wwPDB X-ray Structure Validation Summary Report (i)

May 17, 2020 – 03:25 am BST

PDB ID	:	4TKF
Title	:	Crystal Structure of human Tankyrase 2 in complex with IWR-1.
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	:	2014-05-26
Resolution	:	2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

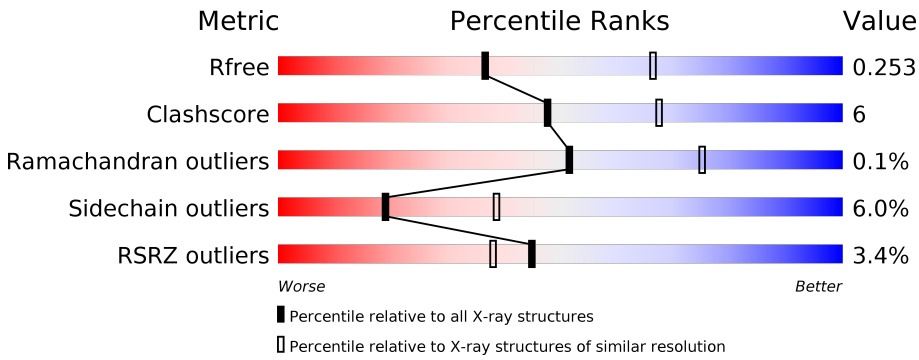
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 >=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 <=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	4% 70% 17% 12%
1	B	227	2% 74% 13% • 10%
1	C	227	% 77% 15% 8%
1	D	227	6% 67% 15% • 17%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6912 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	199	1598	1007	296	284	11	0	0	0
1	B	204	1642	1035	303	293	11	0	0	0
1	C	208	1686	1066	308	301	11	0	1	0
1	D	188	1522	959	284	269	10	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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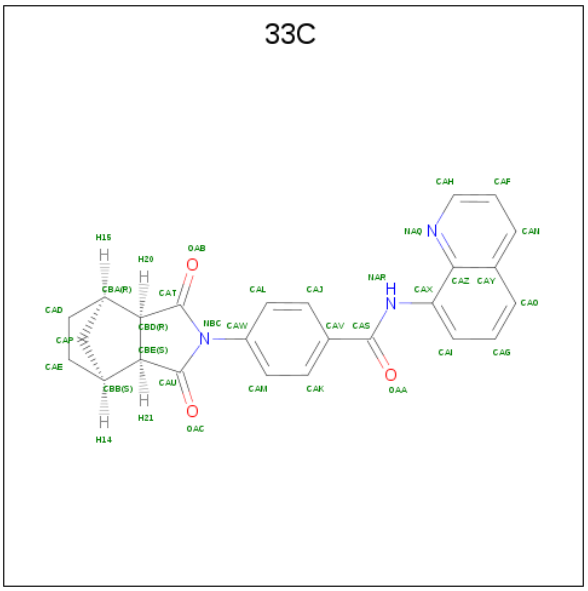
Chain	Residue	Modelled	Actual	Comment	Reference
D	938	MET	-	initiating methionine	UNP Q9H2K2
D	939	GLY	-	expression tag	UNP Q9H2K2
D	940	SER	-	expression tag	UNP Q9H2K2
D	941	SER	-	expression tag	UNP Q9H2K2
D	942	HIS	-	expression tag	UNP Q9H2K2
D	943	HIS	-	expression tag	UNP Q9H2K2
D	944	HIS	-	expression 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).

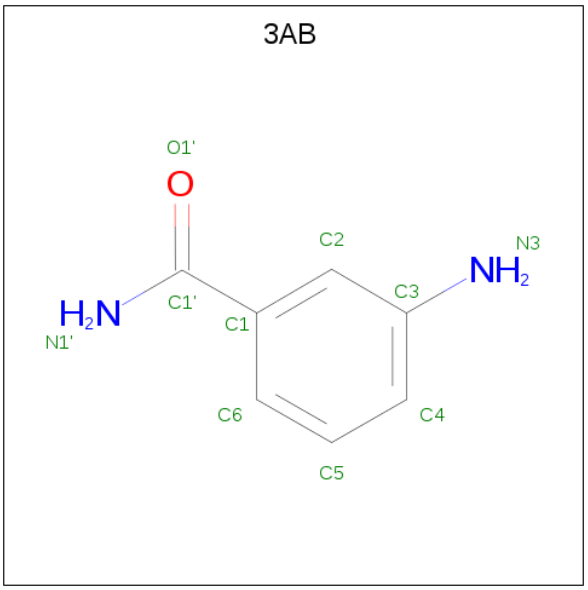
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	B	1	1	1	0	0
2	A	1	1	1	0	0
2	D	1	1	1	0	0
2	C	1	1	1	0	0

