



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 04:54 AM BST

PDB ID : 5DSY  
Title : Crystal structure of constitutively active PARP-2  
Authors : Riccio, A.A.; Pascal, J.M.  
Deposited on : 2015-09-17  
Resolution : 2.70 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 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 : 2.13.1  
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) : 2.13.1

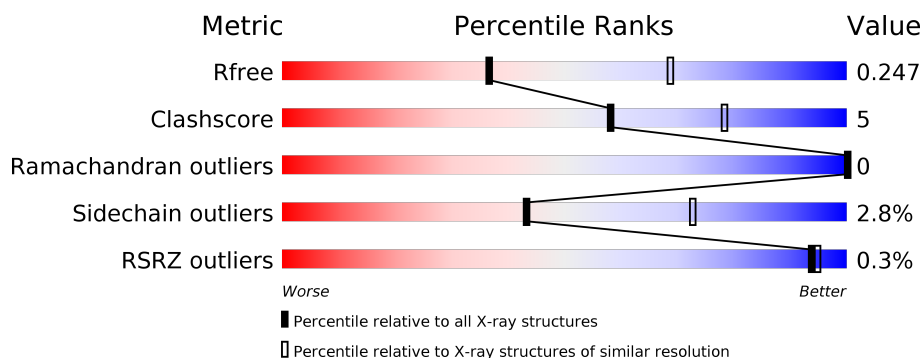
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	280	
1	B	280	
1	C	280	
1	D	280	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8087 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 Poly [ADP-ribose] polymerase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1967	1250	339	367	11			
1	B	251	Total	C	N	O	S	0	0	0
			1988	1265	342	370	11			
1	C	248	Total	C	N	O	S	0	0	0
			1967	1250	340	366	11			
1	D	247	Total	C	N	O	S	0	0	0
			1958	1245	337	365	11			

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	MET	-	initiating methionine	UNP Q9UGN5
A	198	GLY	-	expression tag	UNP Q9UGN5
A	199	SER	-	expression tag	UNP Q9UGN5
A	200	SER	-	expression tag	UNP Q9UGN5
A	201	HIS	-	expression tag	UNP Q9UGN5
A	202	HIS	-	expression tag	UNP Q9UGN5
A	203	HIS	-	expression tag	UNP Q9UGN5
A	204	HIS	-	expression tag	UNP Q9UGN5
A	205	HIS	-	expression tag	UNP Q9UGN5
A	206	HIS	-	expression tag	UNP Q9UGN5
A	207	SER	-	expression tag	UNP Q9UGN5
A	208	SER	-	expression tag	UNP Q9UGN5
A	209	GLY	-	expression tag	UNP Q9UGN5
A	210	LEU	-	expression tag	UNP Q9UGN5
A	211	VAL	-	expression tag	UNP Q9UGN5
A	212	PRO	-	expression tag	UNP Q9UGN5
A	213	ARG	-	expression tag	UNP Q9UGN5
A	214	GLY	-	expression tag	UNP Q9UGN5
A	215	SER	-	expression tag	UNP Q9UGN5
A	216	HIS	-	expression tag	UNP Q9UGN5
A	217	PRO	-	expression tag	UNP Q9UGN5

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	218	GLU	-	expression tag	UNP Q9UGN5
A	219	SER	-	expression tag	UNP Q9UGN5
A	220	GLN	-	expression tag	UNP Q9UGN5
A	221	LEU	-	expression tag	UNP Q9UGN5
A	222	ASP	-	expression tag	UNP Q9UGN5
A	223	LEU	-	expression tag	UNP Q9UGN5
A	224	ARG	-	expression tag	UNP Q9UGN5
A	225	VAL	-	expression tag	UNP Q9UGN5
A	226	GLN	-	expression tag	UNP Q9UGN5
A	227	GLU	-	expression tag	UNP Q9UGN5
A	228	LEU	-	expression tag	UNP Q9UGN5
A	229	ILE	-	expression tag	UNP Q9UGN5
A	230	LYS	-	expression tag	UNP Q9UGN5
A	231	LEU	-	expression tag	UNP Q9UGN5
A	232	ILE	-	expression tag	UNP Q9UGN5
A	233	CYS	-	expression tag	UNP Q9UGN5
A	234	ASN	-	expression tag	UNP Q9UGN5
A	329	VAL	-	expression tag	UNP Q9UGN5
A	330	GLN	-	expression tag	UNP Q9UGN5
A	331	ALA	-	expression tag	UNP Q9UGN5
A	332	MET	-	expression tag	UNP Q9UGN5
A	333	GLU	-	expression tag	UNP Q9UGN5
A	334	GLU	-	expression tag	UNP Q9UGN5
B	197	MET	-	initiating methionine	UNP Q9UGN5
B	198	GLY	-	expression tag	UNP Q9UGN5
B	199	SER	-	expression tag	UNP Q9UGN5
B	200	SER	-	expression tag	UNP Q9UGN5
B	201	HIS	-	expression tag	UNP Q9UGN5
B	202	HIS	-	expression tag	UNP Q9UGN5
B	203	HIS	-	expression tag	UNP Q9UGN5
B	204	HIS	-	expression tag	UNP Q9UGN5
B	205	HIS	-	expression tag	UNP Q9UGN5
B	206	HIS	-	expression tag	UNP Q9UGN5
B	207	SER	-	expression tag	UNP Q9UGN5
B	208	SER	-	expression tag	UNP Q9UGN5
B	209	GLY	-	expression tag	UNP Q9UGN5
B	210	LEU	-	expression tag	UNP Q9UGN5
B	211	VAL	-	expression tag	UNP Q9UGN5
B	212	PRO	-	expression tag	UNP Q9UGN5
B	213	ARG	-	expression tag	UNP Q9UGN5
B	214	GLY	-	expression tag	UNP Q9UGN5
B	215	SER	-	expression tag	UNP Q9UGN5

