



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 12:44 PM EST

PDB ID : 4TK5  
Title : Crystal Structure of human Tankyrase 2 in complex with EB47.  
Authors : Qiu, W.; Lam, R.; Romanov, V.; Gordon, R.; Gebremeskel, S.; Vodsedalek, J.; Thompson, C.; Beletskaya, I.; Battaile, K.P.; Pai, E.F.; Chirgadze, N.Y.  
Deposited on : 2014-05-25  
Resolution : 2.02 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

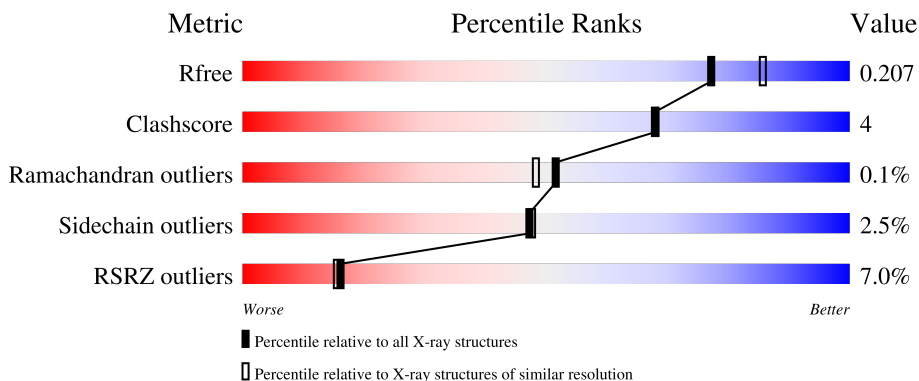
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.02 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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  $\geq 3$ , 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	 6% 81% 7% 11%
1	B	227	 3% 82% 7% 11%
1	C	227	 4% 83% 7% • 8%
1	D	227	 12% 78% 8% • 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UHB	A	1202	X	-	-	-
3	UHB	B	1202	X	-	-	-
3	UHB	D	1201	X	-	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7494 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 Tankyrase-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	201	Total 1620	C 1020	N 299	O 290	S 11	0	0	0
1	B	203	Total 1641	C 1036	N 302	O 292	S 11	0	0	0
1	C	208	Total 1673	C 1055	N 308	O 299	S 11	0	0	0
1	D	199	Total 1598	C 1008	N 297	O 282	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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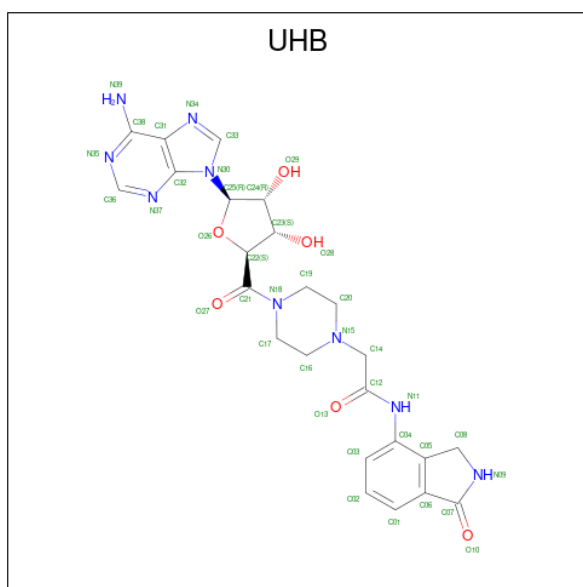
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Chain	Residue	Modelled	Actual	Comment	Reference
D	938	MET	-	initiating methionine	UNP Q9H2K2
D	939	GLY	-	expression tag	UNP Q9H2K2
D	940	SER	-	expression tag	UNP Q9H2K2
D	941	SER	-	expression tag	UNP Q9H2K2
D	942	HIS	-	expression tag	UNP Q9H2K2
D	943	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	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is 2-[4-[(2S,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]carbon ylpiperazin-1-yl]-N-(1-oxidanylidene-2,3-dihydroisoindol-4-yl)ethanamide (three-letter code: UHB) (formula: C<sub>24</sub>H<sub>27</sub>N<sub>9</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	39	24	9	6	0	0
3	B	1	39	24	9	6	0	0
3	C	1	39	24	9	6	0	0
3	D	1	39	24	9	6	0	0

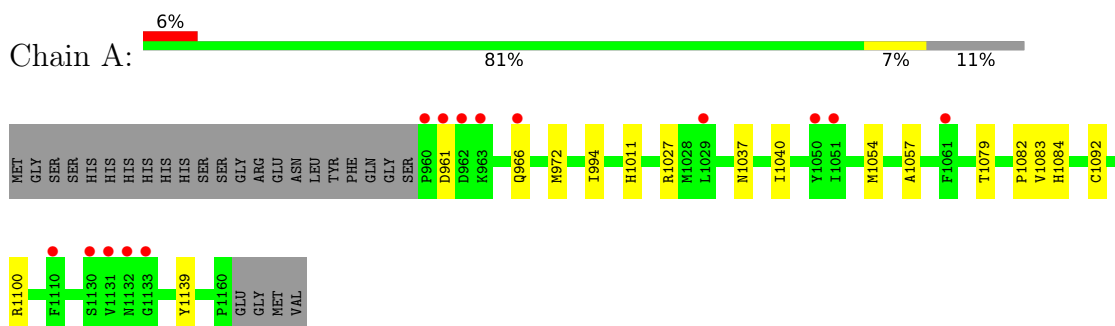
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	206	206	206	0	0
4	B	221	221	221	0	0
4	C	216	216	216	0	0
4	D	160	160	160	0	0

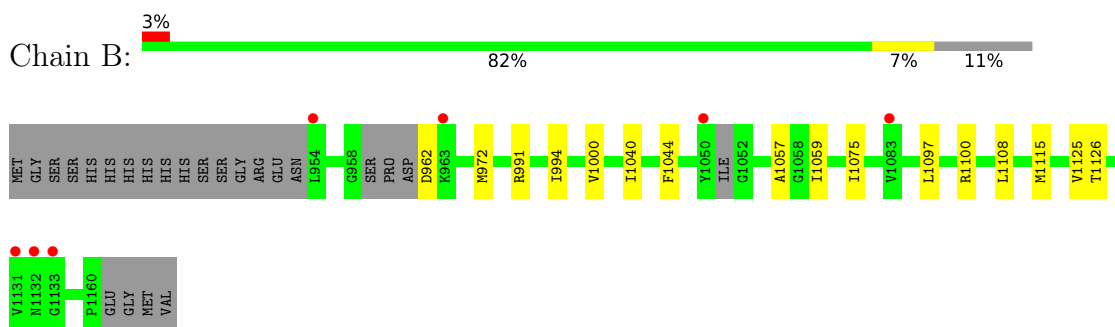
### 3 Residue-property plots [i](#)