- Molecule 3 is 4-[(3aR,4R,7S,7aS)-1,3-dioxooctahydro-2H-4,7-methanoisoindol-2-yl]-N-(quinolin-8-yl)benzamide (three-letter code: 33C) (formula: $C_{25}H_{21}N_3O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	31	25	3	3	0	0
			Total	C	N	O		
3	B	1	31	25	3	3	0	0
			Total	C	N	O		
3	C	1	31	25	3	3	0	0
			Total	C	N	O		
3	D	1	31	25	3	3	0	0

- Molecule 4 is 3-aminobenzamide (three-letter code: 3AB) (formula: $C_7H_8N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	10	7	2	1	0	0
			Total	C	N	O		
4	C	1	10	7	2	1	0	0

- Molecule 5 is water.

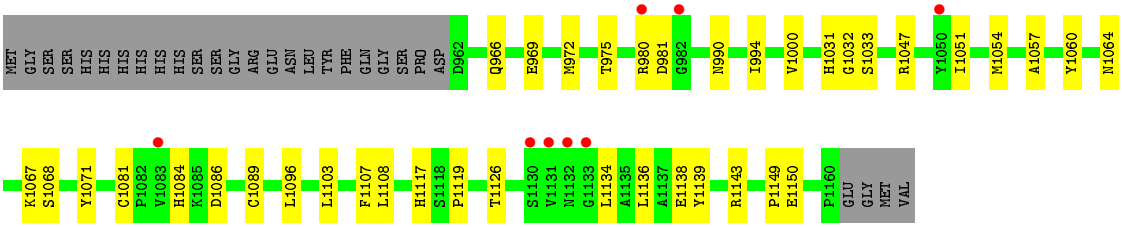
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	68	68	68	0	0
			Total	O		
5	B	80	80	80	0	0
			Total	O		
5	C	104	104	104	0	0
			Total	O		
5	D	64	64	64	0	0

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.

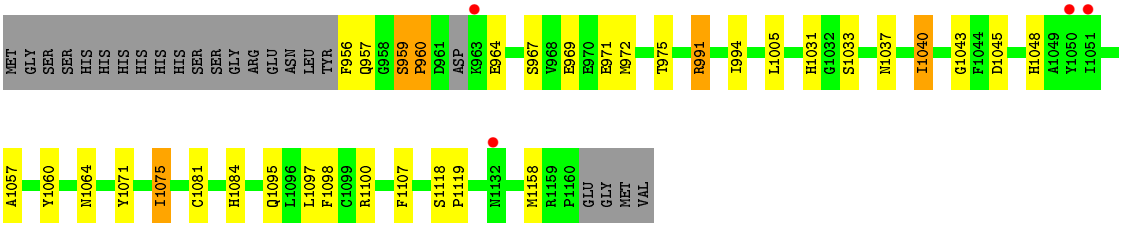
- Molecule 1: Tankyrase-2

Chain A:



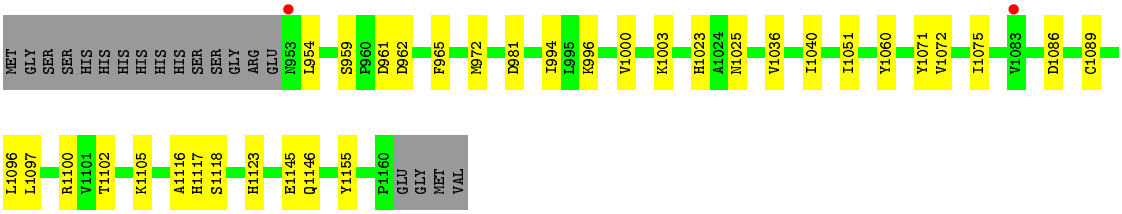
- Molecule 1: Tankyrase-2

Chain B:



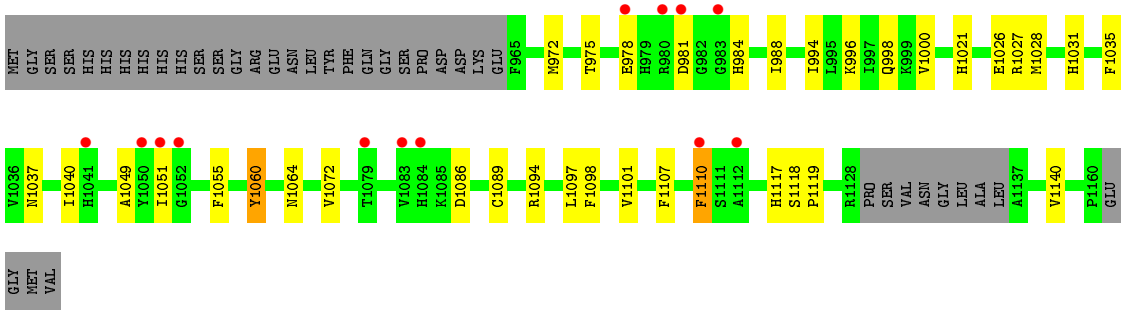
- Molecule 1: Tankyrase-2

Chain C:



- Molecule 1: Tankyrase-2

Chain D:


GLY
MET
VAL
V1036
N1037
I1040
H1041
A1049
Y1050
I1051
G1052
F1055
Y1060
N1064
V1072
T1079
V1083
H1084
K1085
D1086
C1089
R1094
L1097
F1098
V1101
F1107
F1110
S1111
A1112
H1117
S1118
P1119
R1128
PRO
SER
VAL
ASN
GLY
LEU
ALA
LEU
A1137
V1140
P1160
GLU
MET
GLY
SER
SER
HIS
HIS
HIS
HIS
HIS
HIS
SER
SER
GLY
ARG
GLU
ASN
LEU
TYR
PHE
GLN
GLY
SER
PRO
ASP
ASP
LYS
GLU
F965
M972
T975
E978
H979
R980
D981
G982
G983
H984
I988
I994
L995
K996
I997
Q998
K999
V1000
H1021
E1026
R1027
M1028
H1031
F1035

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.36Å 78.59Å 151.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.60 – 2.60 19.65 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.60-2.60) 99.8 (19.65-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 2.59Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.166 , 0.251 0.171 , 0.253	Depositor DCC
R_{free} test set	1389 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 65.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6912	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 3AB, ZN, 33C

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	0.50	0/1641	0.74	0/2207
1	B	0.56	1/1686 (0.1%)	0.79	1/2265 (0.0%)
1	C	0.53	0/1736	0.75	0/2335
1	D	0.50	0/1563	0.72	0/2098
All	All	0.52	1/6626 (0.0%)	0.75	1/8905 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	960	PRO	N-CD	5.11	1.54	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	959	SER	C-N-CD	5.85	140.69	128.40

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	1598	0	1528	22	0
1	B	1642	0	1572	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1686	0	1612	20	0
1	D	1522	0	1452	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	21	3	0
3	B	31	0	21	3	0
3	C	31	0	21	7	0
3	D	31	0	21	2	0
4	A	10	0	8	2	0
4	C	10	0	8	3	0
5	A	68	0	0	0	0
5	B	80	0	0	0	0
5	C	104	0	0	1	0
5	D	64	0	0	1	0
All	All	6912	0	6264	79	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 6.

The worst 5 of 79 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	1.27	0.81
1:D:1000:VAL:HG21	1:D:1040:ILE:HD12	1.64	0.79
1:D:1110:PHE:H	1:D:1110:PHE:HD1	1.40	0.70
1:C:1040:ILE:HD11	1:C:1097:LEU:HD21	1.74	0.67
1:A:1060:TYR:CD1	3:A:1202:33C:H20	2.30	0.67

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%)	190 (96%)	6 (3%)	1 (0%)	29	52
1	B	200/227 (88%)	193 (96%)	7 (4%)	0	100	100
1	C	207/227 (91%)	200 (97%)	7 (3%)	0	100	100
1	D	184/227 (81%)	176 (96%)	8 (4%)	0	100	100
All	All	788/908 (87%)	759 (96%)	28 (4%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	980	ARG

