:ILE:HG12	1.92	0.51
1:A:226:ILE:HD13	3:A:441:HOH:O	2.10	0.51
1:A:56:PRO:HG2	1:A:134:ASN:HB2	1.93	0.51
1:B:72:GLN:NE2	1:B:75:LEU:HD12	2.25	0.51
1:B:108:ASN:HB3	3:B:2478:HOH:O	2.11	0.50
1:A:1:MET:HE2	3:B:2480:HOH:O	2.11	0.49
1:B:193:LYS:HE3	1:B:201:GLU:OE2	2.13	0.49
1:B:56:PRO:HG2	1:B:134:ASN:HB2	1.94	0.49
1:B:120:LYS:HD2	1:B:120:LYS:C	2.38	0.49
1:B:120:LYS:HE3	1:B:123:LYS:HE2	1.95	0.49
1:A:101:TRP:HE3	1:A:232:LEU:HD21	1.78	0.47
1:A:202:GLY:N	1:A:215:ILE:HD11	2.29	0.47
1:B:72:GLN:NE2	3:B:2476:HOH:O	2.22	0.47
1:B:120:LYS:CE	1:B:123:LYS:HE2	2.45	0.47
1:A:59:GLY:HA3	1:A:61:TRP:CZ2	2.49	0.47
1:A:180:ASN:HA	1:A:183:ARG:HH12	1.78	0.47
1:B:207:ILE:HD12	1:B:207:ILE:O	2.14	0.47
1:B:101:TRP:CE2	1:B:102:PRO:HB3	2.49	0.47
1:B:181:LEU:HD11	3:B:2498:HOH:O	2.14	0.47
1:B:75:LEU:HD22	1:B:124:ILE:CD1	2.45	0.47
1:A:100:LYS:HB3	1:A:104:ASP:HB2	1.97	0.46
1:B:32:GLU:HG3	3:B:2408:HOH:O	2.14	0.46
1:B:8:ILE:O	1:B:11:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LYS:HB3	1:A:135:LYS:HZ3	1.81	0.45
1:B:41:LYS:HG2	1:B:42:GLN:N	2.31	0.45
1:A:217:LEU:HD12	1:A:217:LEU:N	2.32	0.45
1:B:154:LEU:HD13	3:B:2480:HOH:O	2.17	0.45
1:B:62:LEU:C	1:B:62:LEU:HD12	2.41	0.45
1:B:100:LYS:HD2	1:B:106:LEU:HD11	1.99	0.44
1:A:62:LEU:C	1:A:62:LEU:HD12	2.43	0.44
1:B:176:MET:HE1	1:B:209:ASP:OD2	2.17	0.44
1:A:226:ILE:CD1	3:A:441:HOH:O	2.66	0.44
1:A:11:ARG:HG2	1:A:11:ARG:HH11	1.83	0.43
1:B:59:GLY:HA3	1:B:61:TRP:CZ2	2.53	0.43
1:B:179:LEU:O	1:B:183:ARG:HG3	2.17	0.43
1:B:217:LEU:HD12	1:B:217:LEU:N	2.34	0.43
1:B:72:GLN:HE22	1:B:75:LEU:HD12	1.83	0.43
1:A:193:LYS:HG3	1:A:201:GLU:HG2	2.00	0.43
1:B:44:MET:HA	1:B:44:MET:HE2	2.00	0.43
1:B:203:ILE:N	1:B:203:ILE:HD12	2.32	0.43
1:B:52:LYS:HG3	3:B:2392:HOH:O	2.18	0.43
1:B:205:GLU:O	1:B:206:ASP:HB2	2.17	0.43
1:B:154:LEU:CD1	3:B:2480:HOH:O	2.67	0.42
1:B:207:ILE:HD12	1:B:207:ILE:C	2.43	0.42
1:A:235:LEU:N	1:A:235:LEU:HD12	2.34	0.42
1:A:227:TYR:HE2	3:A:364:HOH:O	2.01	0.42
1:A:201:GLU:OE2	1:A:235:LEU:HD21	2.20	0.42
1:B:24:GLU:HG2	1:B:46:HIS:HE1	1.84	0.42
1:A:119:GLY:HA3	1:A:124:ILE:HD13	2.02	0.41
1:A:191:ARG:HH11	1:A:235:LEU:CD2	2.32	0.41
1:A:233:ARG:CZ	1:A:234:PHE:H	2.34	0.41
1:A:233:ARG:HH11	1:A:233:ARG:HD2	1.72	0.41
1:B:176:MET:HE1	1:B:209:ASP:CG	2.45	0.41
1:A:212:ARG:HD3	1:A:226:ILE:CD1	2.51	0.41
1:A:232:LEU:N	1:A:232:LEU:HD23	2.36	0.41
1:B:101:TRP:CD2	1:B:102:PRO:HB3	2.56	0.41
1:A:192:VAL:HG12	1:A:234:PHE:CD1	2.56	0.41
1:B:2:LEU:CD2	3:B:2480:HOH:O	2.69	0.40
1:A:98:ARG:NH2	3:A:356:HOH:O	2.50	0.40
1:A:226:ILE:CD1	3:A:493:HOH:O	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	227/235 (97%)	220 (97%)	6 (3%)	1 (0%)	30	8
1	B	217/235 (92%)	213 (98%)	4 (2%)	0	100	100
All	All	444/470 (94%)	433 (98%)	10 (2%)	1 (0%)	43	16