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

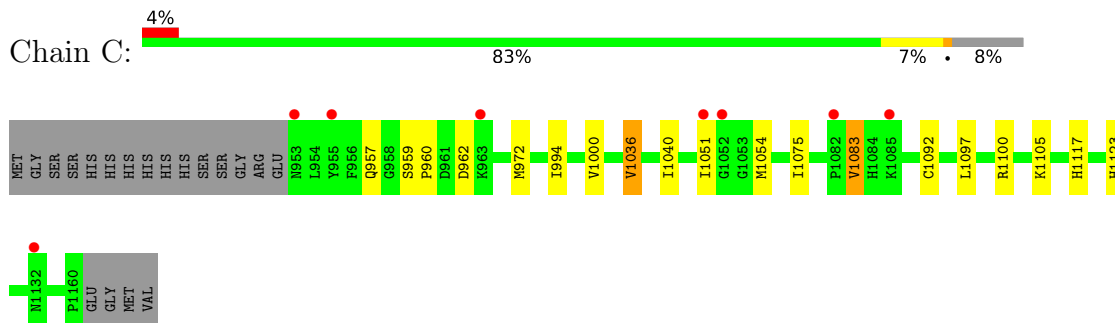
- Molecule 1: Tankyrase-2



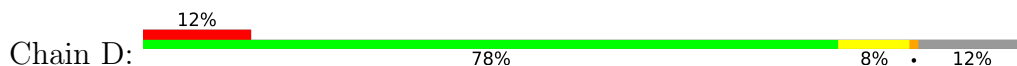
- Molecule 1: Tankyrase-2



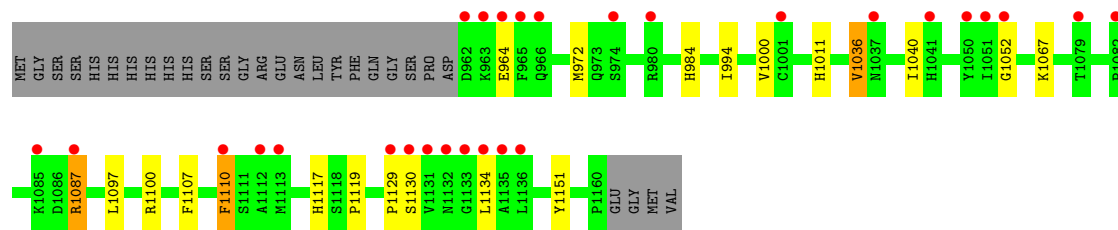
- Molecule 1: Tankyrase-2



- Molecule 1: Tankyrase-2







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.02Å 79.62Å 153.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.57 – 2.02 28.92 – 2.02	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.57-2.02) 99.6 (28.92-2.02)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 2.03Å)	Xtrriage
Refinement program	BUSTER-TNT BUSTER 2.10.0, BUSTER 2.10.0	Depositor
R, $R_{free}$	0.177 , 0.212 0.177 , 0.207	Depositor DCC
$R_{free}$ test set	980 reflections (1.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtrriage
Anisotropy	0.426	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 65.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7494	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.26% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UHB, 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	0.49	0/1664	0.65	0/2237
1	B	0.48	0/1684	0.66	0/2260
1	C	0.45	0/1718	0.66	1/2310 (0.0%)
1	D	0.49	0/1641	0.65	0/2206
All	All	0.48	0/6707	0.65	1/9013 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	960	PRO	N-CA-CB	5.50	109.90	103.30

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	1620	0	1553	11	0
1	B	1641	0	1568	11	0
1	C	1673	0	1595	13	0
1	D	1598	0	1538	17	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
3	A	39	0	26	0	0
3	B	39	0	26	1	0
3	C	39	0	27	1	0
3	D	39	0	26	0	0
4	A	206	0	0	3	0
4	B	221	0	0	1	0
4	C	216	0	0	0	0
4	D	160	0	0	3	0
All	All	7494	0	6359	50	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 4.