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	216	HIS	-	expression tag	UNP Q9UGN5
B	217	PRO	-	expression tag	UNP Q9UGN5
B	218	GLU	-	expression tag	UNP Q9UGN5
B	219	SER	-	expression tag	UNP Q9UGN5
B	220	GLN	-	expression tag	UNP Q9UGN5
B	221	LEU	-	expression tag	UNP Q9UGN5
B	222	ASP	-	expression tag	UNP Q9UGN5
B	223	LEU	-	expression tag	UNP Q9UGN5
B	224	ARG	-	expression tag	UNP Q9UGN5
B	225	VAL	-	expression tag	UNP Q9UGN5
B	226	GLN	-	expression tag	UNP Q9UGN5
B	227	GLU	-	expression tag	UNP Q9UGN5
B	228	LEU	-	expression tag	UNP Q9UGN5
B	229	ILE	-	expression tag	UNP Q9UGN5
B	230	LYS	-	expression tag	UNP Q9UGN5
B	231	LEU	-	expression tag	UNP Q9UGN5
B	232	ILE	-	expression tag	UNP Q9UGN5
B	233	CYS	-	expression tag	UNP Q9UGN5
B	234	ASN	-	expression tag	UNP Q9UGN5
B	329	VAL	-	expression tag	UNP Q9UGN5
B	330	GLN	-	expression tag	UNP Q9UGN5
B	331	ALA	-	expression tag	UNP Q9UGN5
B	332	MET	-	expression tag	UNP Q9UGN5
B	333	GLU	-	expression tag	UNP Q9UGN5
B	334	GLU	-	expression tag	UNP Q9UGN5
C	197	MET	-	initiating methionine	UNP Q9UGN5
C	198	GLY	-	expression tag	UNP Q9UGN5
C	199	SER	-	expression tag	UNP Q9UGN5
C	200	SER	-	expression tag	UNP Q9UGN5
C	201	HIS	-	expression tag	UNP Q9UGN5
C	202	HIS	-	expression tag	UNP Q9UGN5
C	203	HIS	-	expression tag	UNP Q9UGN5
C	204	HIS	-	expression tag	UNP Q9UGN5
C	205	HIS	-	expression tag	UNP Q9UGN5
C	206	HIS	-	expression tag	UNP Q9UGN5
C	207	SER	-	expression tag	UNP Q9UGN5
C	208	SER	-	expression tag	UNP Q9UGN5
C	209	GLY	-	expression tag	UNP Q9UGN5
C	210	LEU	-	expression tag	UNP Q9UGN5
C	211	VAL	-	expression tag	UNP Q9UGN5
C	212	PRO	-	expression tag	UNP Q9UGN5
C	213	ARG	-	expression tag	UNP Q9UGN5

*Continued on next page...*

*Continued from previous page...*

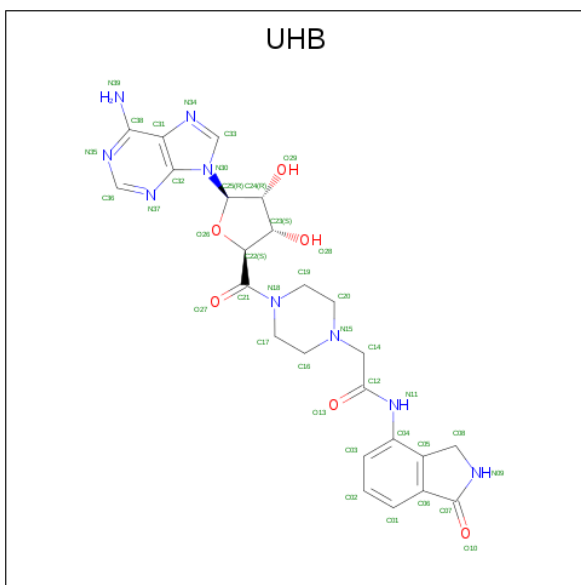
Chain	Residue	Modelled	Actual	Comment	Reference
C	214	GLY	-	expression tag	UNP Q9UGN5
C	215	SER	-	expression tag	UNP Q9UGN5
C	216	HIS	-	expression tag	UNP Q9UGN5
C	217	PRO	-	expression tag	UNP Q9UGN5
C	218	GLU	-	expression tag	UNP Q9UGN5
C	219	SER	-	expression tag	UNP Q9UGN5
C	220	GLN	-	expression tag	UNP Q9UGN5
C	221	LEU	-	expression tag	UNP Q9UGN5
C	222	ASP	-	expression tag	UNP Q9UGN5
C	223	LEU	-	expression tag	UNP Q9UGN5
C	224	ARG	-	expression tag	UNP Q9UGN5
C	225	VAL	-	expression tag	UNP Q9UGN5
C	226	GLN	-	expression tag	UNP Q9UGN5
C	227	GLU	-	expression tag	UNP Q9UGN5
C	228	LEU	-	expression tag	UNP Q9UGN5
C	229	ILE	-	expression tag	UNP Q9UGN5
C	230	LYS	-	expression tag	UNP Q9UGN5
C	231	LEU	-	expression tag	UNP Q9UGN5
C	232	ILE	-	expression tag	UNP Q9UGN5
C	233	CYS	-	expression tag	UNP Q9UGN5
C	234	ASN	-	expression tag	UNP Q9UGN5
C	329	VAL	-	expression tag	UNP Q9UGN5
C	330	GLN	-	expression tag	UNP Q9UGN5
C	331	ALA	-	expression tag	UNP Q9UGN5
C	332	MET	-	expression tag	UNP Q9UGN5
C	333	GLU	-	expression tag	UNP Q9UGN5
C	334	GLU	-	expression tag	UNP Q9UGN5
D	197	MET	-	initiating methionine	UNP Q9UGN5
D	198	GLY	-	expression tag	UNP Q9UGN5
D	199	SER	-	expression tag	UNP Q9UGN5
D	200	SER	-	expression tag	UNP Q9UGN5
D	201	HIS	-	expression tag	UNP Q9UGN5
D	202	HIS	-	expression tag	UNP Q9UGN5
D	203	HIS	-	expression tag	UNP Q9UGN5
D	204	HIS	-	expression tag	UNP Q9UGN5
D	205	HIS	-	expression tag	UNP Q9UGN5
D	206	HIS	-	expression tag	UNP Q9UGN5
D	207	SER	-	expression tag	UNP Q9UGN5
D	208	SER	-	expression tag	UNP Q9UGN5
D	209	GLY	-	expression tag	UNP Q9UGN5
D	210	LEU	-	expression tag	UNP Q9UGN5
D	211	VAL	-	expression tag	UNP Q9UGN5

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	212	PRO	-	expression tag	UNP Q9UGN5
D	213	ARG	-	expression tag	UNP Q9UGN5
D	214	GLY	-	expression tag	UNP Q9UGN5
D	215	SER	-	expression tag	UNP Q9UGN5
D	216	HIS	-	expression tag	UNP Q9UGN5
D	217	PRO	-	expression tag	UNP Q9UGN5
D	218	GLU	-	expression tag	UNP Q9UGN5
D	219	SER	-	expression tag	UNP Q9UGN5
D	220	GLN	-	expression tag	UNP Q9UGN5
D	221	LEU	-	expression tag	UNP Q9UGN5
D	222	ASP	-	expression tag	UNP Q9UGN5
D	223	LEU	-	expression tag	UNP Q9UGN5
D	224	ARG	-	expression tag	UNP Q9UGN5
D	225	VAL	-	expression tag	UNP Q9UGN5
D	226	GLN	-	expression tag	UNP Q9UGN5
D	227	GLU	-	expression tag	UNP Q9UGN5
D	228	LEU	-	expression tag	UNP Q9UGN5
D	229	ILE	-	expression tag	UNP Q9UGN5
D	230	LYS	-	expression tag	UNP Q9UGN5
D	231	LEU	-	expression tag	UNP Q9UGN5
D	232	ILE	-	expression tag	UNP Q9UGN5
D	233	CYS	-	expression tag	UNP Q9UGN5
D	234	ASN	-	expression tag	UNP Q9UGN5
D	329	VAL	-	expression tag	UNP Q9UGN5
D	330	GLN	-	expression tag	UNP Q9UGN5
D	331	ALA	-	expression tag	UNP Q9UGN5
D	332	MET	-	expression tag	UNP Q9UGN5
D	333	GLU	-	expression tag	UNP Q9UGN5
D	334	GLU	-	expression tag	UNP Q9UGN5