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	GLY

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	202/204 (99%)	197 (98%)	5 (2%)	42	8
1	B	193/204 (95%)	190 (98%)	3 (2%)	55	19
All	All	395/408 (97%)	387 (98%)	8 (2%)	48	12

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	A	102	PRO
1	A	135	LYS
1	A	199	SER
1	A	232	LEU

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Mol	Chain	Res	Type
1	B	69	LYS
1	B	102	PRO
1	B	203	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	138	ASN
1	B	46	HIS
1	B	72	GLN

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](#)

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	BT5	B	2301	-	41,42,42	2.14	12 (29%)	60,62,62	1.68	12 (20%)
2	BT5	B	2302	-	41,42,42	2.21	12 (29%)	60,62,62	1.72	12 (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	BT5	B	2301	-	-	6/20/59/59	0/5/5/5
2	BT5	B	2302	-	-	6/20/59/59	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2302	BT5	C9B-CAB	-6.58	1.28	1.52
2	B	2301	BT5	C9B-CAB	-6.50	1.28	1.52
2	B	2302	BT5	P-OBB	5.30	1.70	1.60
2	B	2301	BT5	P-OBB	5.07	1.69	1.60
2	B	2302	BT5	C2-N1	4.35	1.41	1.33
2	B	2302	BT5	C2-N3	4.14	1.41	1.33
2	B	2301	BT5	C2-N1	3.98	1.41	1.33
2	B	2302	BT5	P-O5'	-3.94	1.44	1.59
2	B	2301	BT5	C2-N3	3.63	1.40	1.33
2	B	2301	BT5	P-O5'	-3.59	1.45	1.59
2	B	2302	BT5	P-OP2	-3.48	1.39	1.55
2	B	2301	BT5	P-OP2	-3.45	1.39	1.55
2	B	2302	BT5	C4-N3	3.37	1.40	1.34
2	B	2301	BT5	C4-N3	3.09	1.40	1.34
2	B	2302	BT5	C1'-N9	2.92	1.54	1.46
2	B	2301	BT5	C5'-C4'	-2.63	1.43	1.51
2	B	2301	BT5	C8-N7	2.56	1.36	1.31
2	B	2301	BT5	C1'-N9	2.53	1.53	1.46
2	B	2302	BT5	C5'-C4'	-2.48	1.44	1.51
2	B	2302	BT5	C8-N7	2.40	1.36	1.31
2	B	2302	BT5	C6-N1	2.38	1.42	1.35
2	B	2301	BT5	C6-N1	2.36	1.42	1.35
2	B	2302	BT5	C2B-S1B	-2.26	1.79	1.82
2	B	2301	BT5	C2B-S1B	-2.11	1.79	1.82

