



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:26 pm BST

PDB ID : 4TK0  
Title : Crystal Structure of human Tankyrase 2 in complex with DPQ.  
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Deposited on : 2014-05-25  
Resolution : 1.65 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

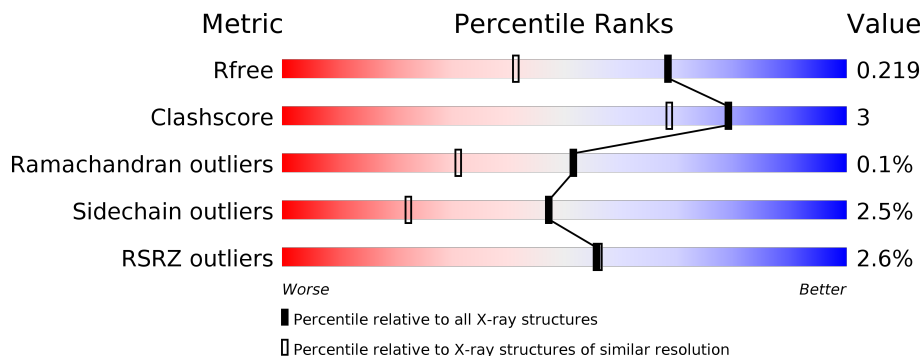
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1827 (1.66-1.66)
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)
RSRZ outliers	127900	1791 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	227	
1	B	227	
1	C	227	
1	D	227	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	3Z	A	1202	-	-	-	X

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7570 atoms, of which 78 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 Tankyrase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	199	Total 1605	C 1011	N 297	O 286	S 11	0	0	0
1	B	205	Total 1657	C 1046	N 304	O 296	S 11	0	0	0
1	C	208	Total 1686	C 1066	N 308	O 301	S 11	0	1	0
1	D	190	Total 1543	C 973	N 286	O 273	S 11	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	938	MET	-	initiating methionine	UNP Q9H2K2
A	939	GLY	-	expression tag	UNP Q9H2K2
A	940	SER	-	expression tag	UNP Q9H2K2
A	941	SER	-	expression tag	UNP Q9H2K2
A	942	HIS	-	expression tag	UNP Q9H2K2
A	943	HIS	-	expression tag	UNP Q9H2K2
A	944	HIS	-	expression tag	UNP Q9H2K2
A	945	HIS	-	expression tag	UNP Q9H2K2
A	946	HIS	-	expression tag	UNP Q9H2K2
A	947	HIS	-	expression tag	UNP Q9H2K2
A	948	SER	-	expression tag	UNP Q9H2K2
A	949	SER	-	expression tag	UNP Q9H2K2
A	950	GLY	-	expression tag	UNP Q9H2K2
A	951	ARG	-	expression tag	UNP Q9H2K2
A	952	GLU	-	expression tag	UNP Q9H2K2
A	953	ASN	-	expression tag	UNP Q9H2K2
A	954	LEU	-	expression tag	UNP Q9H2K2
A	955	TYR	-	expression tag	UNP Q9H2K2
A	956	PHE	-	expression tag	UNP Q9H2K2
A	957	GLN	-	expression tag	UNP Q9H2K2
A	958	GLY	-	expression tag	UNP Q9H2K2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	938	MET	-	initiating methionine	UNP Q9H2K2
B	939	GLY	-	expression tag	UNP Q9H2K2
B	940	SER	-	expression tag	UNP Q9H2K2
B	941	SER	-	expression tag	UNP Q9H2K2
B	942	HIS	-	expression tag	UNP Q9H2K2
B	943	HIS	-	expression tag	UNP Q9H2K2
B	944	HIS	-	expression tag	UNP Q9H2K2
B	945	HIS	-	expression tag	UNP Q9H2K2
B	946	HIS	-	expression tag	UNP Q9H2K2
B	947	HIS	-	expression tag	UNP Q9H2K2
B	948	SER	-	expression tag	UNP Q9H2K2
B	949	SER	-	expression tag	UNP Q9H2K2
B	950	GLY	-	expression tag	UNP Q9H2K2
B	951	ARG	-	expression tag	UNP Q9H2K2
B	952	GLU	-	expression tag	UNP Q9H2K2
B	953	ASN	-	expression tag	UNP Q9H2K2
B	954	LEU	-	expression tag	UNP Q9H2K2
B	955	TYR	-	expression tag	UNP Q9H2K2
B	956	PHE	-	expression tag	UNP Q9H2K2
B	957	GLN	-	expression tag	UNP Q9H2K2
B	958	GLY	-	expression tag	UNP Q9H2K2
C	938	MET	-	initiating methionine	UNP Q9H2K2
C	939	GLY	-	expression tag	UNP Q9H2K2
C	940	SER	-	expression tag	UNP Q9H2K2
C	941	SER	-	expression tag	UNP Q9H2K2
C	942	HIS	-	expression tag	UNP Q9H2K2
C	943	HIS	-	expression tag	UNP Q9H2K2
C	944	HIS	-	expression tag	UNP Q9H2K2
C	945	HIS	-	expression tag	UNP Q9H2K2
C	946	HIS	-	expression tag	UNP Q9H2K2
C	947	HIS	-	expression tag	UNP Q9H2K2
C	948	SER	-	expression tag	UNP Q9H2K2
C	949	SER	-	expression tag	UNP Q9H2K2
C	950	GLY	-	expression tag	UNP Q9H2K2
C	951	ARG	-	expression tag	UNP Q9H2K2
C	952	GLU	-	expression tag	UNP Q9H2K2
C	953	ASN	-	expression tag	UNP Q9H2K2
C	954	LEU	-	expression tag	UNP Q9H2K2
C	955	TYR	-	expression tag	UNP Q9H2K2
C	956	PHE	-	expression tag	UNP Q9H2K2
C	957	GLN	-	expression tag	UNP Q9H2K2
C	958	GLY	-	expression tag	UNP Q9H2K2