- Molecule 2 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
2	A	1	Total 39	C 24	N 9	O 6	0	0
2	B	1	Total 39	C 24	N 9	O 6	0	0
2	C	1	Total 39	C 24	N 9	O 6	0	0
2	D	1	Total 39	C 24	N 9	O 6	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	13	Total O 13 13	0	0
3	B	12	Total O 12 12	0	0
3	C	17	Total O 17 17	0	0
3	D	9	Total O 9 9	0	0

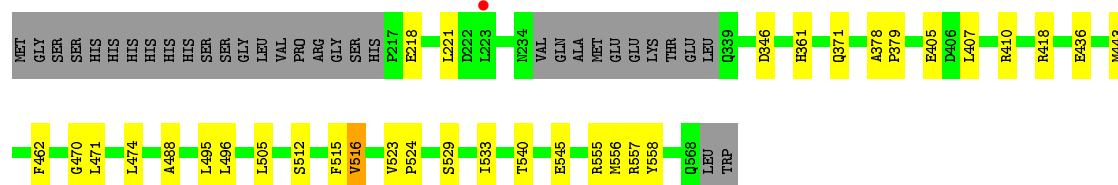


### 3 Residue-property plots [i](#)

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.

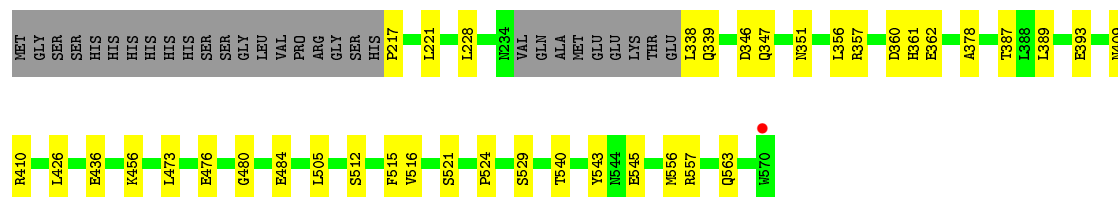
- Molecule 1: Poly [ADP-ribose] polymerase 2

Chain A:



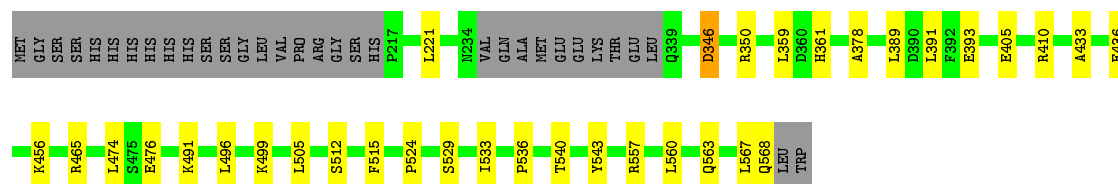
- Molecule 1: Poly [ADP-ribose] polymerase 2

Chain B:



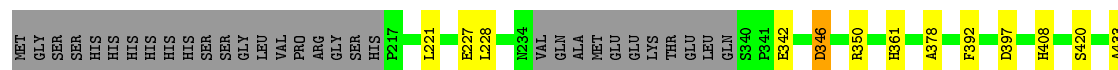
- Molecule 1: Poly [ADP-ribose] polymerase 2

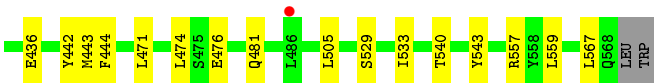
Chain C:



- Molecule 1: Poly [ADP-ribose] polymerase 2

Chain D:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.16 Å 119.90 Å 120.74 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.54 – 2.70 46.54 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (46.54-2.70) 98.3 (46.54-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 2.69 Å)	Xtriage
Refinement program	PHENIX 1.8.2 _1309	Depositor
R, $R_{free}$	0.193 , 0.248 0.192 , 0.247	Depositor DCC
$R_{free}$ test set	1856 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.2	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 29.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.095 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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

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	0.52	0/2015	0.65	0/2729
1	B	0.52	0/2036	0.69	0/2758
1	C	0.52	0/2015	0.68	0/2729
1	D	0.51	0/2006	0.65	0/2717
All	All	0.52	0/8072	0.67	0/10933

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	1967	0	1927	20	0
1	B	1988	0	1951	22	0
1	C	1967	0	1929	23	0
1	D	1958	0	1919	15	0
2	A	39	0	27	0	0
2	B	39	0	27	0	0
2	C	39	0	27	1	0
2	D	39	0	27	0	0
3	A	13	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	0	1	0
3	C	17	0	0	0	0
3	D	9	0	0	0	0
All	All	8087	0	7834	76	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 5.