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2302	BT5	N3-C2-N1	-6.28	119.08	128.58
2	B	2301	BT5	N3-C2-N1	-6.18	119.23	128.58
2	B	2301	BT5	C2B-C4B-C5B	-3.37	104.77	108.89
2	B	2302	BT5	C5-C4-N3	-3.36	122.09	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2301	BT5	C5B-C6B-S1B	-3.30	101.52	106.06
2	B	2302	BT5	C2B-C4B-C5B	-3.25	104.92	108.89
2	B	2302	BT5	C5B-C6B-S1B	-3.25	101.59	106.06
2	B	2301	BT5	C5-C4-N3	-3.06	122.50	126.72
2	B	2301	BT5	N9-C8-N7	-2.88	109.86	113.94
2	B	2302	BT5	C2-N3-C4	2.84	118.77	111.83
2	B	2301	BT5	C2-N3-C4	2.79	118.65	111.83
2	B	2302	BT5	N9-C8-N7	-2.69	110.12	113.94
2	B	2302	BT5	C9B-CAB-CBB	2.69	123.53	113.69
2	B	2302	BT5	N3-C4-N9	2.60	131.58	127.17
2	B	2301	BT5	C2-N1-C6	2.52	122.88	118.73
2	B	2301	BT5	C9B-CAB-CBB	2.48	122.79	113.69
2	B	2302	BT5	C2-N1-C6	2.35	122.60	118.73
2	B	2302	BT5	OP2-P-O5'	2.33	118.15	107.57
2	B	2302	BT5	C5-N7-C8	2.23	106.95	103.45
2	B	2301	BT5	N3-C4-N9	2.20	130.91	127.17
2	B	2301	BT5	C5-N7-C8	2.19	106.90	103.45
2	B	2302	BT5	C2B-C4B-N2B	2.18	115.65	113.34
2	B	2301	BT5	OP2-P-O5'	2.16	117.35	107.57
2	B	2301	BT5	N2B-C3B-N1B	2.02	111.18	108.85

There are no chirality outliers.

All (12) torsion outliers are listed below:

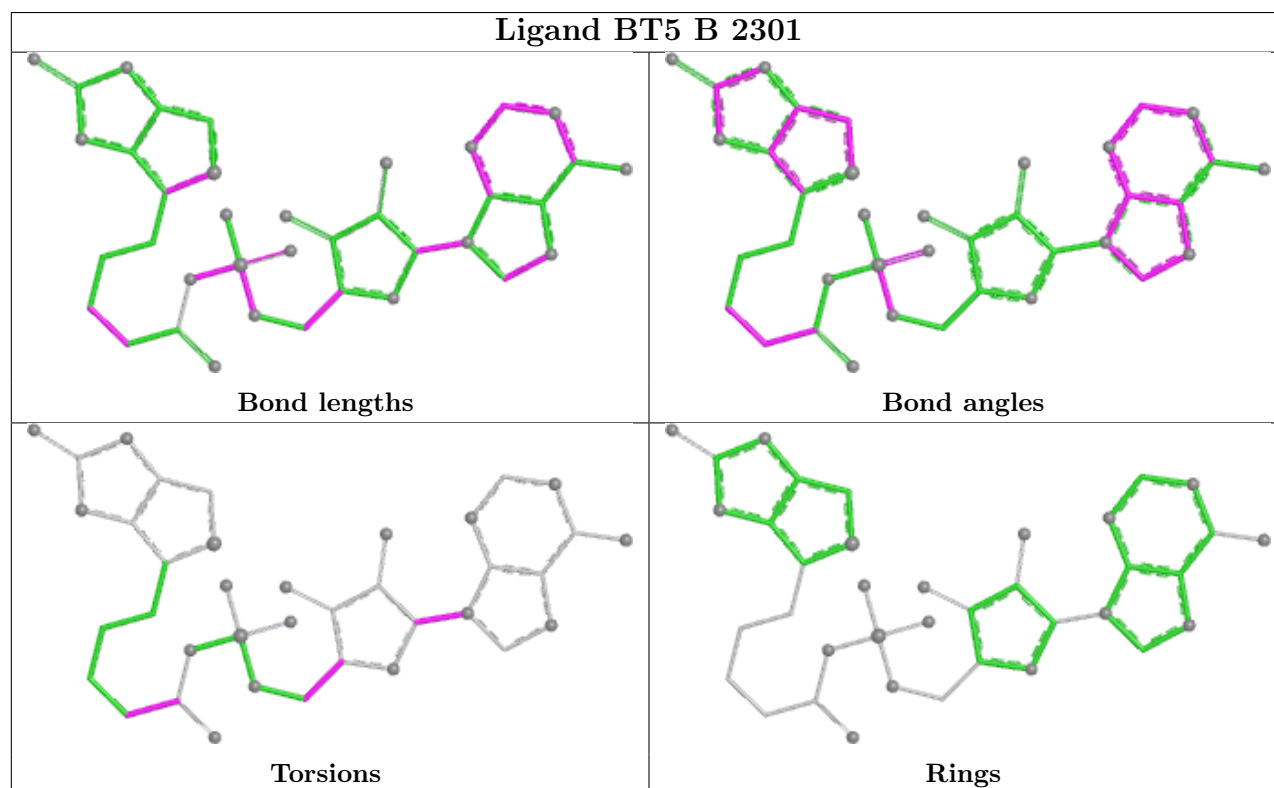
Mol	Chain	Res	Type	Atoms
2	B	2301	BT5	C9B-CAB-CBB-OBB
2	B	2302	BT5	C9B-CAB-CBB-OBB
2	B	2301	BT5	C3'-C4'-C5'-O5'
2	B	2302	BT5	C3'-C4'-C5'-O5'
2	B	2302	BT5	C2'-C1'-N9-C8
2	B	2301	BT5	C2'-C1'-N9-C8
2	B	2301	BT5	O4'-C4'-C5'-O5'
2	B	2302	BT5	C2'-C1'-N9-C4
2	B	2301	BT5	C2'-C1'-N9-C4
2	B	2301	BT5	O4'-C1'-N9-C8
2	B	2302	BT5	O4'-C1'-N9-C8
2	B	2302	BT5	O4'-C4'-C5'-O5'