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	166/192 (86%)	157 (95%)	9 (5%)	22	44
1	B	172/192 (90%)	160 (93%)	12 (7%)	15	30
1	C	177/192 (92%)	167 (94%)	10 (6%)	21	42
1	D	158/192 (82%)	149 (94%)	9 (6%)	20	41
All	All	673/768 (88%)	633 (94%)	40 (6%)	19	39

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1075	ILE
1	C	959	SER
1	D	1051	ILE
1	B	1118	SER
1	C	961	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such

sidechains are listed below:

Mol	Chain	Res	Type
1	C	1117	HIS
1	C	1123	HIS
1	D	1031	HIS
1	B	1095	GLN
1	D	1023	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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
4	3AB	C	1203	-	10,10,10	0.93	0	13,13,13	0.59	0
4	3AB	A	1203	-	10,10,10	0.77	0	13,13,13	0.75	0
3	33C	C	1202	-	36,36,36	2.25	7 (19%)	54,54,54	1.57	12 (22%)
3	33C	D	1202	-	36,36,36	2.28	6 (16%)	54,54,54	1.56	8 (14%)
3	33C	A	1202	-	36,36,36	2.14	5 (13%)	54,54,54	1.65	12 (22%)
3	33C	B	1202	-	36,36,36	2.15	5 (13%)	54,54,54	1.70	13 (24%)

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
4	3AB	C	1203	-	-	0/4/4/4	0/1/1/1
4	3AB	A	1203	-	-	0/4/4/4	0/1/1/1
3	33C	C	1202	-	-	4/12/49/49	0/7/6/6
3	33C	D	1202	-	-	2/12/49/49	0/7/6/6
3	33C	A	1202	-	-	4/12/49/49	0/7/6/6
3	33C	B	1202	-	-	4/12/49/49	0/7/6/6

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1202	33C	CAW-NBC	-7.84	1.32	1.44
3	C	1202	33C	CAW-NBC	-7.41	1.33	1.44
3	B	1202	33C	CAW-NBC	-7.26	1.33	1.44
3	C	1202	33C	CAE-CAD	-7.21	1.34	1.54
3	A	1202	33C	CAE-CAD	-7.12	1.34	1.54

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1202	33C	OAC-CAU-CBE	-3.91	123.08	127.52
3	B	1202	33C	CBD-CAT-NBC	3.89	111.51	108.26
3	D	1202	33C	CAX-CAZ-NAQ	3.89	120.78	117.48
3	C	1202	33C	CAH-NAQ-CAZ	3.82	122.06	117.30
3	D	1202	33C	CAH-NAQ-CAZ	3.82	122.06	117.30

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	33C	NAR-CAS-CAV-CAK
3	C	1202	33C	NAR-CAS-CAV-CAJ
3	C	1202	33C	OAA-CAS-CAV-CAJ
3	A	1202	33C	OAA-CAS-CAV-CAK
3	B	1202	33C	NAR-CAS-CAV-CAK

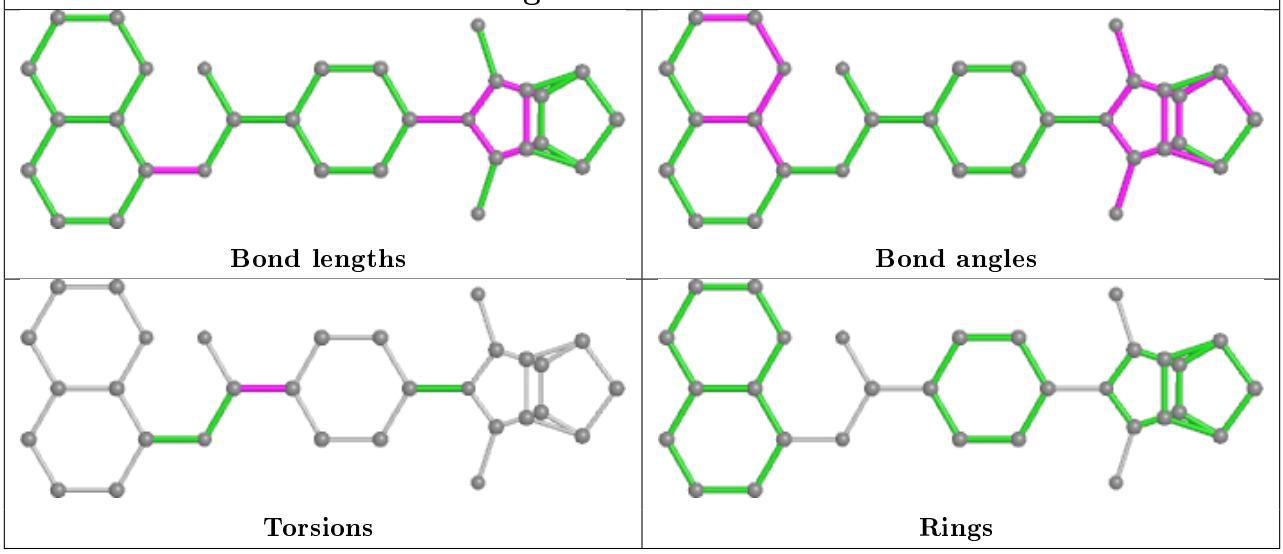
There are no ring outliers.