All (76) 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:D:476:GLU:HG3	1:D:557:ARG:HG3	1.70	0.74
1:A:505:LEU:HB3	1:A:533:ILE:HD13	1.70	0.73
1:A:529:SER:HB3	1:D:529:SER:HB3	1.71	0.72
1:C:405:GLU:HG3	1:C:410:ARG:NH2	2.05	0.70
1:B:347:GLN:O	1:B:351:ASN:ND2	2.24	0.67
1:B:410:ARG:NH1	3:B:1101:HOH:O	2.21	0.67
1:C:476:GLU:HG3	1:C:557:ARG:HG3	1.77	0.67
1:C:405:GLU:HG3	1:C:410:ARG:HH22	1.60	0.66
1:B:529:SER:HB3	1:C:529:SER:HB3	1.81	0.62
1:B:476:GLU:HG3	1:B:557:ARG:HG3	1.80	0.62
1:C:505:LEU:HB3	1:C:533:ILE:HD13	1.83	0.60
1:B:217:PRO:HD3	1:B:339:GLN:HG3	1.86	0.57
1:C:465:ARG:NH2	1:C:567:LEU:O	2.36	0.56
1:C:567:LEU:O	1:C:568:GLN:HB2	2.07	0.55
1:A:516:VAL:HG12	1:A:523:VAL:HB	1.90	0.54
1:C:378:ALA:HB1	1:C:543:TYR:CZ	2.43	0.54
1:B:484:GLU:HB3	1:B:505:LEU:HD11	1.90	0.53
1:A:474:LEU:HB2	1:A:558:TYR:HB2	1.91	0.53
1:D:228:LEU:HD22	1:D:392:PHE:CE2	2.45	0.52
1:B:378:ALA:HB1	1:B:543:TYR:CZ	2.45	0.51
1:D:346:ASP:O	1:D:350:ARG:HG3	2.11	0.50
1:D:505:LEU:HD13	1:D:533:ILE:HD13	1.92	0.50
1:C:512:SER:HA	1:C:515:PHE:CG	2.48	0.49
1:A:556:MET:O	1:A:557:ARG:HD2	2.14	0.48
1:B:389:LEU:HD11	1:B:563:GLN:HB2	1.96	0.48
1:D:378:ALA:HB1	1:D:543:TYR:CZ	2.48	0.47
1:A:495:LEU:HD13	1:C:536:PRO:HB3	1.96	0.47
1:A:436:GLU:HG2	1:A:436:GLU:O	2.15	0.47
1:A:418:ARG:HG2	1:A:462:PHE:HD2	1.80	0.47
1:C:346:ASP:O	1:C:350:ARG:HG3	2.14	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:THR:HB	1:B:563:GLN:HB3	1.97	0.46
1:B:360:ASP:C	1:B:362:GLU:H	2.19	0.46
1:C:378:ALA:HB1	1:C:543:TYR:OH	2.16	0.45
1:B:512:SER:HA	1:B:515:PHE:CD2	2.52	0.45
1:B:228:LEU:HD23	1:B:356:LEU:HD13	1.99	0.45
1:A:378:ALA:HA	1:A:379:PRO:HD3	1.79	0.45
1:B:357:ARG:NH1	1:B:393:GLU:OE2	2.50	0.45
1:C:359:LEU:HD12	1:C:391:LEU:CD2	2.47	0.45
1:A:515:PHE:CD1	1:A:524:PRO:HA	2.52	0.44
1:D:408:HIS:NE2	1:D:481:GLN:OE1	2.45	0.44
1:B:378:ALA:HB1	1:B:543:TYR:OH	2.18	0.44
1:C:491:LYS:NZ	1:D:567:LEU:O	2.50	0.44
1:C:359:LEU:HD21	1:C:393:GLU:HB2	2.00	0.44
1:B:515:PHE:CD1	1:B:524:PRO:HA	2.52	0.44
1:D:342:GLU:OE1	1:D:350:ARG:HD2	2.18	0.43
1:D:433:ALA:HB1	1:D:442:TYR:CZ	2.52	0.43
1:B:436:GLU:O	1:B:436:GLU:HG2	2.18	0.43
1:A:496:LEU:HD23	1:A:496:LEU:HA	1.86	0.43
1:B:360:ASP:OD1	1:B:361:HIS:N	2.52	0.43
1:B:409:ASN:ND2	1:B:480:GLY:O	2.51	0.43
1:B:512:SER:HA	1:B:515:PHE:CG	2.54	0.43
1:C:512:SER:HA	1:C:515:PHE:CD2	2.53	0.43
1:A:405:GLU:HG3	1:A:410:ARG:NH2	2.34	0.42
1:A:443:MET:HG3	1:A:488:ALA:HB1	2.01	0.42
1:C:433:ALA:HB2	2:C:1001:UHB:H19A	2.02	0.42
1:D:436:GLU:HG2	1:D:436:GLU:O	2.20	0.42
1:C:515:PHE:CD1	1:C:524:PRO:HA	2.55	0.42
1:C:436:GLU:O	1:C:436:GLU:HG2	2.21	0.41
1:C:389:LEU:HD11	1:C:563:GLN:HB2	2.02	0.41
1:A:407:LEU:HA	1:A:407:LEU:HD23	1.87	0.41
1:A:555:ARG:NH2	1:A:557:ARG:CZ	2.83	0.41
1:C:560:LEU:N	1:C:560:LEU:HD12	2.35	0.41
1:D:443:MET:HG2	1:D:444:PHE:CE2	2.55	0.41
1:A:474:LEU:HA	1:A:474:LEU:HD23	1.82	0.41
1:A:512:SER:HA	1:A:515:PHE:CG	2.56	0.41
1:D:397:ASP:OD1	1:D:397:ASP:N	2.54	0.41
1:B:456:LYS:NZ	1:B:545:GLU:OE2	2.35	0.41
1:A:470:GLY:O	1:A:471:LEU:HD23	2.21	0.41
1:C:474:LEU:HA	1:C:474:LEU:HD23	1.72	0.41
1:D:474:LEU:HA	1:D:474:LEU:HD23	1.93	0.40
1:D:471:LEU:HD13	1:D:559:LEU:HD21	2.03	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:GLN:NE2	3:A:1102:HOH:O	2.54	0.40
1:B:473:LEU:HD21	1:B:556:MET:HG2	2.03	0.40
1:A:557:ARG:HA	1:A:557:ARG:HD2	1.95	0.40
1:B:426:LEU:HA	1:B:426:LEU:HD23	1.86	0.40
1:C:496:LEU:HD13	1:C:499:LYS:O	2.22	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	244/280 (87%)	239 (98%)	5 (2%)	0	100	100
1	B	247/280 (88%)	239 (97%)	8 (3%)	0	100	100
1	C	244/280 (87%)	237 (97%)	7 (3%)	0	100	100
1	D	243/280 (87%)	235 (97%)	8 (3%)	0	100	100
All	All	978/1120 (87%)	950 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	216/245 (88%)	209 (97%)	7 (3%)	39	68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	218/245 (89%)	212 (97%)	6 (3%)	43	73
1	C	216/245 (88%)	211 (98%)	5 (2%)	50	78
1	D	215/245 (88%)	209 (97%)	6 (3%)	43	73
All	All	865/980 (88%)	841 (97%)	24 (3%)	43	73

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	GLU
1	A	221	LEU
1	A	346	ASP
1	A	361	HIS
1	A	516	VAL
1	A	540	THR
1	A	545	GLU
1	B	221	LEU
1	B	338	LEU
1	B	346	ASP
1	B	516	VAL
1	B	521	SER
1	B	540	THR
1	C	221	LEU
1	C	346	ASP
1	C	361	HIS
1	C	456	LYS
1	C	540	THR
1	D	221	LEU
1	D	227	GLU
1	D	346	ASP
1	D	361	HIS
1	D	420	SER
1	D	540	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

4 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	UHB	D	1001	-	41,44,44	0.50	0	50,65,65	0.63	1 (2%)
2	UHB	A	1001	-	41,44,44	0.48	0	50,65,65	0.70	1 (2%)
2	UHB	C	1001	-	41,44,44	0.51	0	50,65,65	0.59	1 (2%)
2	UHB	B	1001	-	41,44,44	0.51	0	50,65,65	0.81	1 (2%)