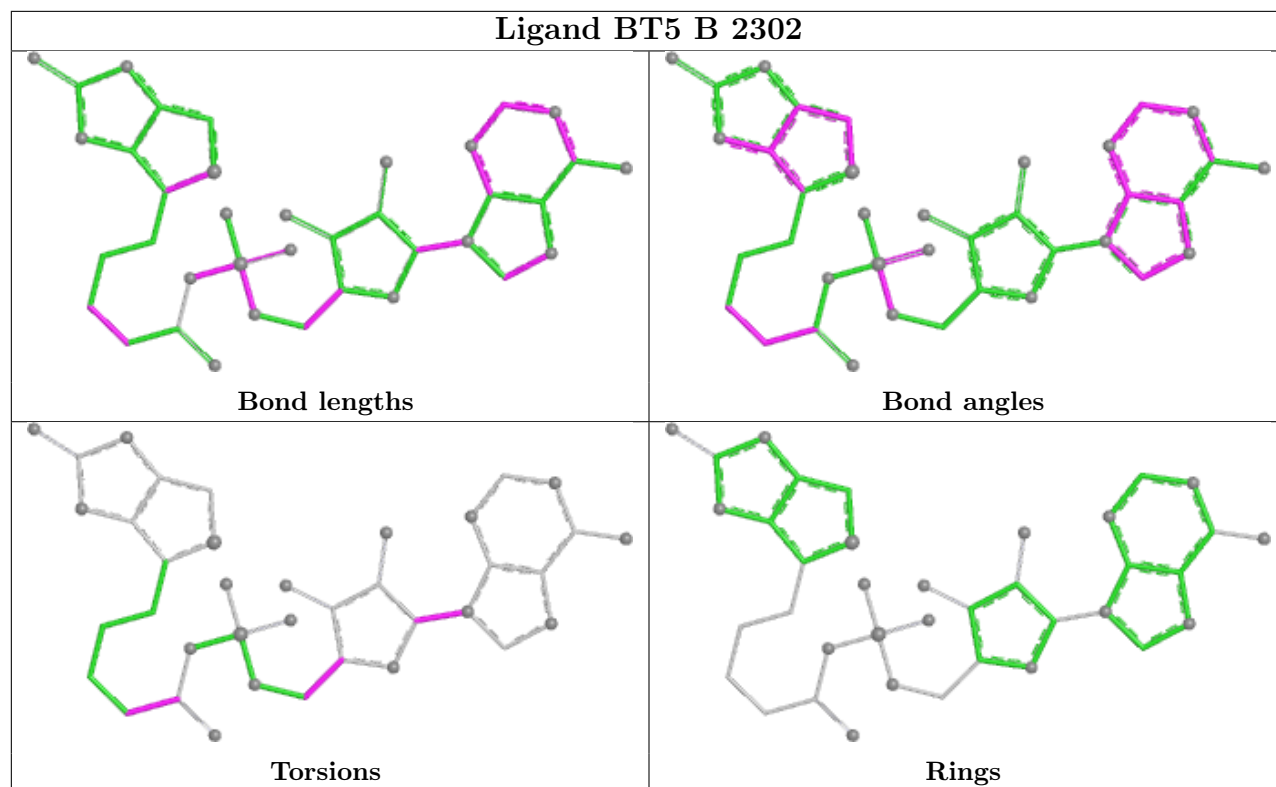
There are no ring outliers.