6 monomers are involved in 17 short contacts:

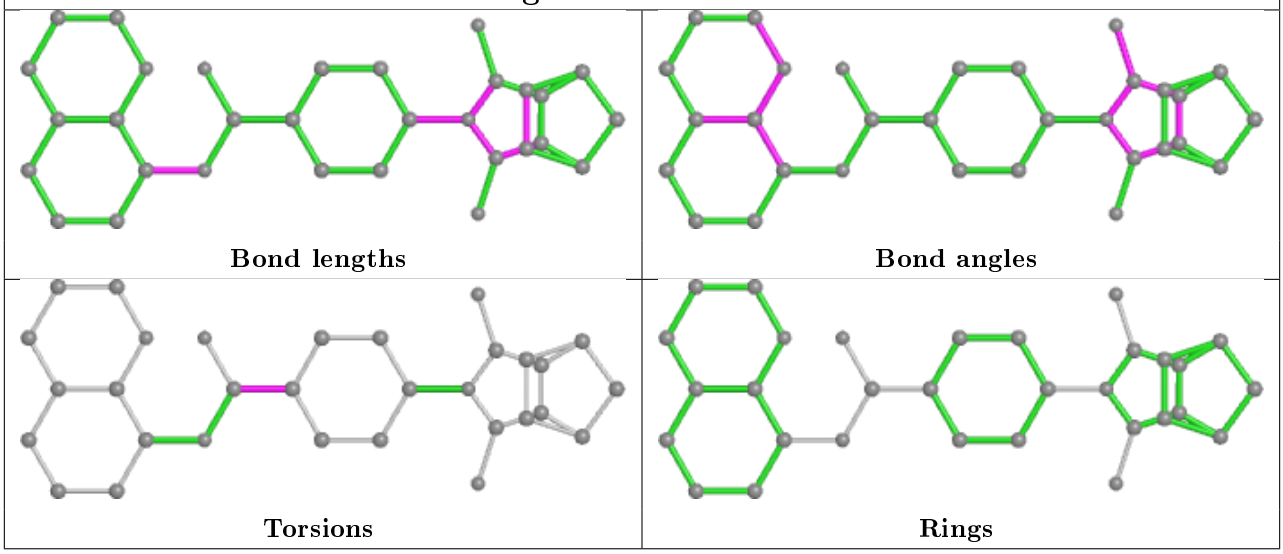
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1203	3AB	3	0
4	A	1203	3AB	2	0
3	C	1202	33C	7	0
3	D	1202	33C	2	0
3	A	1202	33C	3	0
3	B	1202	33C	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