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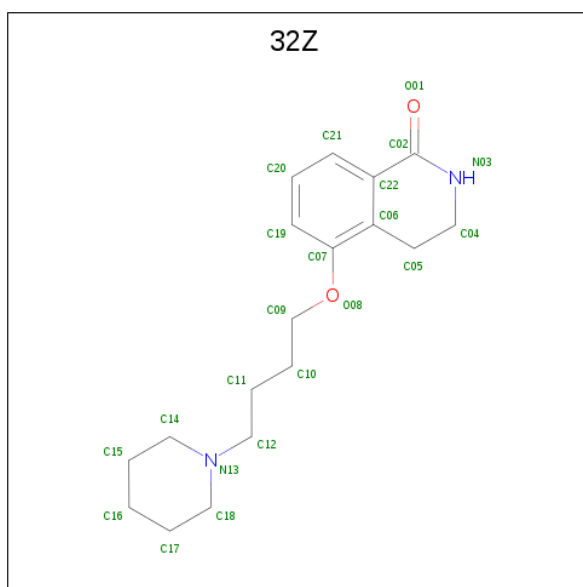
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Chain	Residue	Modelled	Actual	Comment	Reference
D	938	MET	-	initiating methionine	UNP Q9H2K2
D	939	GLY	-	expression tag	UNP Q9H2K2
D	940	SER	-	expression tag	UNP Q9H2K2
D	941	SER	-	expression tag	UNP Q9H2K2
D	942	HIS	-	expression tag	UNP Q9H2K2
D	943	HIS	-	expression tag	UNP Q9H2K2
D	944	HIS	-	expression tag	UNP Q9H2K2
D	945	HIS	-	expression tag	UNP Q9H2K2
D	946	HIS	-	expression tag	UNP Q9H2K2
D	947	HIS	-	expression tag	UNP Q9H2K2
D	948	SER	-	expression tag	UNP Q9H2K2
D	949	SER	-	expression tag	UNP Q9H2K2
D	950	GLY	-	expression tag	UNP Q9H2K2
D	951	ARG	-	expression tag	UNP Q9H2K2
D	952	GLU	-	expression tag	UNP Q9H2K2
D	953	ASN	-	expression tag	UNP Q9H2K2
D	954	LEU	-	expression tag	UNP Q9H2K2
D	955	TYR	-	expression tag	UNP Q9H2K2
D	956	PHE	-	expression tag	UNP Q9H2K2
D	957	GLN	-	expression tag	UNP Q9H2K2
D	958	GLY	-	expression tag	UNP Q9H2K2

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is 5-[4-(piperidin-1-yl)butoxy]-3,4-dihydroisoquinolin-1(2H)-one (three-letter code: 3Z) (formula: C<sub>18</sub>H<sub>26</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	H	N			O
3	A	1	48	18	26	2	2	0	0
3	B	1	48	18	26	2	2	0	0
3	C	1	48	18	26	2	2	0	0

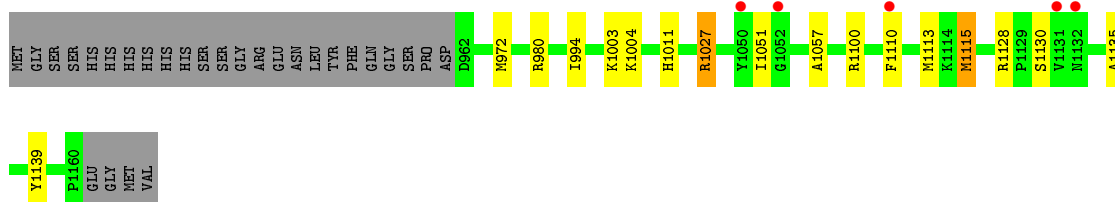
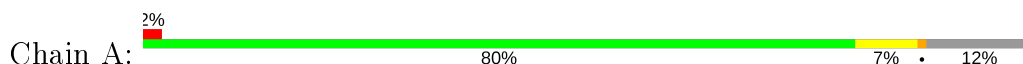
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	227	Total	O	0	0
			227	227		
4	B	239	Total	O	0	0
			239	239		
4	C	255	Total	O	0	0
			255	255		
4	D	211	Total	O	0	0
			211	211		

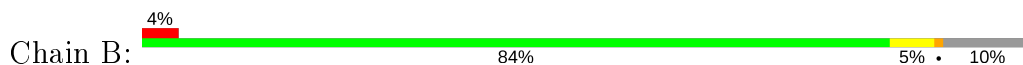
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

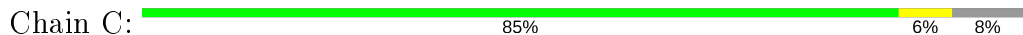
- Molecule 1: Tankyrase-2



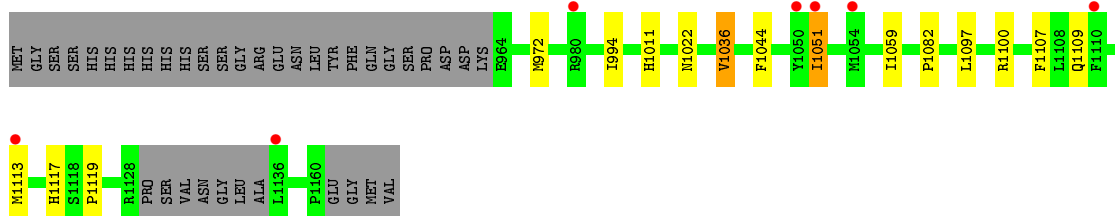
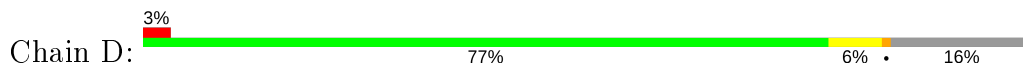
- Molecule 1: Tankyrase-2