All (50) 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:1105:LYS:H	1:C:1123:HIS:HD2	1.15	0.92
1:C:1000:VAL:HG21	1:C:1040:ILE:HD12	1.64	0.80
1:D:1000:VAL:HG21	1:D:1040:ILE:HD12	1.65	0.78
1:B:1000:VAL:HG21	1:B:1040:ILE:HD12	1.66	0.78
1:D:984:HIS:CD2	1:D:1087:ARG:HH22	2.11	0.68
1:D:1087:ARG:HH11	1:D:1087:ARG:HG3	1.61	0.66
1:B:1115:MET:HE1	1:B:1125:VAL:HG21	1.78	0.65
1:B:1075:ILE:HD11	3:B:1202:UHB:H16	1.80	0.63
1:B:1057:ALA:O	1:D:1117:HIS:HE1	1.81	0.62
1:C:1105:LYS:H	1:C:1123:HIS:CD2	2.07	0.61
1:D:1129:PRO:HA	1:D:1134:LEU:HB3	1.83	0.61
1:A:1057:ALA:O	1:C:1117:HIS:HE1	1.85	0.60
1:C:1075:ILE:HD11	3:C:1202:UHB:H20	1.83	0.59
1:D:1087:ARG:HG3	1:D:1087:ARG:NH1	2.19	0.57
1:C:972:MET:HG2	1:C:994:ILE:HD11	1.87	0.55
1:C:1083:VAL:HG13	1:C:1092:CYS:SG	2.47	0.54
1:D:984:HIS:CD2	1:D:1087:ARG:NH2	2.75	0.54
1:A:972:MET:HG2	1:A:994:ILE:HD11	1.90	0.53
1:D:972:MET:HG2	1:D:994:ILE:HD11	1.92	0.51
1:B:972:MET:HG2	1:B:994:ILE:HD11	1.93	0.50
1:B:1115:MET:CE	1:B:1125:VAL:HG21	2.42	0.48
1:A:1079:THR:HG23	4:A:1320:HOH:O	2.12	0.48
1:D:1036:VAL:HG22	1:D:1097:LEU:HG	1.95	0.48
1:C:1036:VAL:HG22	1:C:1097:LEU:HG	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1083:VAL:HG23	1:A:1084:HIS:CE1	2.50	0.47
1:D:1040:ILE:HD11	1:D:1097:LEU:CD2	2.45	0.47
1:D:1117:HIS:HD2	4:D:1335:HOH:O	1.96	0.47
1:B:1040:ILE:HD11	1:B:1097:LEU:CD2	2.45	0.46
1:B:1115:MET:HG2	4:B:1475:HOH:O	2.16	0.46
1:A:1037:ASN:HA	1:A:1040:ILE:HG12	1.97	0.46
1:C:1040:ILE:HD11	1:C:1097:LEU:CD2	2.47	0.45
1:B:1040:ILE:HD11	1:B:1097:LEU:HD21	1.99	0.44
1:D:1107:PHE:CG	1:D:1119:PRO:HG2	2.52	0.44
1:A:1083:VAL:HG23	1:A:1084:HIS:ND1	2.32	0.44
1:D:964:GLU:HG2	1:D:1151:TYR:OH	2.18	0.44
1:A:1027:ARG:NH1	1:A:1139:TYR:OH	2.51	0.44
1:C:959:SER:HB2	1:C:962:ASP:HB2	1.99	0.44
1:A:1011:HIS:HE1	4:A:1413:HOH:O	2.01	0.43
1:A:1082:PRO:HD2	4:A:1422:HOH:O	2.18	0.43
1:D:1011:HIS:HE1	4:D:1378:HOH:O	2.02	0.43
1:A:1083:VAL:HG22	1:A:1092:CYS:SG	2.59	0.42
1:D:1040:ILE:HD11	1:D:1097:LEU:HD21	2.00	0.42
1:D:1067:LYS:HE3	4:D:1411:HOH:O	2.20	0.42
1:D:1110:PHE:HB2	1:D:1130:SER:HB3	2.02	0.41
1:B:1044:PHE:HB3	1:B:1059:ILE:HD13	2.00	0.41
1:C:1040:ILE:HD11	1:C:1097:LEU:HD21	2.01	0.41
1:A:1083:VAL:CG2	1:A:1092:CYS:SG	3.09	0.41
1:B:1108:LEU:HD12	1:B:1126:THR:HB	2.03	0.41
1:C:972:MET:HG2	1:C:994:ILE:CD1	2.51	0.40
1:C:1000:VAL:HG21	1:C:1040:ILE:CD1	2.44	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	199/227 (88%)	195 (98%)	4 (2%)	0	100	100
1	B	197/227 (87%)	197 (100%)	0	0	100	100
1	C	206/227 (91%)	206 (100%)	0	0	100	100
1	D	197/227 (87%)	192 (98%)	4 (2%)	1 (0%)	29	22
All	All	799/908 (88%)	790 (99%)	8 (1%)	1 (0%)	51	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1052	GLY

### 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	170/192 (88%)	166 (98%)	4 (2%)	49	49
1	B	171/192 (89%)	168 (98%)	3 (2%)	59	61
1	C	174/192 (91%)	168 (97%)	6 (3%)	37	35
1	D	166/192 (86%)	162 (98%)	4 (2%)	49	49
All	All	681/768 (89%)	664 (98%)	17 (2%)	47	48

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

Mol	Chain	Res	Type
1	A	961	ASP
1	A	966	GLN
1	A	1054	MET
1	A	1100	ARG
1	B	962	ASP
1	B	991	ARG
1	B	1100	ARG
1	C	957	GLN
1	C	1036	VAL
1	C	1051	ILE

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Mol	Chain	Res	Type
1	C	1054	MET
1	C	1083	VAL
1	C	1100	ARG
1	D	1036	VAL
1	D	1087	ARG
1	D	1100	ARG
1	D	1110	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1011	HIS
1	A	1048	HIS
1	B	1011	HIS
1	B	1048	HIS
1	C	1048	HIS
1	C	1117	HIS
1	C	1123	HIS
1	D	1011	HIS
1	D	1023	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 monosaccharides in this entry.

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

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	UHB	C	1202	-	41,44,44	2.12	9 (21%)	50,65,65	2.04	13 (26%)
3	UHB	A	1202	-	41,44,44	2.22	16 (39%)	50,65,65	2.02	15 (30%)
3	UHB	B	1202	-	41,44,44	2.14	12 (29%)	50,65,65	2.01	16 (32%)
3	UHB	D	1201	-	41,44,44	3.21	16 (39%)	50,65,65	3.09	20 (40%)

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	UHB	C	1202	-	-	2/16/55/55	0/6/6/6
3	UHB	A	1202	-	1/1/9/11	2/16/55/55	0/6/6/6
3	UHB	B	1202	-	1/1/9/11	2/16/55/55	0/6/6/6
3	UHB	D	1201	-	2/2/9/11	5/16/55/55	1/6/6/6