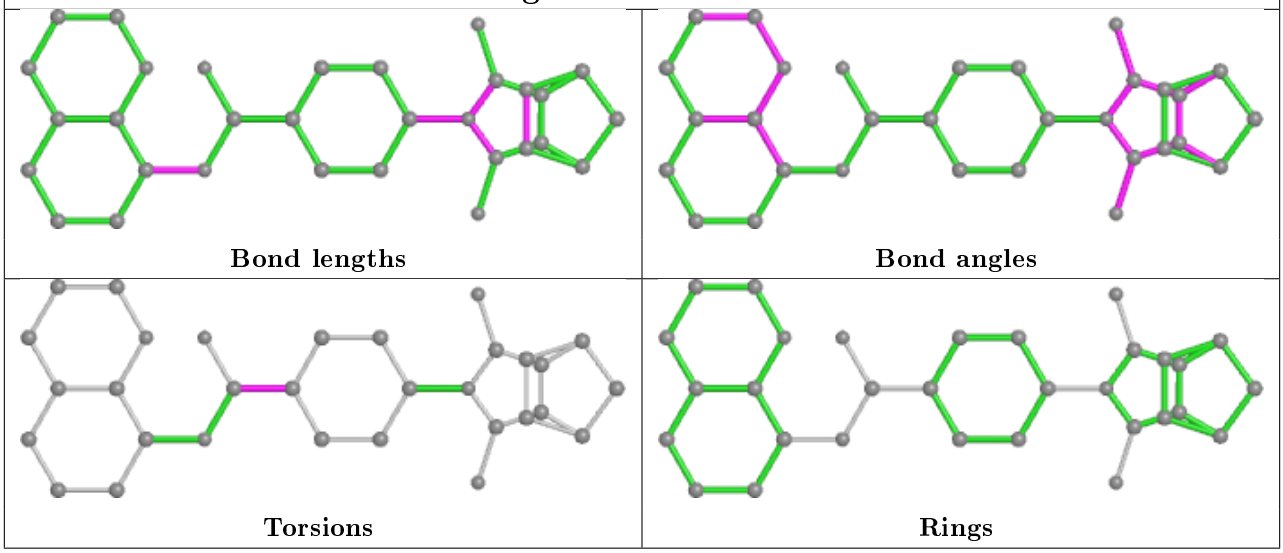
Ligand 33C C 1202



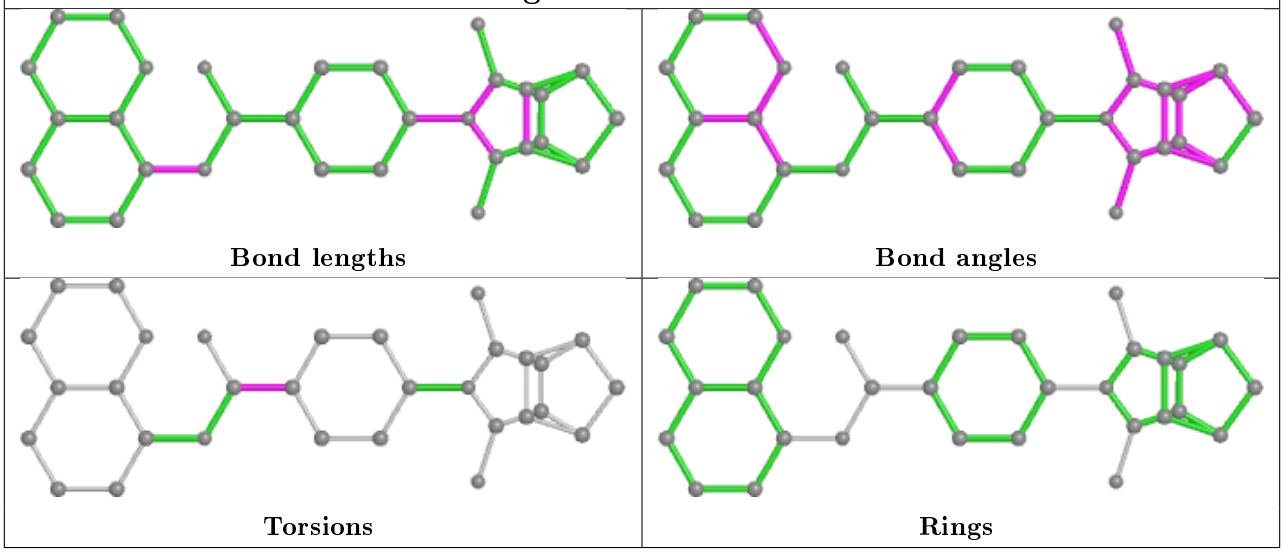
Ligand 33C D 1202



Ligand 33C A 1202



Ligand 33C B 1202



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 (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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	199/227 (87%)	-0.09	8 (4%)	38	31	19, 39, 72, 90	0
1	B	204/227 (89%)	-0.30	4 (1%)	65	60	17, 35, 64, 78	0
1	C	208/227 (91%)	-0.26	2 (0%)	82	80	17, 33, 58, 79	0
1	D	188/227 (82%)	-0.07	13 (6%)	16	12	19, 39, 73, 97	0
All	All	799/908 (87%)	-0.18	27 (3%)	45	38	17, 36, 69, 97	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1130	SER	5.5
1	D	980	ARG	4.9
1	A	1132	ASN	4.8
1	D	978	GLU	4.2
1	A	1133	GLY	3.6