- Molecule 1: Tankyrase-2



- Molecule 1: Tankyrase-2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.04Å 79.57Å 153.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.82 – 1.65 70.66 – 1.65	Depositor EDS
% Data completeness (in resolution range)	92.0 (76.82-1.65) 92.0 (70.66-1.65)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 1.65Å)	Xtrriage
Refinement program	BUSTER-TNT BUSTER 2.10.0, BUSTER 2.10.0	Depositor
R, $R_{free}$	0.187 , 0.225 0.188 , 0.219	Depositor DCC
$R_{free}$ test set	997 reflections (0.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtrriage
Anisotropy	0.431	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7570	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 3Z, ZN

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	0.51	0/1648	0.67	0/2215
1	B	0.57	1/1701 (0.1%)	0.72	3/2285 (0.1%)
1	C	0.51	0/1736	0.67	0/2335
1	D	0.50	0/1584	0.64	0/2126
All	All	0.52	1/6669 (0.0%)	0.68	3/8961 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	962	ASP	CB-CG	5.60	1.63	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	1053	GLY	N-CA-C	-5.92	98.29	113.10
1	B	1052	GLY	N-CA-C	5.24	126.20	113.10
1	B	991	ARG	N-CA-CB	-5.01	101.58	110.60

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	1605	0	1541	9	0
1	B	1657	0	1584	5	0
1	C	1686	0	1612	13	0
1	D	1543	0	1480	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	22	26	26	1	0
3	B	22	26	26	0	0
3	C	22	26	26	0	0
4	A	227	0	0	4	0
4	B	239	0	0	0	0
4	C	255	0	0	4	0
4	D	211	0	0	4	0
All	All	7492	78	6295	36	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 3.

All (36) 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:C:1023:HIS:HD2	1:C:1025:ASN:H	1.14	0.92
1:C:1105:LYS:H	1:C:1123:HIS:HD2	1.21	0.82
1:C:1023:HIS:CD2	1:C:1025:ASN:H	2.01	0.78
1:B:961:ASP:HB3	1:B:966:GLN:HE21	1.52	0.71
1:C:1023:HIS:HD2	1:C:1025:ASN:N	1.93	0.60
1:A:1057:ALA:O	1:C:1117:HIS:HE1	1.85	0.59
1:B:1057:ALA:O	1:D:1117:HIS:HE1	1.86	0.59
1:C:1036:VAL:HG22	1:C:1097:LEU:HG	1.83	0.58
1:A:980:ARG:HE	1:A:1135:ALA:HB2	1.69	0.58
1:A:1115:MET:CE	4:A:1434:HOH:O	2.54	0.55
1:A:1110:PHE:HD2	1:A:1130:SER:HB3	1.72	0.54
1:A:1115:MET:HE2	4:A:1434:HOH:O	2.07	0.54
1:D:1109:GLN:NE2	1:D:1113:MET:SD	2.80	0.54
1:C:1011:HIS:HE1	4:C:1449:HOH:O	1.91	0.53
1:A:1011:HIS:HE1	4:A:1473:HOH:O	1.92	0.52
1:A:972:MET:HG2	1:A:994:ILE:HD11	1.92	0.52
1:D:1117:HIS:HD2	4:D:1295:HOH:O	1.92	0.52
1:C:972:MET:HG2	1:C:994:ILE:HD11	1.91	0.51
1:A:1027:ARG:NH1	1:A:1139:TYR:OH	2.43	0.51
1:C:1023:HIS:HE1	1:D:1022:ASN:O	1.94	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1036:VAL:HG22	1:D:1097:LEU:HG	1.91	0.50
1:C:1082:PRO:HD2	4:C:1524:HOH:O	2.10	0.50
1:A:1113:MET:HG2	1:A:1115:MET:HE3	1.95	0.48
1:C:1117:HIS:HD2	4:C:1354:HOH:O	1.95	0.48
1:C:1083:VAL:CG1	1:C:1092:CYS:SG	3.02	0.48
1:D:972:MET:HG2	1:D:994:ILE:HD11	1.96	0.47
1:C:1083:VAL:HG12	4:C:1524:HOH:O	2.13	0.47
1:B:972:MET:HG2	1:B:994:ILE:HD11	1.96	0.47
1:D:1011:HIS:HE1	4:D:1231:HOH:O	2.00	0.45
1:D:1107:PHE:CG	1:D:1119:PRO:HG2	2.54	0.43
1:B:1051:ILE:HG23	1:B:1051:ILE:O	2.19	0.42
3:A:1202:3Z:H042	4:A:1485:HOH:O	2.20	0.41
1:D:1113:MET:HE1	4:D:1411:HOH:O	2.20	0.41
1:D:1082:PRO:HD2	4:D:1319:HOH:O	2.20	0.41
1:B:1044:PHE:HB3	1:B:1059:ILE:HD13	2.04	0.40
1:D:1044:PHE:HB3	1:D:1059:ILE:HD13	2.03	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	197/227 (87%)	192 (98%)	5 (2%)	0	100	100
1	B	201/227 (88%)	198 (98%)	3 (2%)	0	100	100
1	C	207/227 (91%)	205 (99%)	2 (1%)	0	100	100
1	D	186/227 (82%)	181 (97%)	4 (2%)	1 (0%)	29	11
All	All	791/908 (87%)	776 (98%)	14 (2%)	1 (0%)	51	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1051	ILE