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	UHB	D	1001	-	-	2/16/55/55	0/6/6/6
2	UHB	A	1001	-	-	2/16/55/55	0/6/6/6
2	UHB	C	1001	-	-	2/16/55/55	0/6/6/6
2	UHB	B	1001	-	-	2/16/55/55	0/6/6/6

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	UHB	C31-C38-N39	2.16	123.63	120.35
2	B	1001	UHB	C31-C38-N39	2.12	123.58	120.35
2	A	1001	UHB	C31-C38-N39	2.12	123.57	120.35
2	C	1001	UHB	C31-C38-N39	2.11	123.56	120.35

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1001	UHB	C12-C14-N15-C16
2	A	1001	UHB	C12-C14-N15-C16
2	D	1001	UHB	C05-C04-N11-C12
2	B	1001	UHB	C05-C04-N11-C12
2	B	1001	UHB	C12-C14-N15-C16
2	C	1001	UHB	C05-C04-N11-C12
2	A	1001	UHB	C05-C04-N11-C12
2	D	1001	UHB	C12-C14-N15-C16

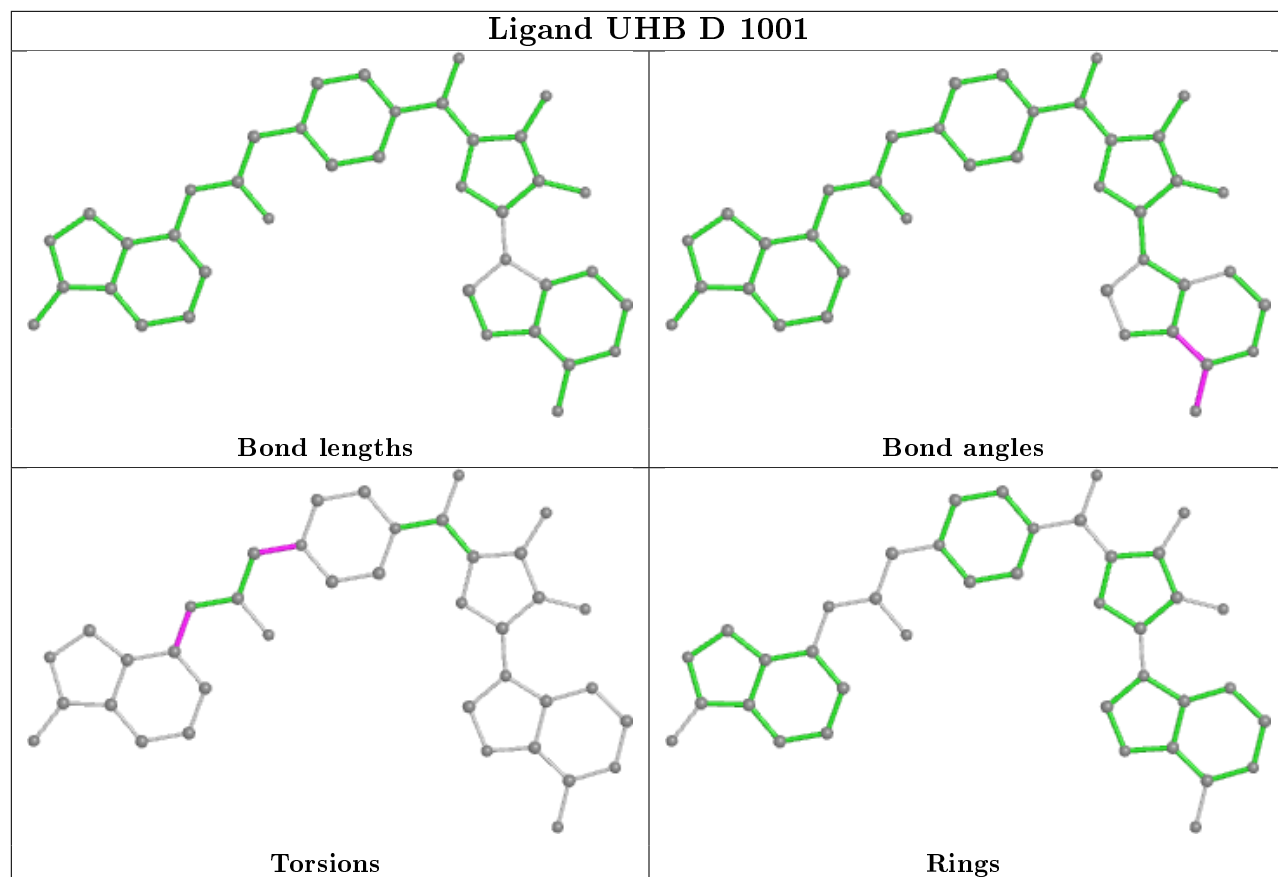
There are no ring outliers.

1 monomer is involved in 1 short contact:

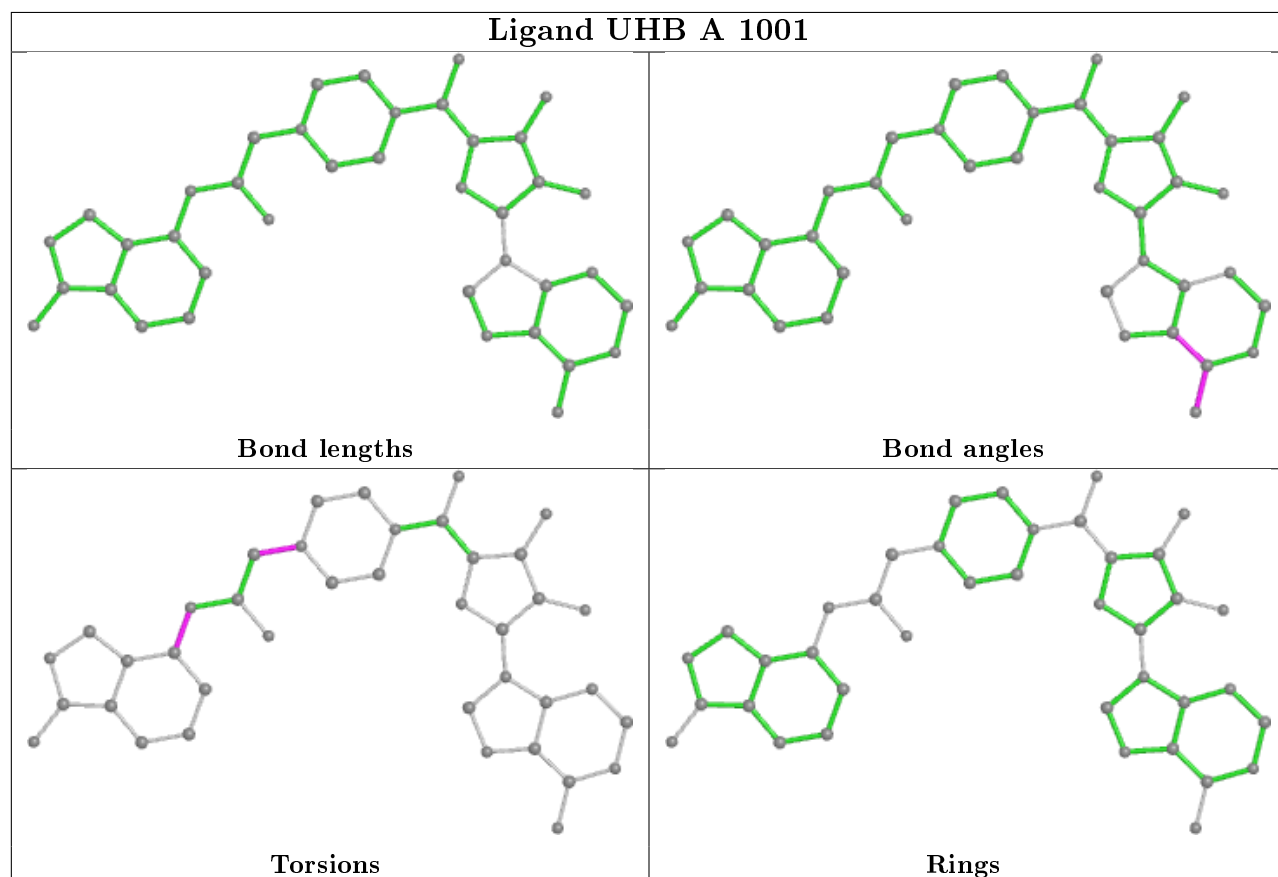
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	UHB	1	0

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.