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

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	231/235 (98%)	1.37	59 (25%) 1 2	7, 13, 26, 41	0
1	B	221/235 (94%)	1.61	66 (29%) 1 1	8, 15, 26, 35	0
All	All	452/470 (96%)	1.49	125 (27%) 1 2	7, 14, 26, 41	0

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	119	GLY	7.3
1	B	109	TYR	6.7
1	B	121	GLY	6.6
1	B	122	ASP	6.3
1	B	209	ASP	6.0
1	B	210	PHE	5.8
1	A	230	VAL	5.8
1	A	231	SER	5.7
1	B	75	LEU	5.6
1	A	122	ASP	5.5
1	A	232	LEU	5.4
1	A	229	ASP	5.4
1	A	235	LEU	5.3
1	A	194	ILE	5.3
1	B	192	VAL	5.0
1	B	50	ASN	4.9
1	A	119	GLY	4.8
1	B	200	PHE	4.7
1	B	70	VAL	4.6
1	B	30	TYR	4.4
1	A	210	PHE	4.4
1	B	67	SER	4.4
1	B	180	ASN	4.4
1	A	227	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	121	GLY	4.1
1	A	226	ILE	4.1
1	B	76	PRO	4.1
1	A	228	GLY	4.1
1	B	207	ILE	4.0
1	B	226	ILE	3.9
1	A	233	ARG	3.8
1	A	138	ASN	3.8
1	A	71	PRO	3.7
1	A	180	ASN	3.6
1	A	183	ARG	3.5
1	B	184	ASP	3.5
1	B	57	GLU	3.5
1	A	199	SER	3.5
1	A	68	PRO	3.5
1	A	192	VAL	3.5
1	B	188	LEU	3.4
1	A	151	VAL	3.3
1	B	69	LYS	3.3
1	A	203	ILE	3.3
1	A	215	ILE	3.3
1	A	148	GLY	3.3
1	B	124	ILE	3.3
1	A	1	MET	3.2
1	A	217	LEU	3.2
1	B	199	SER	3.2
1	B	49	LEU	3.2
1	A	72	GLN	3.2
1	B	68	PRO	3.2
1	A	149	SER	3.1
1	B	108	ASN	3.1
1	A	184	ASP	3.1
1	B	72	GLN	3.1
1	A	150	GLU	3.0
1	B	190	VAL	3.0
1	B	138	ASN	3.0
1	B	217	LEU	3.0
1	B	193	LYS	3.0
1	B	44	MET	3.0
1	B	28	THR	2.9
1	B	204	ALA	2.9
1	A	200	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	49	LEU	2.8
1	A	234	PHE	2.8
1	A	32	GLU	2.8
1	B	140	ALA	2.8
1	B	71	PRO	2.7
1	B	148	GLY	2.7
1	A	124	ILE	2.7
1	B	11	ARG	2.7
1	A	70	VAL	2.7
1	A	147	LEU	2.7
1	A	193	LYS	2.7
1	B	107	VAL	2.7
1	B	183	ARG	2.6
1	B	48	ALA	2.6
1	A	80	PHE	2.5
1	B	203	ILE	2.5
1	B	98	ARG	2.5
1	B	145	LEU	2.5
1	A	225	VAL	2.5
1	B	225	VAL	2.5
1	B	123	LYS	2.4
1	A	75	LEU	2.4
1	B	32	GLU	2.4
1	B	120	LYS	2.4
1	A	207	ILE	2.4
1	A	50	ASN	2.4
1	B	43	THR	2.4
1	A	139	GLY	2.4
1	A	201	GLU	2.3
1	B	206	ASP	2.3
1	A	202	GLY	2.3
1	B	179	LEU	2.3
1	A	220	GLY	2.3
1	A	187	ILE	2.3
1	A	222	VAL	2.3
1	B	189	GLY	2.2
1	A	188	LEU	2.2
1	B	219	SER	2.2
1	B	73	LYS	2.2
1	B	117	VAL	2.2
1	A	206	ASP	2.2
1	B	176	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	149	SER	2.2
1	A	76	PRO	2.2
1	B	46	HIS	2.1
1	A	136	VAL	2.1
1	A	120	LYS	2.1
1	B	136	VAL	2.1
1	B	94	SER	2.1
1	B	139	GLY	2.1
1	A	179	LEU	2.1
1	A	186	MET	2.1
1	B	215	ILE	2.1
1	A	67	SER	2.0
1	B	29	SER	2.0
1	A	209	ASP	2.0
1	B	41	LYS	2.0
1	B	12	ARG	2.0
1	B	151	VAL	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](#)