### 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	168/192 (88%)	161 (96%)	7 (4%)	30	8
1	B	173/192 (90%)	169 (98%)	4 (2%)	50	25
1	C	177/192 (92%)	174 (98%)	3 (2%)	60	39
1	D	161/192 (84%)	158 (98%)	3 (2%)	57	34
All	All	679/768 (88%)	662 (98%)	17 (2%)	47	22

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1003	LYS
1	A	1004	LYS
1	A	1027	ARG
1	A	1051	ILE
1	A	1100	ARG
1	A	1115	MET
1	A	1128	ARG
1	B	991	ARG
1	B	1051	ILE
1	B	1100	ARG
1	B	1131	VAL
1	C	957	GLN
1	C	1036	VAL
1	C	1100	ARG
1	D	1036	VAL
1	D	1051	ILE
1	D	1100	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1011	HIS
1	A	1048	HIS
1	B	966	GLN
1	B	1011	HIS
1	B	1037	ASN
1	B	1041	HIS
1	B	1048	HIS
1	B	1070	GLN
1	C	1011	HIS
1	C	1023	HIS
1	C	1037	ASN
1	C	1117	HIS
1	C	1123	HIS
1	D	1011	HIS
1	D	1117	HIS

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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
3	32Z	B	1202	-	23,24,24	1.51	5 (21%)	30,31,31	1.73	9 (30%)
3	32Z	C	1202	-	23,24,24	1.29	1 (4%)	30,31,31	1.29	5 (16%)
3	32Z	A	1202	-	23,24,24	1.76	7 (30%)	30,31,31	1.68	5 (16%)

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
3	32Z	B	1202	-	-	2/8/26/26	0/3/3/3
3	32Z	C	1202	-	-	5/8/26/26	0/3/3/3
3	32Z	A	1202	-	-	4/8/26/26	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1202	32Z	C07-C06	3.87	1.45	1.40
3	C	1202	32Z	C12-N13	3.57	1.55	1.47
3	B	1202	32Z	C20-C19	3.41	1.46	1.38
3	A	1202	32Z	C12-N13	2.89	1.54	1.47
3	A	1202	32Z	C22-C02	2.77	1.51	1.47
3	A	1202	32Z	C20-C19	2.72	1.44	1.38
3	B	1202	32Z	C04-N03	2.44	1.51	1.46
3	B	1202	32Z	C14-N13	2.39	1.53	1.46
3	A	1202	32Z	C15-C14	2.37	1.59	1.51
3	A	1202	32Z	C14-N13	2.32	1.53	1.46
3	B	1202	32Z	C12-N13	2.30	1.52	1.47
3	A	1202	32Z	C22-C06	2.12	1.43	1.40
3	B	1202	32Z	C18-N13	2.04	1.52	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1202	32Z	C09-O08-C07	4.02	127.52	117.69
3	A	1202	32Z	C15-C14-N13	3.80	117.42	111.33
3	B	1202	32Z	C15-C14-N13	3.78	117.40	111.33
3	B	1202	32Z	C17-C18-N13	3.15	116.38	111.33
3	B	1202	32Z	C18-N13-C14	3.12	115.86	108.83
3	B	1202	32Z	O08-C07-C06	-2.96	111.44	115.71
3	A	1202	32Z	C05-C04-N03	2.76	114.97	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1202	32Z	C21-C22-C06	2.42	122.64	119.78
3	A	1202	32Z	C17-C18-N13	2.32	115.05	111.33
3	B	1202	32Z	O08-C07-C19	2.26	128.86	123.97
3	A	1202	32Z	C21-C22-C06	2.21	122.40	119.78
3	C	1202	32Z	C12-N13-C14	2.19	116.84	111.23
3	B	1202	32Z	C09-O08-C07	2.13	122.90	117.69
3	C	1202	32Z	C15-C14-N13	2.12	114.73	111.33
3	B	1202	32Z	C12-N13-C18	-2.10	105.86	111.23
3	B	1202	32Z	C06-C22-C02	-2.09	119.38	120.58
3	C	1202	32Z	C21-C22-C06	2.08	122.24	119.78
3	C	1202	32Z	C06-C22-C02	-2.03	119.42	120.58
3	C	1202	32Z	C05-C04-N03	2.01	113.64	110.13

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1202	32Z	C10-C11-C12-N13
3	B	1202	32Z	O08-C09-C10-C11
3	A	1202	32Z	C09-C10-C11-C12
3	C	1202	32Z	C10-C09-O08-C07
3	C	1202	32Z	O08-C09-C10-C11
3	A	1202	32Z	C19-C07-O08-C09
3	B	1202	32Z	C10-C11-C12-N13
3	A	1202	32Z	C06-C07-O08-C09
3	A	1202	32Z	O08-C09-C10-C11
3	C	1202	32Z	C19-C07-O08-C09
3	C	1202	32Z	C06-C07-O08-C09

There are no ring outliers.