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1201	UHB	C24-C25	9.14	1.67	1.53
3	D	1201	UHB	C21-N18	7.12	1.45	1.34
3	D	1201	UHB	C17-N18	-6.96	1.34	1.47
3	D	1201	UHB	C08-N09	-6.39	1.39	1.45
3	C	1202	UHB	C23-C22	6.29	1.62	1.53
3	A	1202	UHB	C07-N09	5.82	1.39	1.35
3	A	1202	UHB	C23-C22	5.79	1.61	1.53
3	D	1201	UHB	O29-C24	-5.69	1.29	1.43
3	C	1202	UHB	C21-N18	5.53	1.42	1.34
3	B	1202	UHB	C21-N18	5.39	1.42	1.34
3	B	1202	UHB	C07-N09	5.36	1.39	1.35
3	B	1202	UHB	C23-C22	5.16	1.60	1.53
3	D	1201	UHB	C23-C22	5.14	1.60	1.53
3	C	1202	UHB	C07-N09	4.84	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1201	UHB	C22-C21	4.75	1.64	1.53
3	D	1201	UHB	O26-C22	-4.74	1.37	1.43
3	A	1202	UHB	C21-N18	4.69	1.41	1.34
3	B	1202	UHB	C08-N09	-4.67	1.41	1.45
3	A	1202	UHB	C08-C05	3.95	1.53	1.50
3	D	1201	UHB	O26-C25	-3.79	1.35	1.41
3	C	1202	UHB	C36-N37	3.44	1.37	1.32
3	D	1201	UHB	C04-C05	3.37	1.44	1.40
3	C	1202	UHB	C12-N11	3.22	1.42	1.35
3	A	1202	UHB	C16-N15	3.14	1.55	1.46
3	D	1201	UHB	C07-N09	3.03	1.37	1.35
3	A	1202	UHB	O29-C24	-3.00	1.35	1.43
3	B	1202	UHB	C16-N15	2.97	1.55	1.46
3	D	1201	UHB	C12-N11	2.96	1.42	1.35
3	B	1202	UHB	O29-C24	-2.92	1.36	1.43
3	D	1201	UHB	C24-C23	-2.86	1.45	1.53
3	C	1202	UHB	C16-N15	2.82	1.54	1.46
3	D	1201	UHB	C14-C12	-2.79	1.48	1.52
3	C	1202	UHB	C03-C04	2.79	1.44	1.39
3	B	1202	UHB	C04-C05	2.78	1.43	1.40
3	A	1202	UHB	C04-C05	2.58	1.43	1.40
3	B	1202	UHB	C36-N37	2.54	1.36	1.32
3	B	1202	UHB	C12-N11	2.54	1.41	1.35
3	D	1201	UHB	C17-C16	2.47	1.60	1.51
3	A	1202	UHB	C12-N11	2.47	1.41	1.35
3	D	1201	UHB	O28-C23	-2.34	1.37	1.43
3	A	1202	UHB	C32-N37	2.33	1.38	1.35
3	A	1202	UHB	O28-C23	-2.32	1.37	1.43
3	C	1202	UHB	C24-C25	2.23	1.57	1.53
3	B	1202	UHB	C03-C04	2.21	1.43	1.39
3	A	1202	UHB	C19-N18	-2.20	1.43	1.47
3	B	1202	UHB	C17-N18	-2.19	1.43	1.47
3	C	1202	UHB	C36-N35	2.17	1.38	1.33
3	A	1202	UHB	C24-C25	2.15	1.57	1.53
3	A	1202	UHB	C08-N09	-2.14	1.43	1.45
3	A	1202	UHB	C36-N37	2.09	1.35	1.32
3	A	1202	UHB	O27-C21	2.07	1.26	1.22
3	B	1202	UHB	C36-N35	2.04	1.37	1.33
3	A	1202	UHB	C20-N15	2.03	1.52	1.46

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1201	UHB	C14-N15-C20	9.16	125.30	111.09
3	D	1201	UHB	C22-C21-N18	6.59	131.63	118.34
3	D	1201	UHB	C14-C12-N11	6.21	125.79	114.12
3	D	1201	UHB	C24-C23-C22	-5.82	94.85	101.64
3	D	1201	UHB	C08-C05-C06	-5.80	105.10	109.70
3	C	1202	UHB	C14-C12-N11	5.69	124.81	114.12
3	D	1201	UHB	C14-N15-C16	5.67	119.89	111.09
3	D	1201	UHB	O27-C21-N18	-5.43	115.31	121.67
3	C	1202	UHB	C14-N15-C20	5.19	119.14	111.09
3	D	1201	UHB	C05-C08-N09	5.12	107.07	101.77
3	A	1202	UHB	C08-C05-C06	-4.95	105.77	109.70
3	D	1201	UHB	O13-C12-C14	-4.88	112.53	121.08
3	C	1202	UHB	C08-C05-C06	-4.85	105.85	109.70
3	B	1202	UHB	C14-N15-C20	4.78	118.50	111.09
3	B	1202	UHB	C08-C05-C06	-4.68	105.99	109.70
3	A	1202	UHB	C14-N15-C20	4.34	117.82	111.09
3	A	1202	UHB	C14-C12-N11	4.32	122.25	114.12
3	D	1201	UHB	C03-C04-C05	-4.17	115.53	120.68
3	C	1202	UHB	O13-C12-C14	-4.06	113.97	121.08
3	B	1202	UHB	C14-C12-N11	4.02	121.68	114.12
3	C	1202	UHB	C03-C04-C05	-4.01	115.72	120.68
3	A	1202	UHB	C12-C14-N15	3.68	121.90	113.36
3	B	1202	UHB	C03-C04-C05	-3.63	116.19	120.68
3	B	1202	UHB	C12-C14-N15	3.63	121.78	113.36
3	A	1202	UHB	C03-C04-C05	-3.62	116.21	120.68
3	B	1202	UHB	C05-C08-N09	3.61	105.51	101.77
3	D	1201	UHB	C31-C38-N39	3.46	125.61	120.35
3	A	1202	UHB	C05-C08-N09	3.37	105.26	101.77
3	C	1202	UHB	C05-C08-N09	3.35	105.23	101.77
3	B	1202	UHB	O27-C21-N18	-3.33	117.77	121.67
3	B	1202	UHB	C23-C24-C25	3.31	105.96	100.98
3	D	1201	UHB	C12-C14-N15	3.26	120.92	113.36
3	D	1201	UHB	C05-C04-N11	3.08	125.80	119.56
3	A	1202	UHB	O27-C21-N18	-3.05	118.09	121.67
3	A	1202	UHB	C31-C38-N39	3.00	124.92	120.35
3	C	1202	UHB	C12-C14-N15	2.97	120.25	113.36
3	A	1202	UHB	C05-C06-C07	2.96	110.72	108.39
3	D	1201	UHB	O26-C22-C21	2.82	115.59	111.01
3	C	1202	UHB	C31-C38-N39	2.81	124.63	120.35
3	A	1202	UHB	C23-C24-C25	2.75	105.12	100.98
3	B	1202	UHB	C31-C38-N39	2.74	124.51	120.35
3	D	1201	UHB	O27-C21-C22	-2.73	113.06	119.69
3	B	1202	UHB	C22-C21-N18	2.70	123.79	118.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1202	UHB	O27-C21-N18	-2.68	118.53	121.67
3	C	1202	UHB	C05-C06-C07	2.66	110.48	108.39
3	C	1202	UHB	O26-C25-C24	-2.61	103.11	106.93
3	A	1202	UHB	O26-C22-C21	-2.60	106.79	111.01
3	A	1202	UHB	C05-C04-N11	2.57	124.76	119.56
3	A	1202	UHB	O13-C12-C14	-2.52	116.66	121.08
3	B	1202	UHB	C05-C04-N11	2.43	124.48	119.56
3	D	1201	UHB	C05-C06-C07	2.43	110.30	108.39
3	A	1202	UHB	C22-C21-N18	2.41	123.19	118.34
3	A	1202	UHB	C01-C06-C07	-2.39	124.58	129.37
3	B	1202	UHB	O13-C12-C14	-2.36	116.95	121.08
3	C	1202	UHB	C22-C21-N18	2.19	122.76	118.34
3	B	1202	UHB	C20-N15-C16	2.18	113.74	108.83
3	D	1201	UHB	C25-O26-C22	-2.17	105.34	109.11
3	D	1201	UHB	N39-C38-N35	-2.15	114.11	118.57
3	D	1201	UHB	C06-C07-N09	-2.15	105.11	106.35
3	D	1201	UHB	C20-C19-N18	2.09	114.92	110.44
3	B	1202	UHB	O26-C22-C21	-2.07	107.66	111.01
3	B	1202	UHB	C05-C06-C07	2.05	110.00	108.39
3	C	1202	UHB	C01-C06-C07	-2.03	125.31	129.37
3	B	1202	UHB	C17-C16-N15	2.03	114.81	110.64