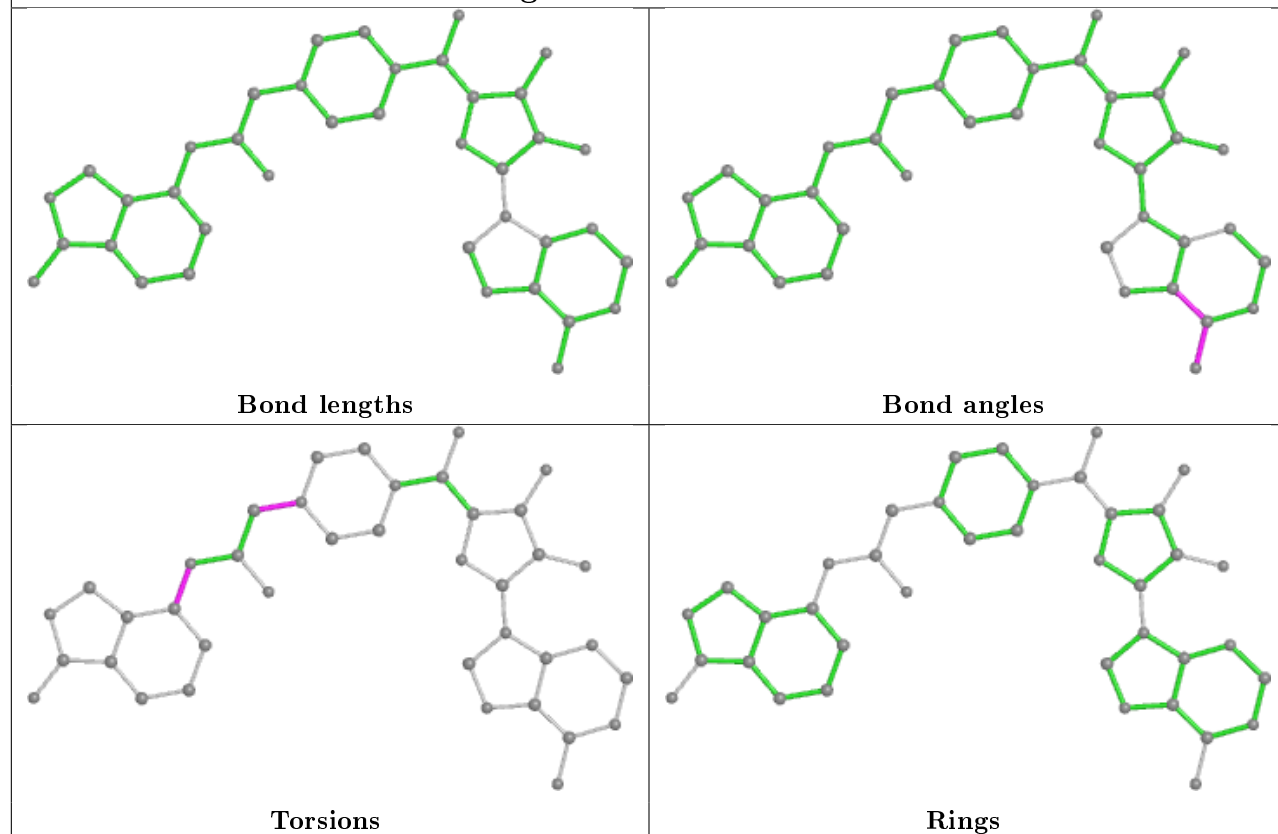
## Ligand UHB D 1001



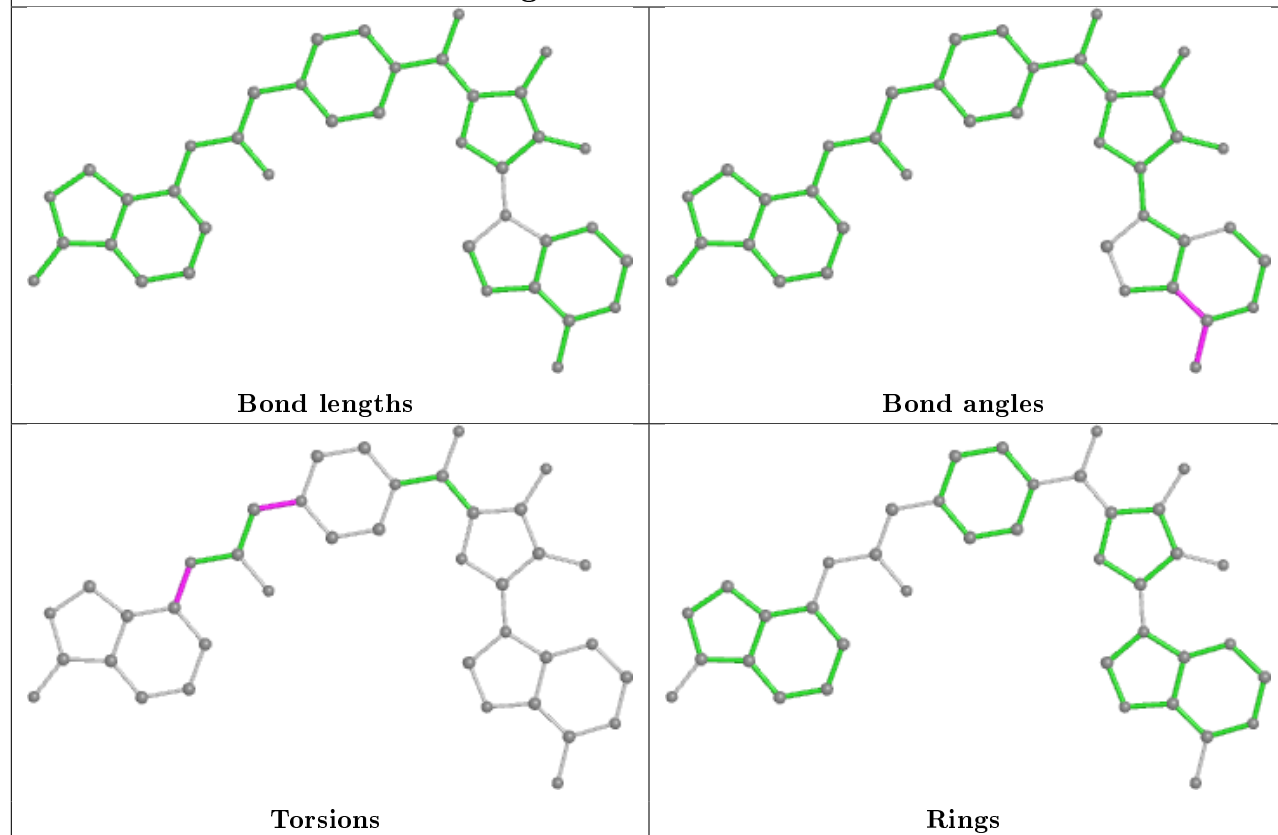
## Ligand UHB A 1001



## Ligand UHB C 1001



## Ligand UHB B 1001



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	248/280 (88%)	0.05	1 (0%) 92 93	34, 48, 73, 96	0
1	B	251/280 (89%)	0.07	1 (0%) 92 93	33, 53, 76, 99	0
1	C	248/280 (88%)	0.05	0 100 100	34, 54, 81, 92	0
1	D	247/280 (88%)	0.09	1 (0%) 92 93	39, 57, 80, 93	0
All	All	994/1120 (88%)	0.07	3 (0%) 94 95	33, 53, 78, 99	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	570	TRP	3.5
1	A	223	LEU	2.1
1	D	486	LEU	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](#)

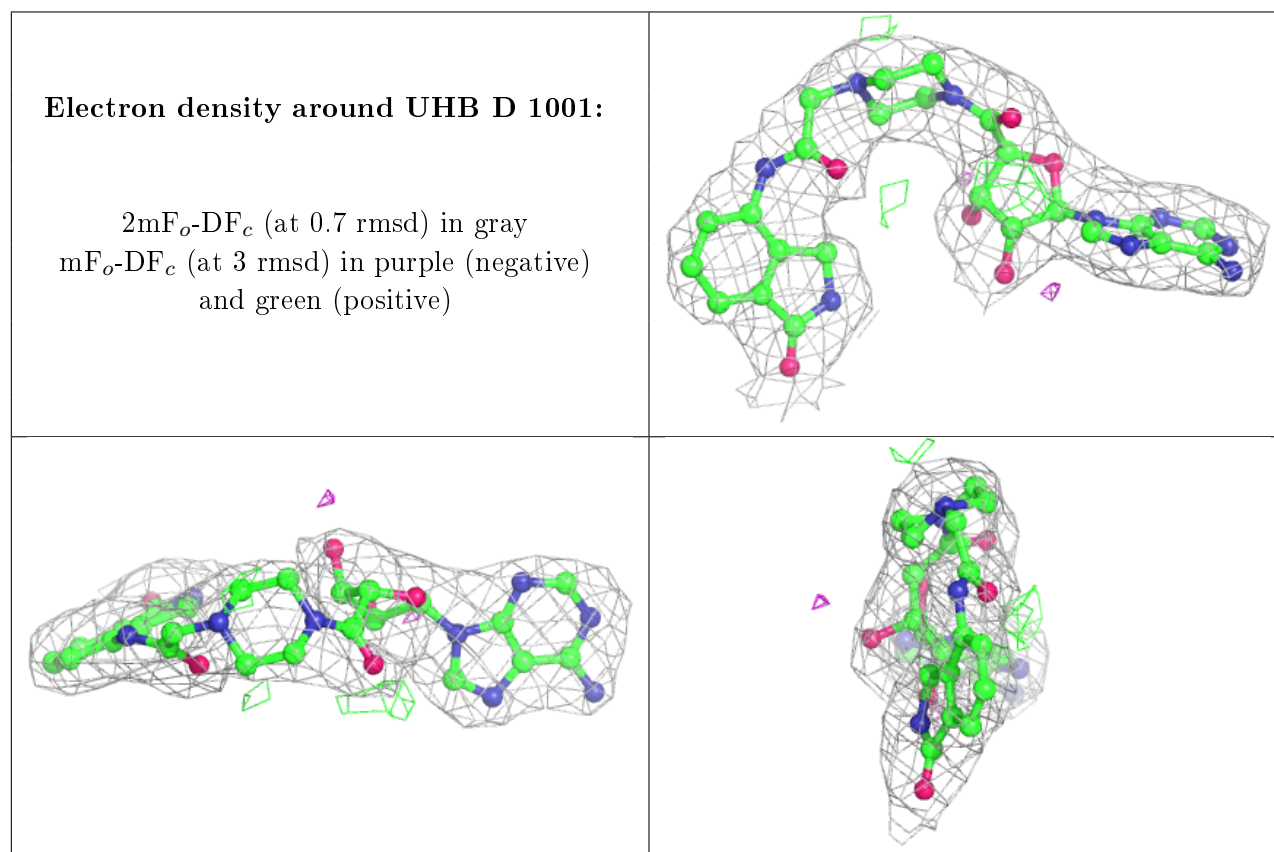
There are no monosaccharides in this entry.