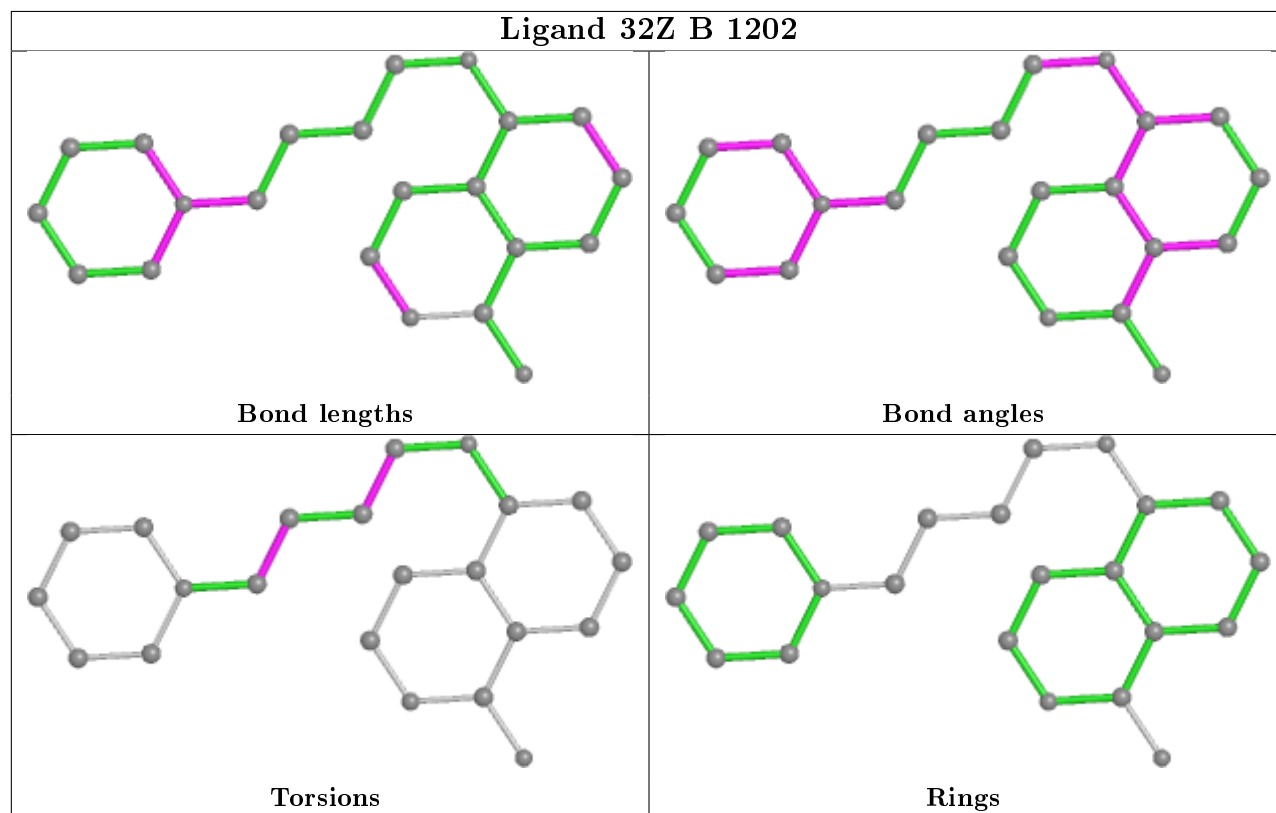
1 monomer is involved in 1 short contact:

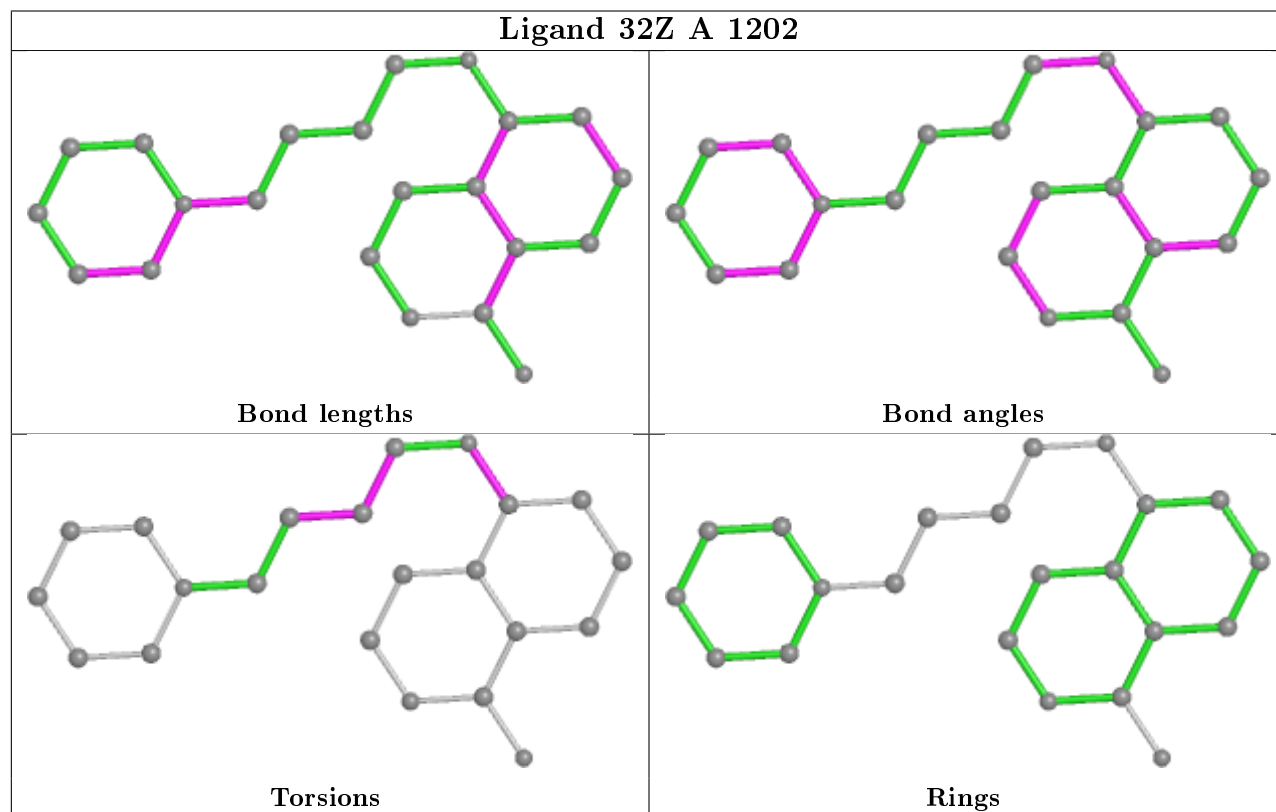
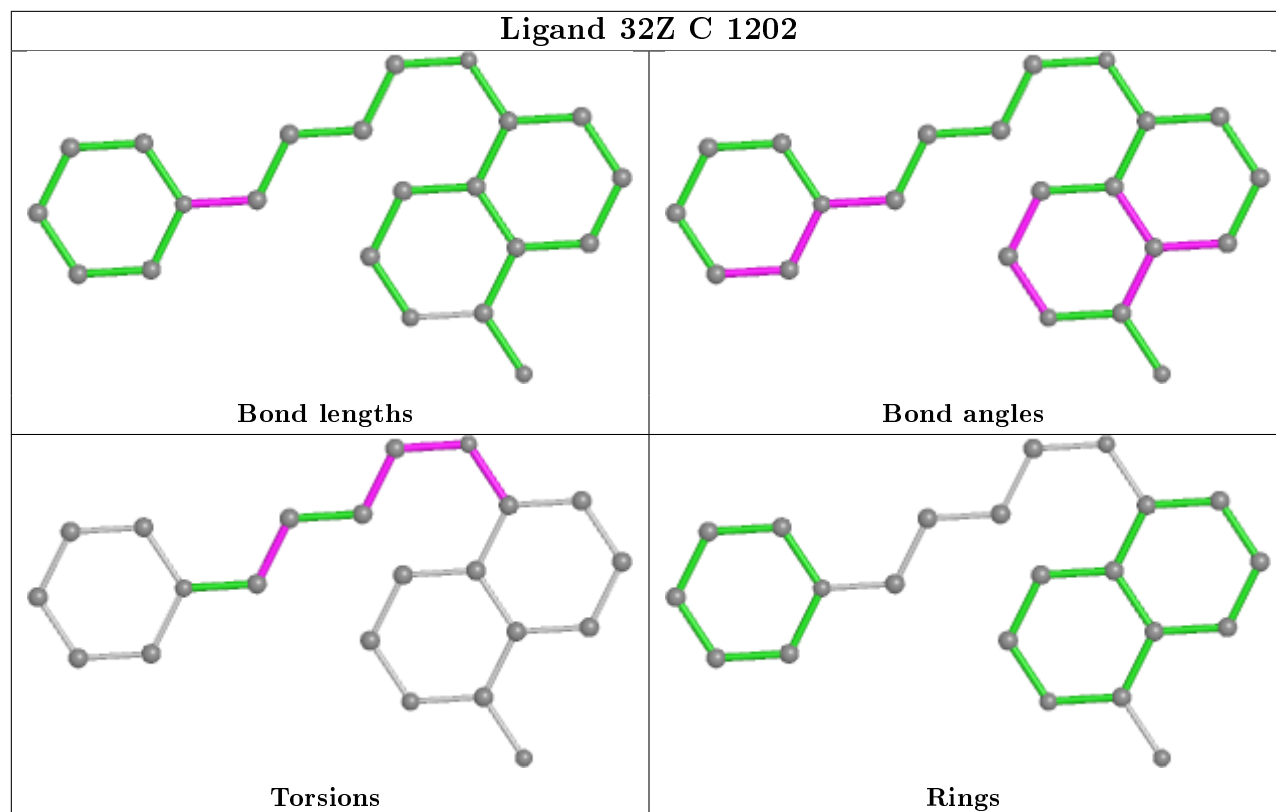
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1202	32Z	1	0

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



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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	199/227 (87%)	-0.21	5 (2%) 57 58	14, 25, 52, 76	0
1	B	205/227 (90%)	-0.19	8 (3%) 39 39	15, 24, 51, 73	0
1	C	208/227 (91%)	-0.25	1 (0%) 91 92	14, 23, 45, 60	0
1	D	190/227 (83%)	-0.02	7 (3%) 41 41	17, 30, 57, 83	0
All	All	802/908 (88%)	-0.17	21 (2%) 56 56	14, 26, 52, 83	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1110	PHE	5.3
1	D	1113	MET	4.9
1	A	1132	ASN	4.1
1	A	1050	TYR	3.9
1	A	1052	GLY	3.8
1	D	1054	MET	3.8
1	B	1051	ILE	3.4
1	D	1136	LEU	3.4
1	D	1051	ILE	3.3
1	D	980	ARG	3.3
1	A	1131	VAL	3.3
1	C	965[A]	PHE	3.0
1	B	1052	GLY	2.7
1	B	1132	ASN	2.6
1	B	958	GLY	2.5
1	B	1049	ALA	2.4
1	B	1131	VAL	2.3
1	D	1050	TYR	2.3
1	B	1050	TYR	2.2
1	A	1110	PHE	2.1
1	B	961	ASP	2.1