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1202	UHB	C24
3	B	1202	UHB	C24
3	D	1201	UHB	C22
3	D	1201	UHB	C24

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1201	UHB	N18-C21-C22-C23
3	D	1201	UHB	O27-C21-C22-C23
3	B	1202	UHB	C05-C04-N11-C12
3	D	1201	UHB	C05-C04-N11-C12
3	D	1201	UHB	C12-C14-N15-C20
3	C	1202	UHB	C05-C04-N11-C12
3	A	1202	UHB	C05-C04-N11-C12
3	B	1202	UHB	C03-C04-N11-C12
3	C	1202	UHB	C03-C04-N11-C12

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Mol	Chain	Res	Type	Atoms
3	D	1201	UHB	C03-C04-N11-C12
3	A	1202	UHB	C03-C04-N11-C12

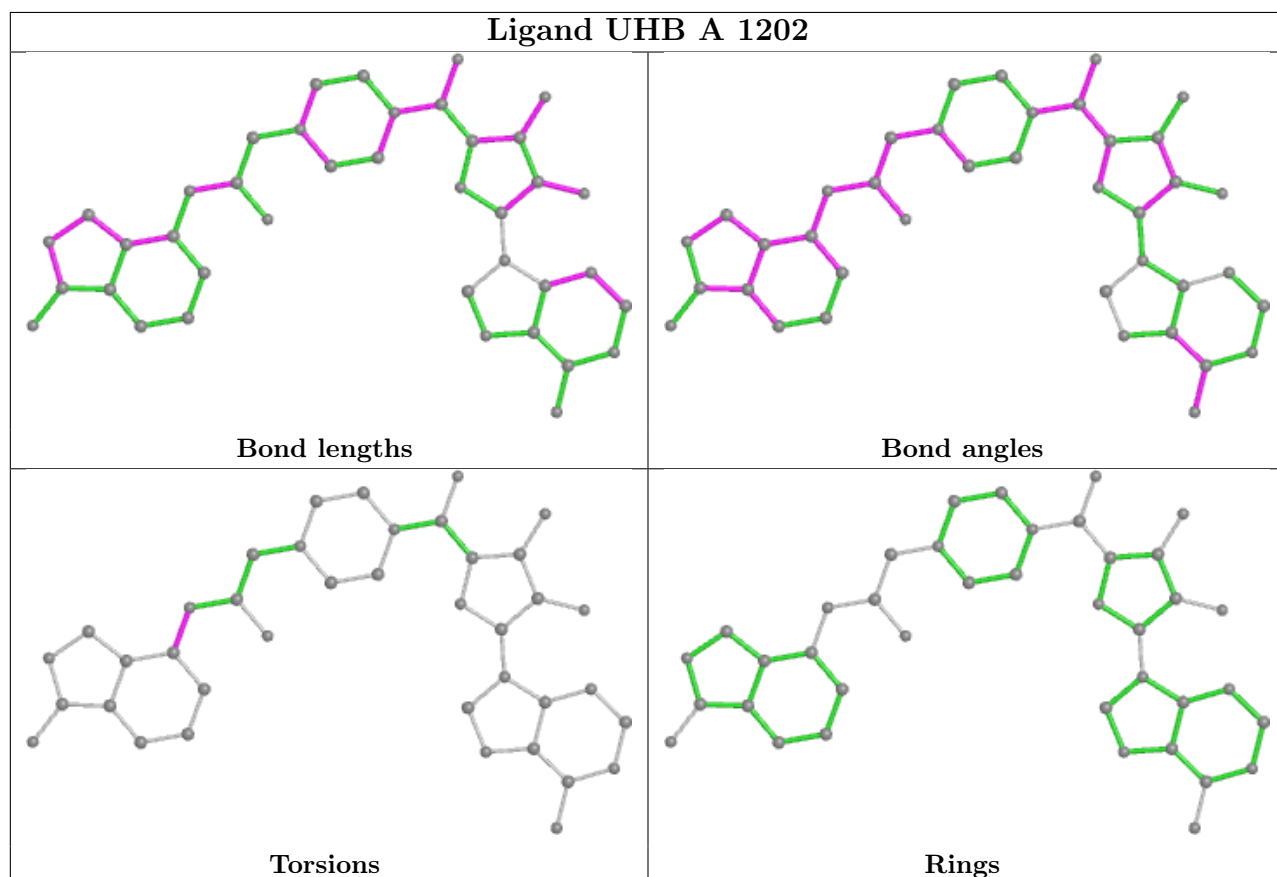
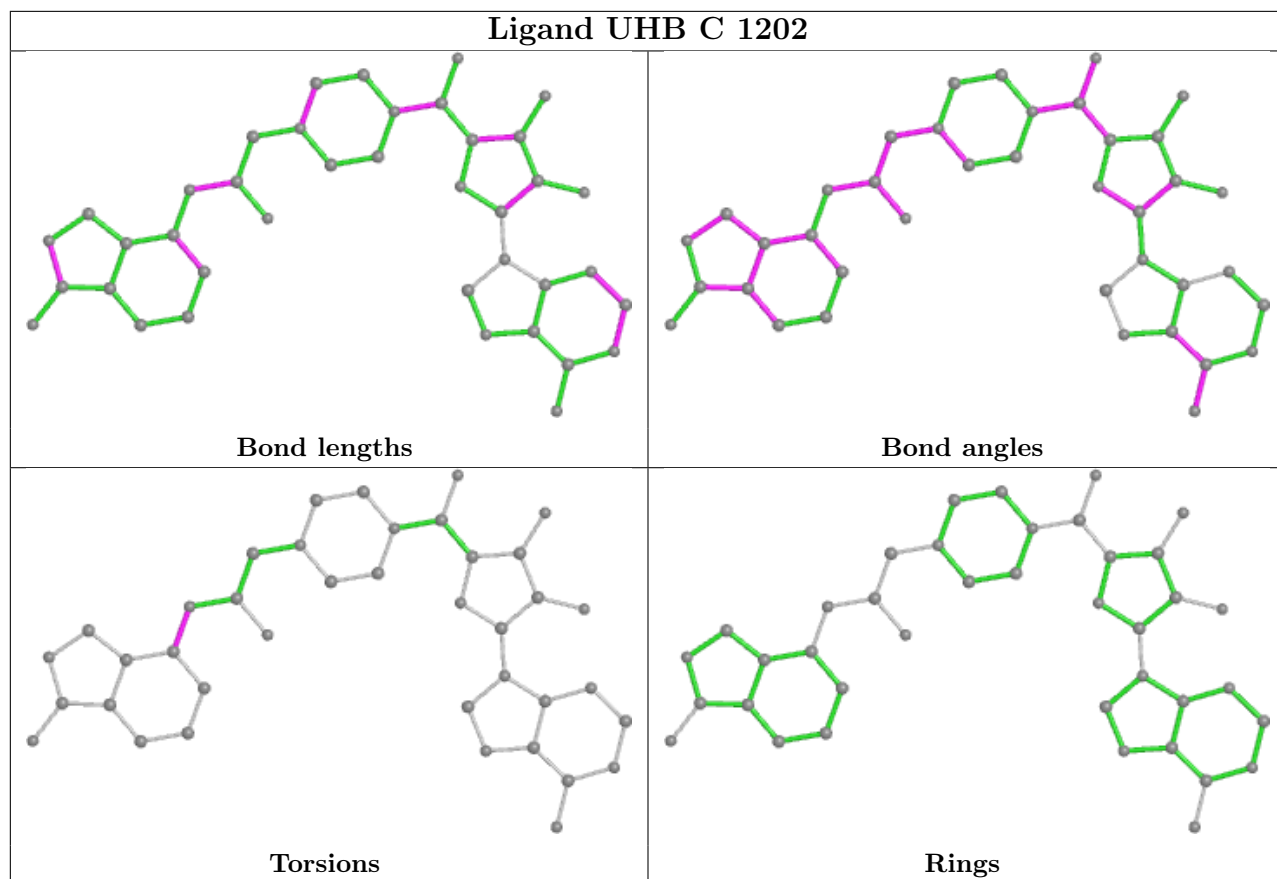
All (1) ring outliers are listed below:

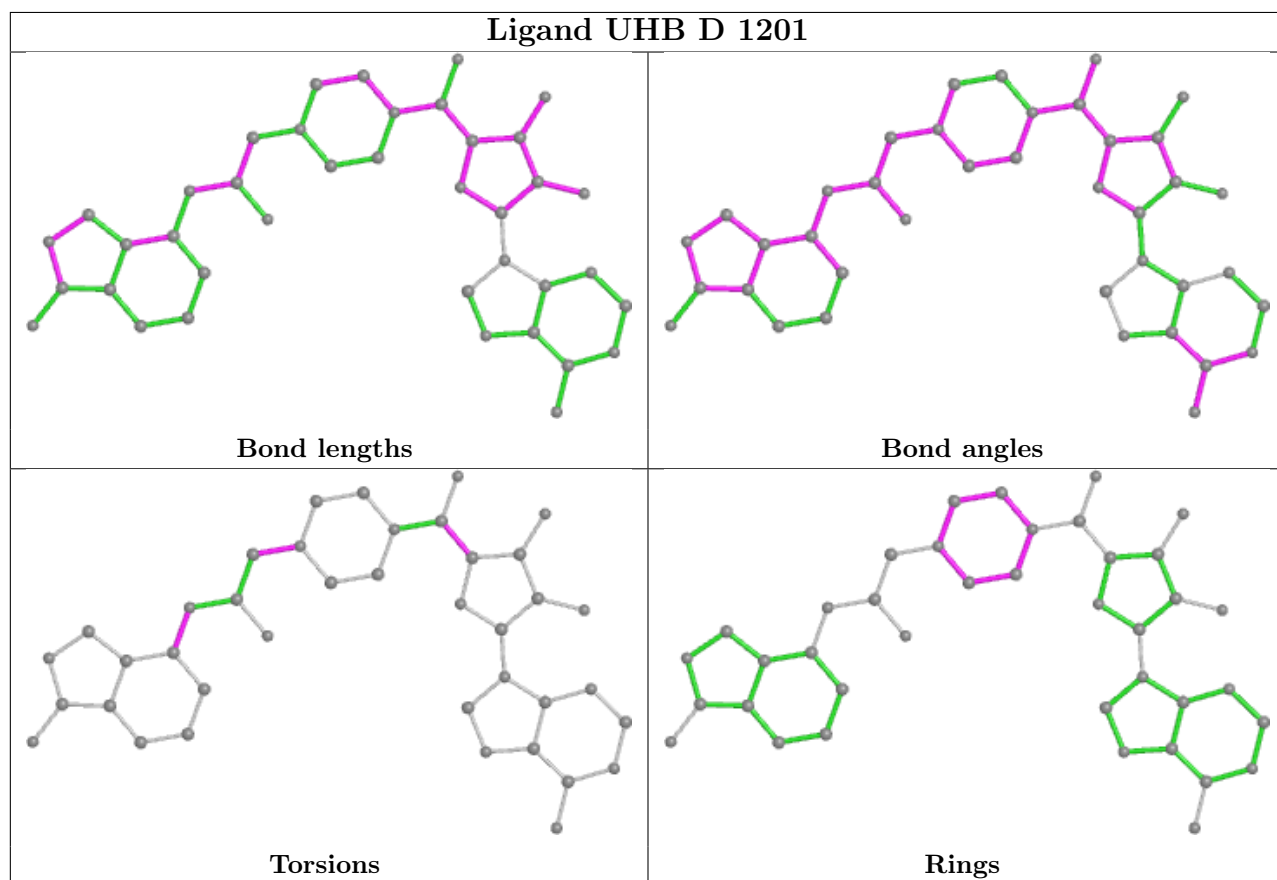
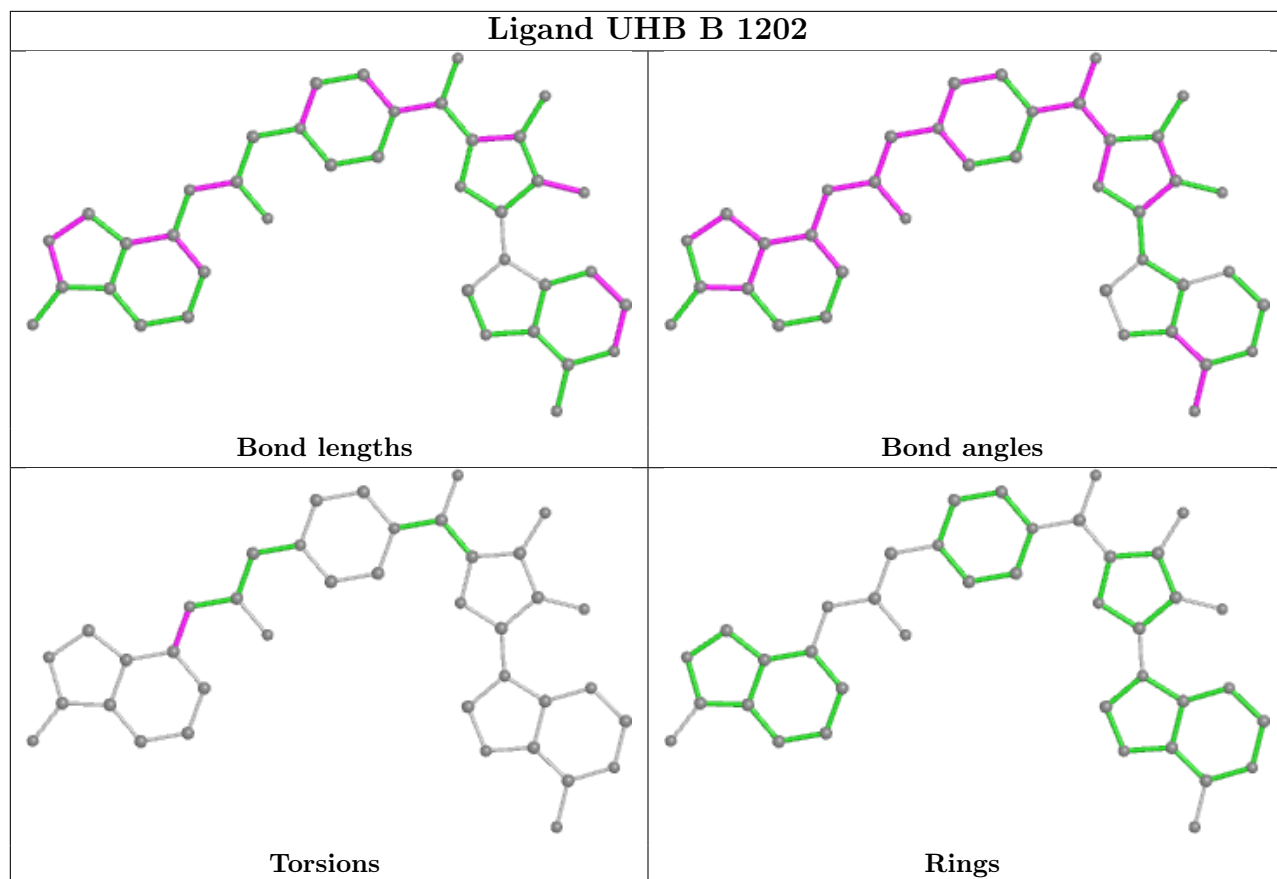
Mol	Chain	Res	Type	Atoms
3	D	1201	UHB	C16-C17-C19-C20-N15-N18