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)

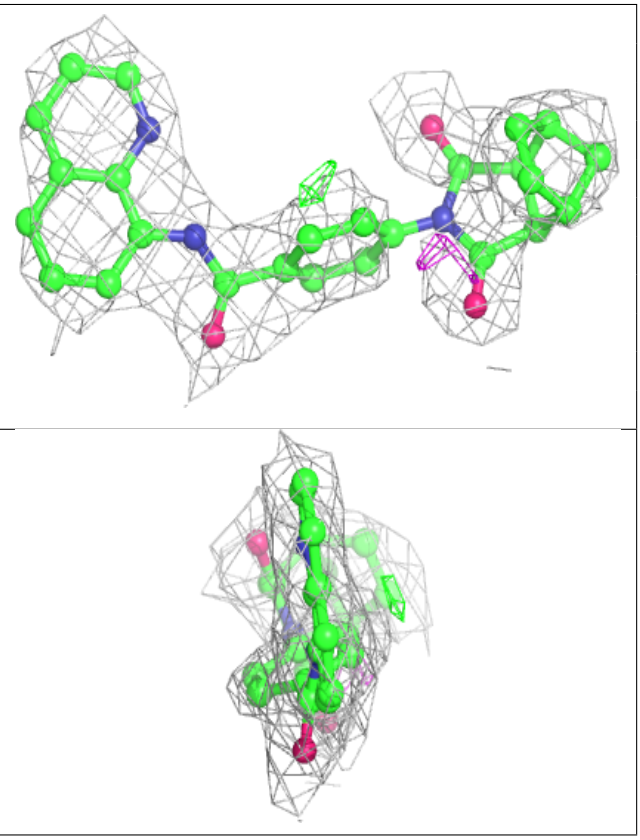
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	33C	C	1202	31/31	0.92	0.22	23,53,144,184	0
4	3AB	A	1203	10/10	0.93	0.24	34,71,144,162	0
3	33C	D	1202	31/31	0.94	0.16	19,35,72,76	0
3	33C	B	1202	31/31	0.94	0.15	15,35,84,142	0
4	3AB	C	1203	10/10	0.95	0.19	22,46,96,123	0
3	33C	A	1202	31/31	0.96	0.13	11,31,67,144	0
2	ZN	D	1201	1/1	0.98	0.03	57,57,57,57	0
2	ZN	B	1201	1/1	0.99	0.04	50,50,50,50	0
2	ZN	A	1201	1/1	0.99	0.03	53,53,53,53	0
2	ZN	C	1201	1/1	1.00	0.05	50,50,50,50	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.

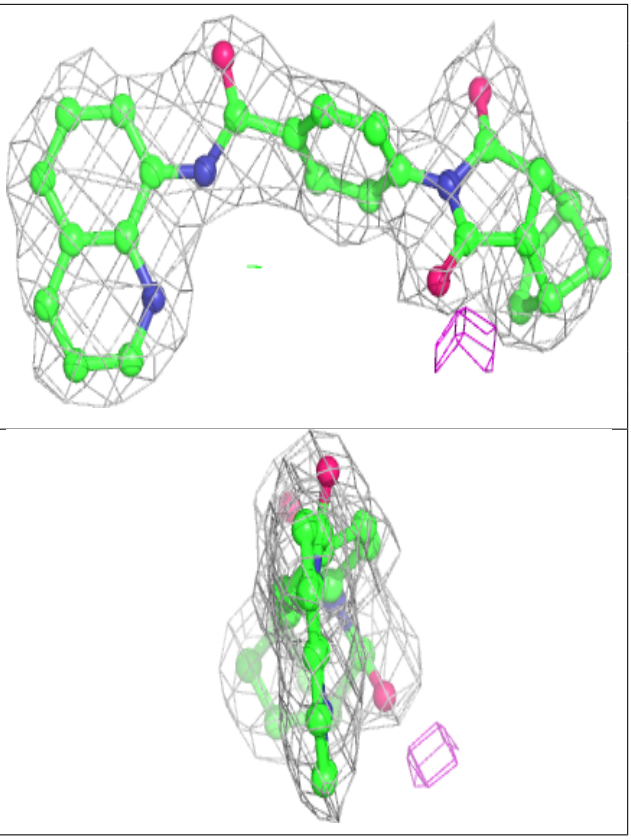
Electron density around 33C C 1202:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