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

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

## 6.3 Carbohydrates [i](#)

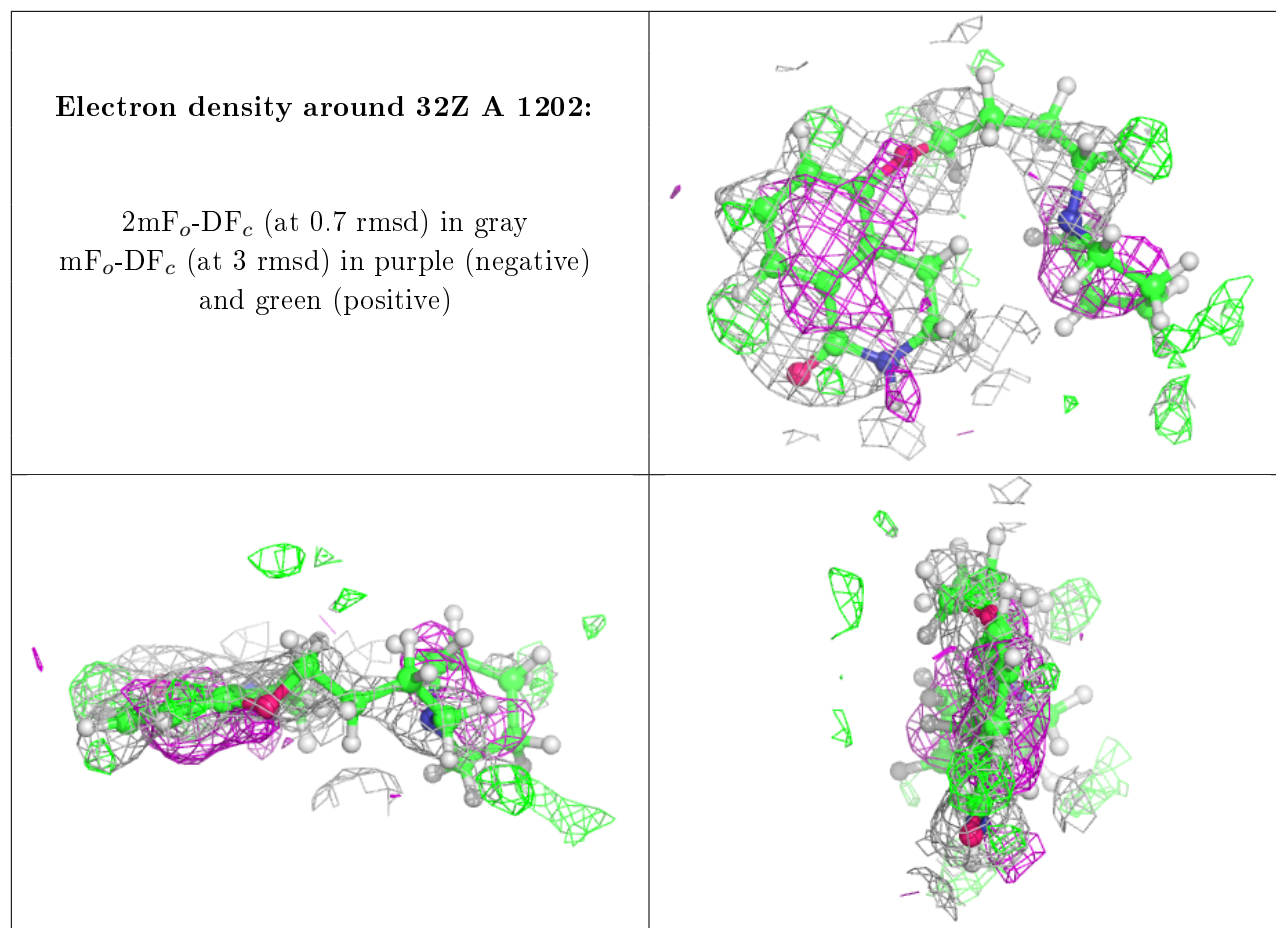
There are no carbohydrates in this entry.

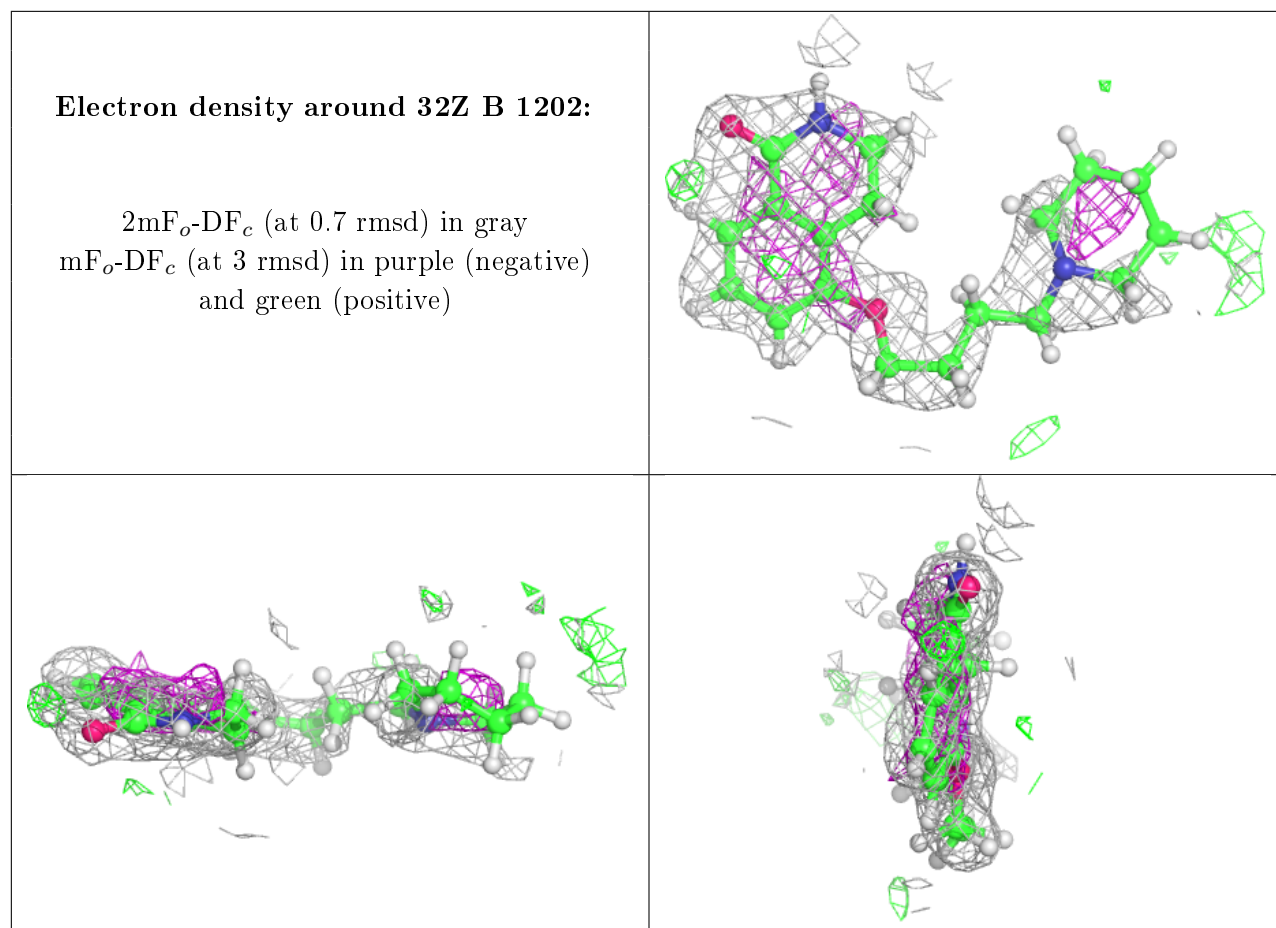
## 6.4 Ligands [i](#)