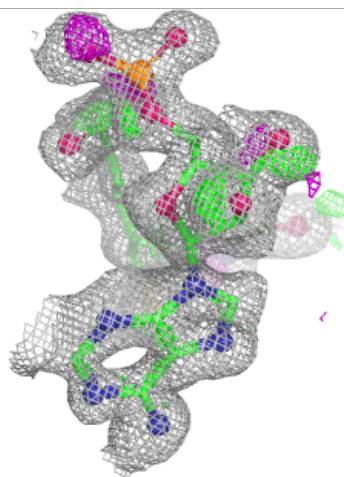
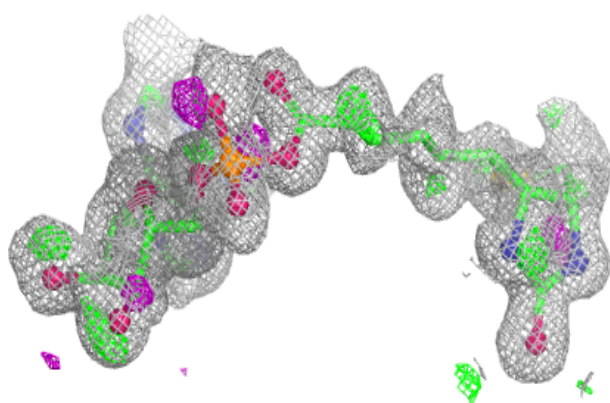
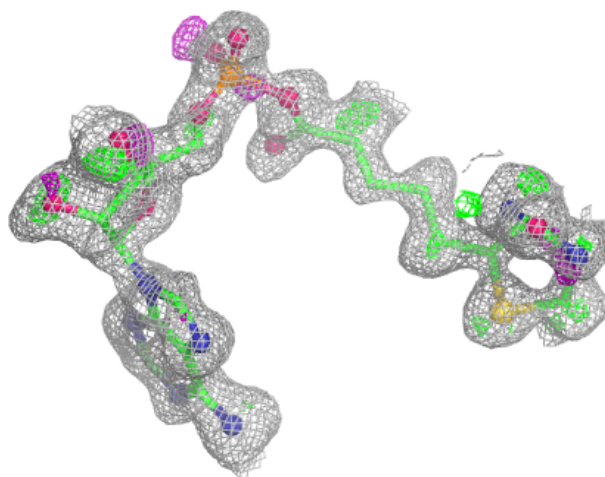
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