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1202	UHB	1	0
3	B	1202	UHB	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	201/227 (88%)	0.29	14 (6%) 16 15	18, 27, 58, 87	0
1	B	203/227 (89%)	0.15	7 (3%) 45 45	16, 27, 55, 80	0
1	C	208/227 (91%)	0.03	8 (3%) 40 40	16, 27, 53, 66	0
1	D	199/227 (87%)	0.66	28 (14%) 2 2	19, 35, 64, 86	0
All	All	811/908 (89%)	0.28	57 (7%) 16 15	16, 29, 58, 87	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	960	PRO	8.6
1	D	1131	VAL	8.3
1	D	963	LYS	5.6
1	D	962	ASP	5.6
1	D	1132	ASN	5.6
1	A	962	ASP	5.4
1	D	1052	GLY	5.4
1	A	1132	ASN	5.2
1	D	1110	PHE	4.8
1	C	1051	ILE	4.7
1	D	964	GLU	4.7
1	A	1131	VAL	4.6
1	D	1133	GLY	4.5
1	B	1132	ASN	4.3
1	A	1051	ILE	4.3
1	C	955	TYR	4.2
1	D	1135	ALA	4.0
1	D	1001	CYS	3.9
1	C	963	LYS	3.9
1	D	1112	ALA	3.9
1	A	1133	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	1113	MET	3.8
1	A	1130	SER	3.6
1	D	965	PHE	3.5
1	B	1131	VAL	3.5
1	A	1110	PHE	3.4
1	D	980	ARG	3.3
1	B	1050	TYR	3.2
1	D	1082	PRO	3.0
1	B	954	LEU	3.0
1	D	1129	PRO	2.9
1	A	961	ASP	2.9
1	B	1083	VAL	2.9
1	C	953	ASN	2.9
1	D	1134	LEU	2.9
1	D	1051	ILE	2.9
1	A	1050	TYR	2.9
1	D	966	GLN	2.9
1	D	1050	TYR	2.8
1	D	1085	LYS	2.7
1	D	1130	SER	2.7
1	B	1133	GLY	2.6
1	A	963	LYS	2.5
1	B	963	LYS	2.5
1	C	1132	ASN	2.4
1	D	974	SER	2.4
1	C	1052	GLY	2.3
1	D	1041	HIS	2.3
1	C	1082	PRO	2.3
1	D	1037	ASN	2.3
1	A	1061	PHE	2.2
1	C	1085	LYS	2.2
1	D	1136	LEU	2.1
1	A	1029	LEU	2.1
1	D	1087	ARG	2.1
1	A	966	GLN	2.1
1	D	1079	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