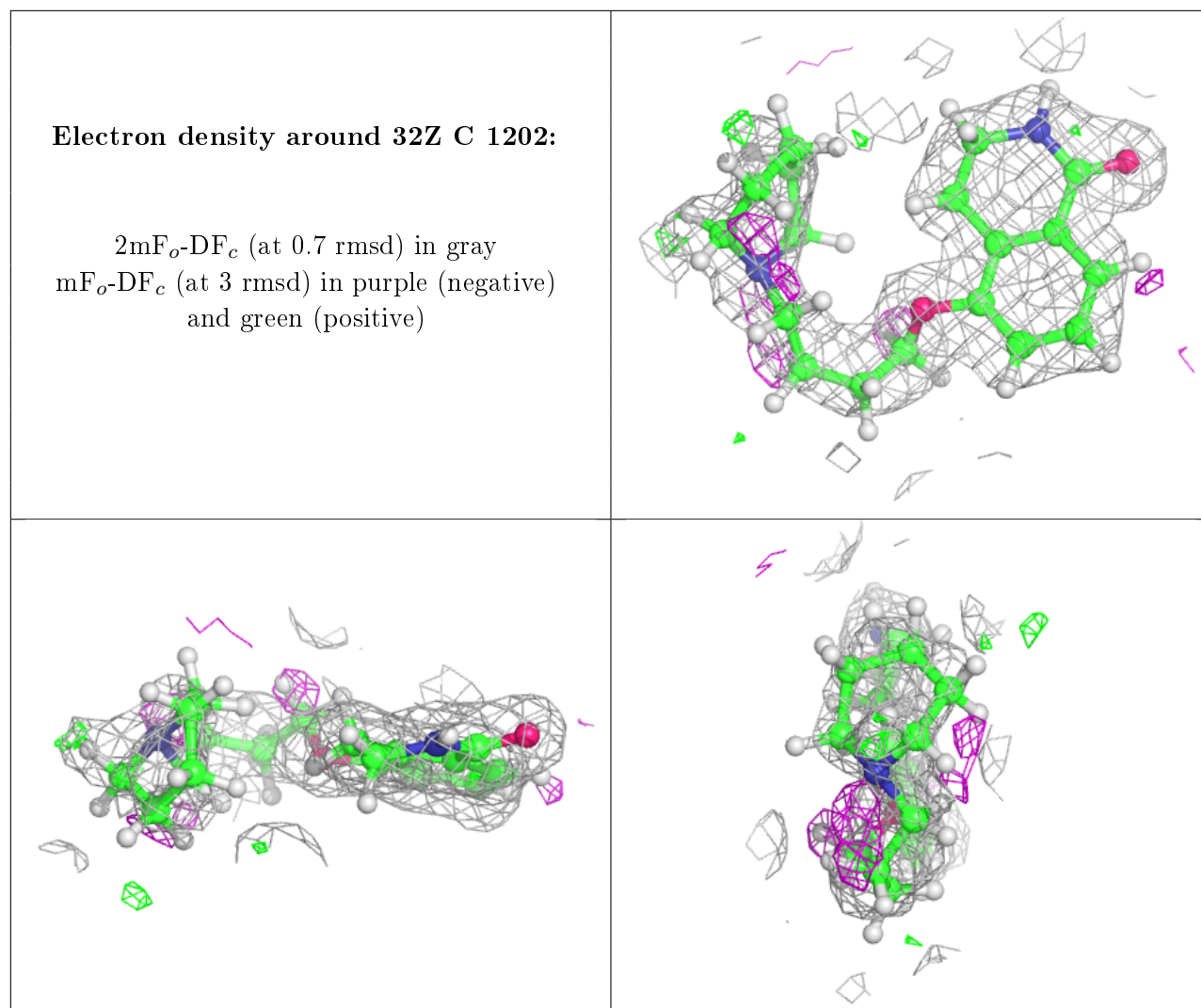
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	32Z	A	1202	22/22	0.69	0.41	27,59,78,78	0
3	32Z	B	1202	22/22	0.83	0.26	15,44,70,70	0
3	32Z	C	1202	22/22	0.94	0.15	17,42,55,56	0
2	ZN	B	1201	1/1	0.99	0.07	33,33,33,33	0
2	ZN	C	1201	1/1	0.99	0.09	32,32,32,32	0
2	ZN	A	1201	1/1	0.99	0.04	33,33,33,33	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.