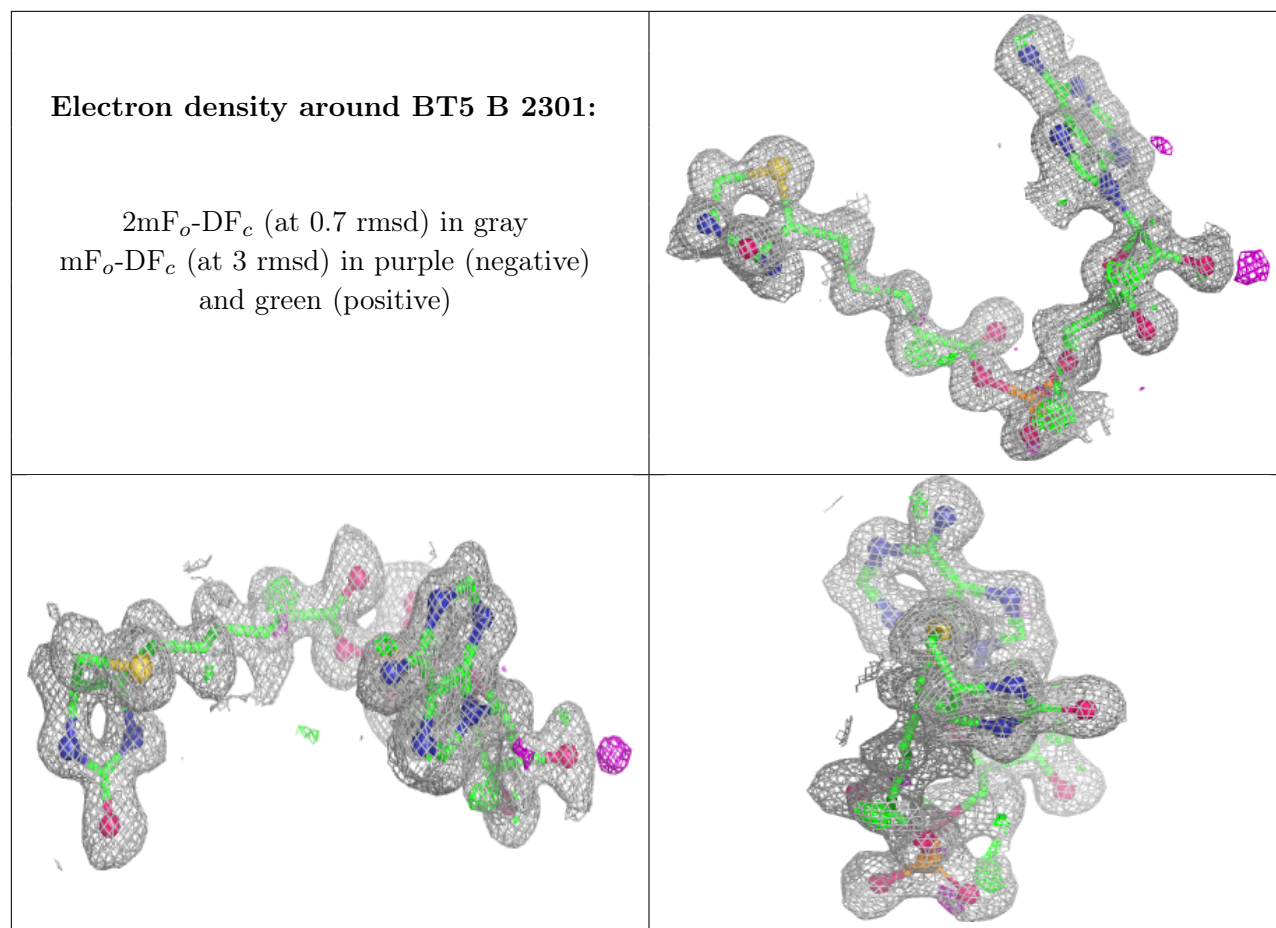
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BT5	B	2302	38/38	0.93	0.11	10,15,20,21	0
2	BT5	B	2301	38/38	0.96	0.08	7,10,16,16	0

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 BT5 B 2302:

$2mF_o-DF_c$ (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.