### 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.

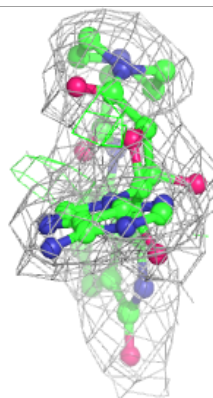
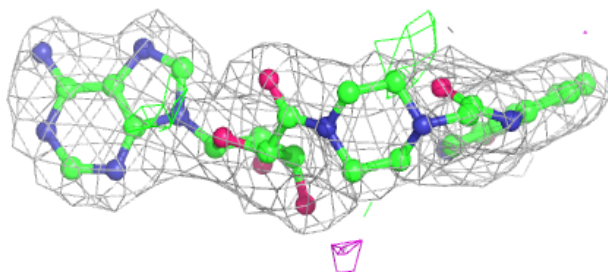
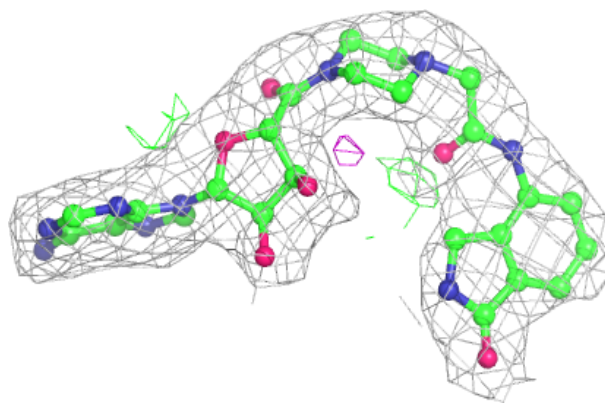
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	UHB	D	1001	39/39	0.98	0.18	38,45,53,53	0
2	UHB	A	1001	39/39	0.98	0.16	31,39,47,48	0
2	UHB	C	1001	39/39	0.98	0.17	32,44,49,55	0
2	UHB	B	1001	39/39	0.98	0.17	30,41,48,50	0

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.

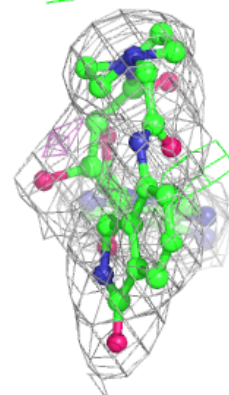
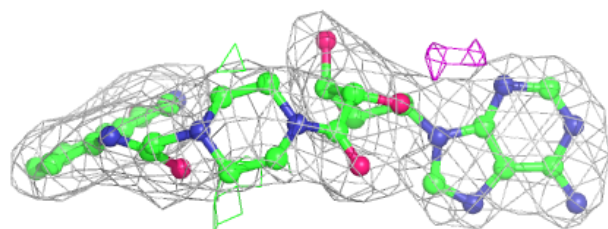
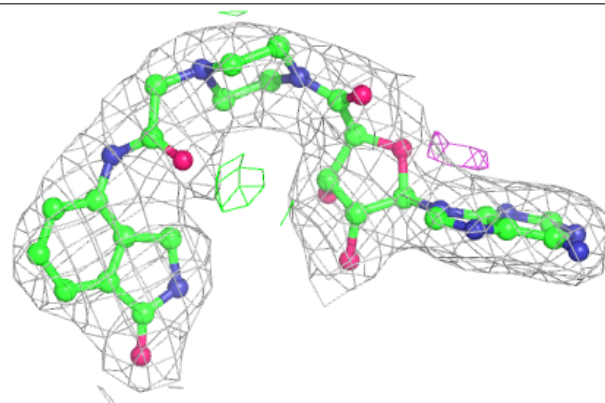


**Electron density around UHB A 1001:**

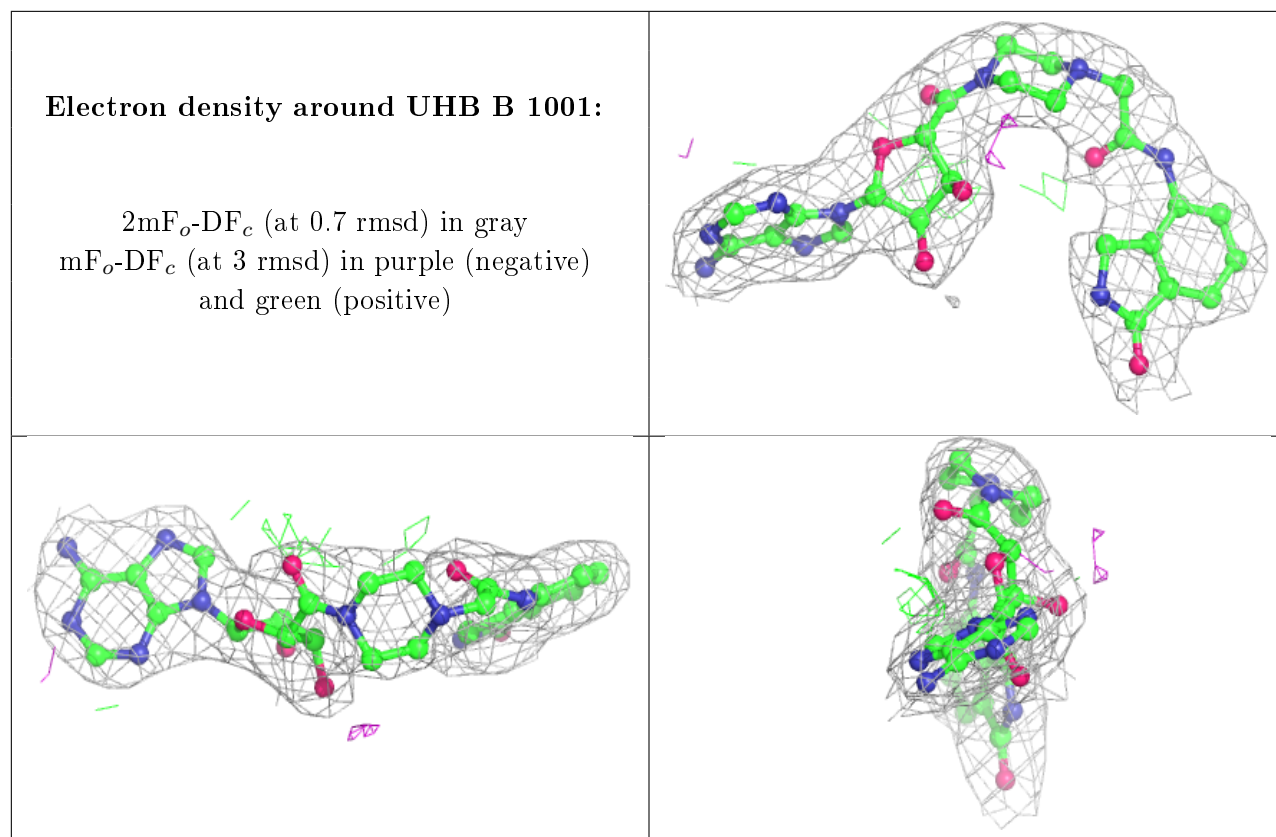
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around UHB C 1001:**

$2mF_o-DF_c$  (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.