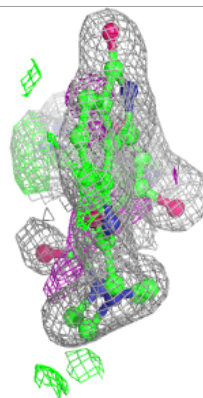
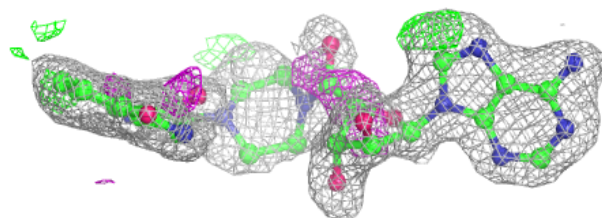
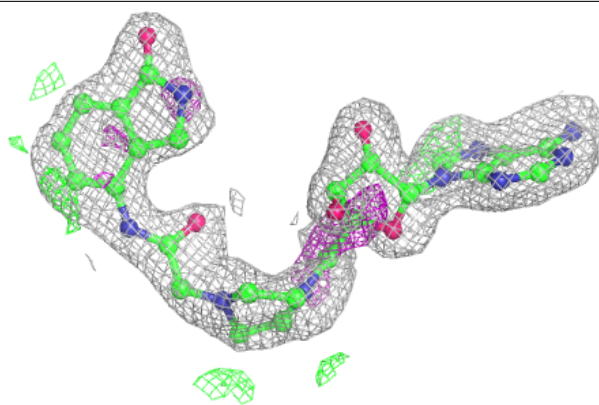
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	UHB	D	1201	39/39	0.72	0.22	43,48,57,58	0
3	UHB	C	1202	39/39	0.83	0.17	20,40,49,54	0
3	UHB	A	1202	39/39	0.88	0.15	22,29,37,43	0
3	UHB	B	1202	39/39	0.88	0.14	22,30,40,42	0
2	ZN	C	1201	1/1	0.99	0.03	34,34,34,34	0
2	ZN	B	1201	1/1	1.00	0.03	36,36,36,36	0
2	ZN	A	1201	1/1	1.00	0.03	32,32,32,32	0

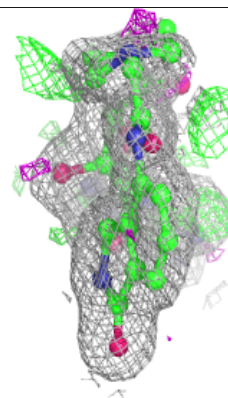
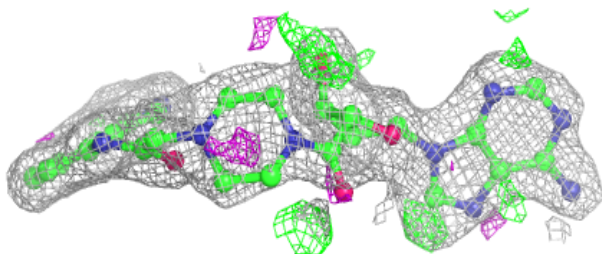
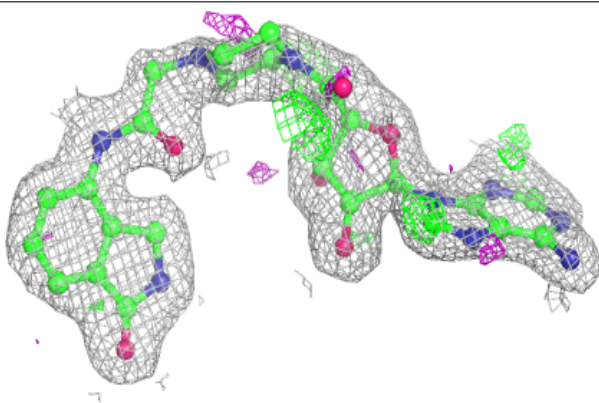
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around UHB D 1201:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

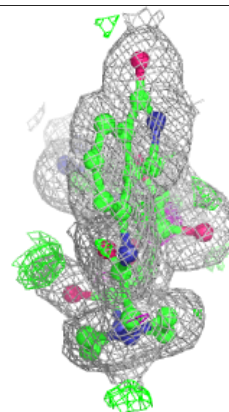
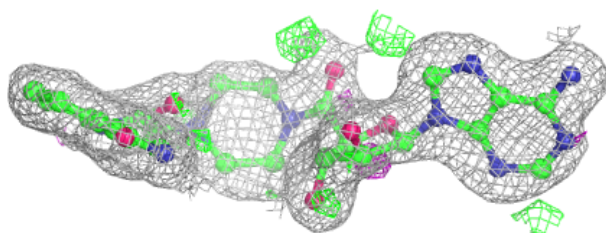
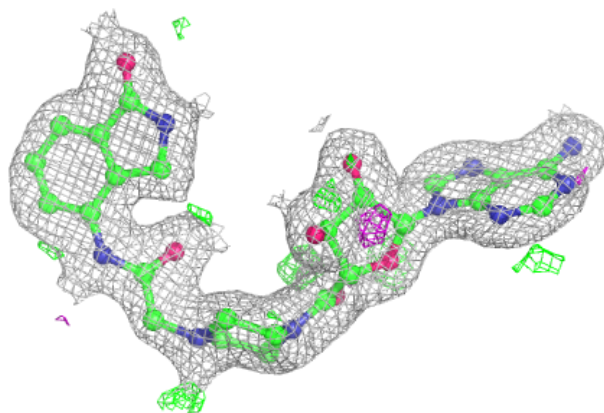
**Electron density around UHB C 1202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

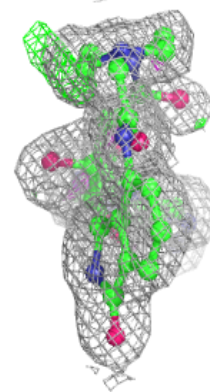
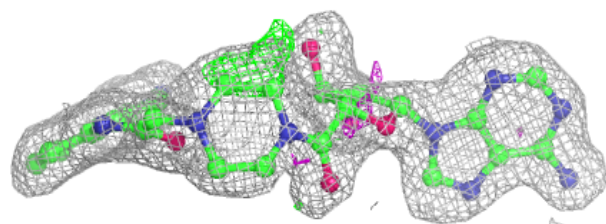
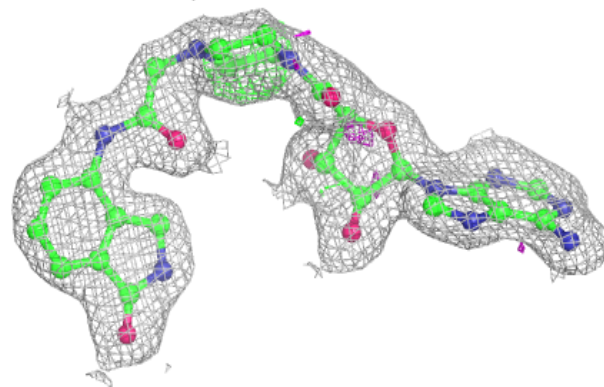


**Electron density around UHB A 1202:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around UHB B 1202:**

$2mF_o-DF_c$  (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.