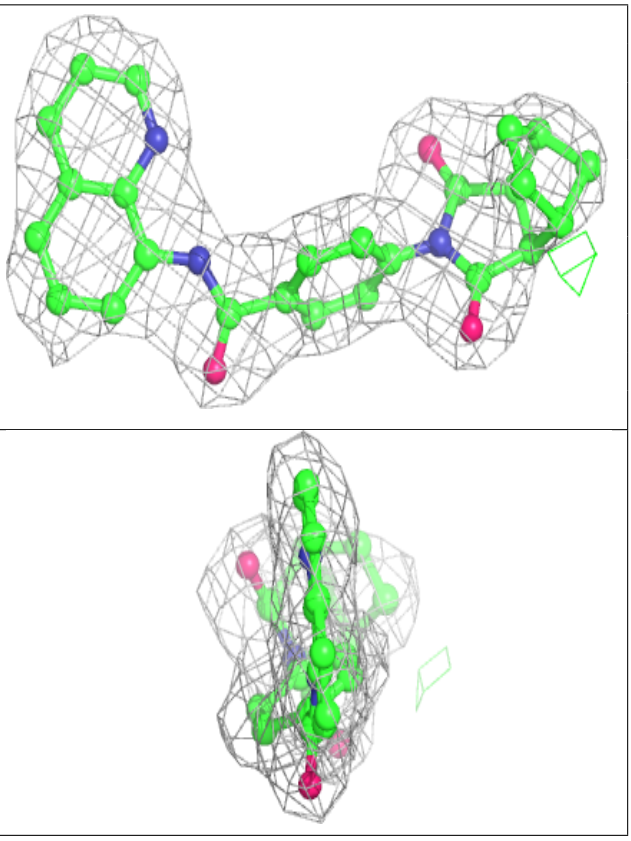
Electron density around 33C D 1202:

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



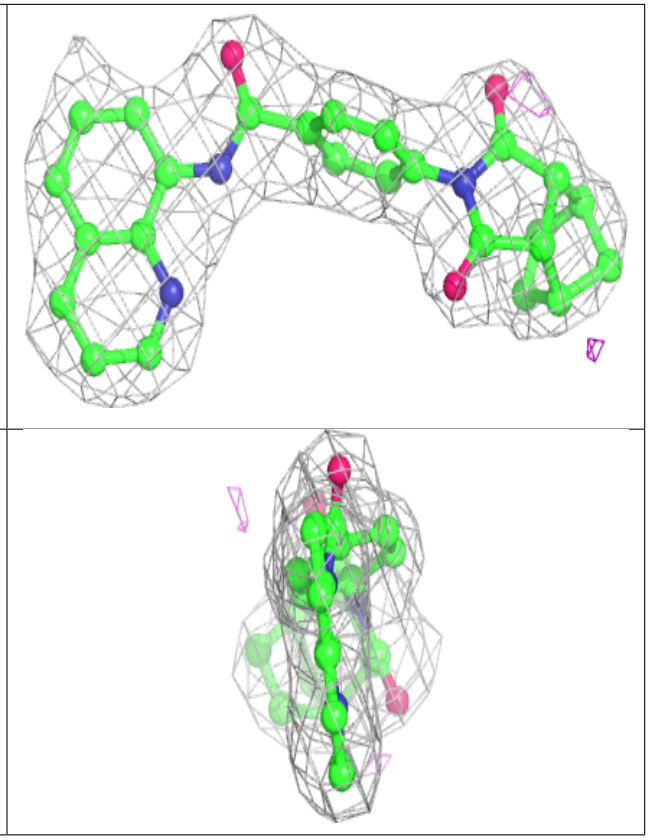
Electron density around 33C B 1202:

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



Electron density around 33C 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)



6.5 Other polymers (i)

There are no such residues in this entry.