



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 17, 2026 – 02:08 PM EDT

PDB ID : 11TN / pdb_000011tn
Title : Candida glabrata Glycogen Debranching Enzyme (GDE) in complex with Miglustat
Authors : Mishra, N.; Paz, A.
Deposited on : 2026-03-12
Resolution : 3.24 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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

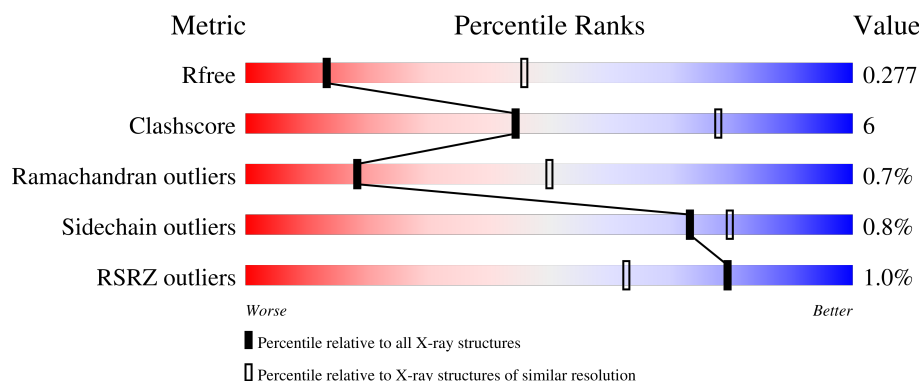
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2153 (3.28-3.20)
Clashscore	190562	2275 (3.28-3.20)
Ramachandran outliers	187476	2233 (3.28-3.20)
Sidechain outliers	187428	2232 (3.28-3.20)
RSRZ outliers	180081	2153 (3.28-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1524	
1	B	1524	

2 Entry composition [i](#)

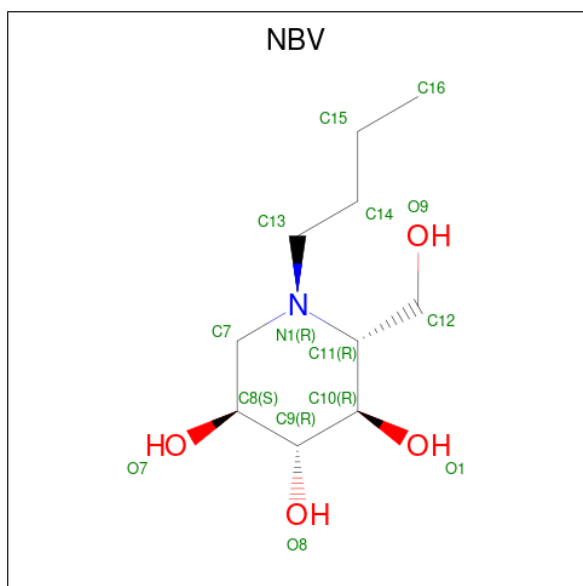
There are 2 unique types of molecules in this entry. The entry contains 23473 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycogen debranching enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1524	Total	C	N	O	S	0	0	0
			12264	7821	2061	2330	52			
1	B	1388	Total	C	N	O	S	0	0	0
			11179	7131	1884	2114	50			

- Molecule 2 is (2R,3R,4R,5S)-1-BUTYL-2-(HYDROXYMETHYL)PIPERIDINE-3,4,5-TRIOL (CCD ID: NBV) (formula: C₁₀H₂₁NO₄) (labeled as "Ligand of Interest" by depositor).

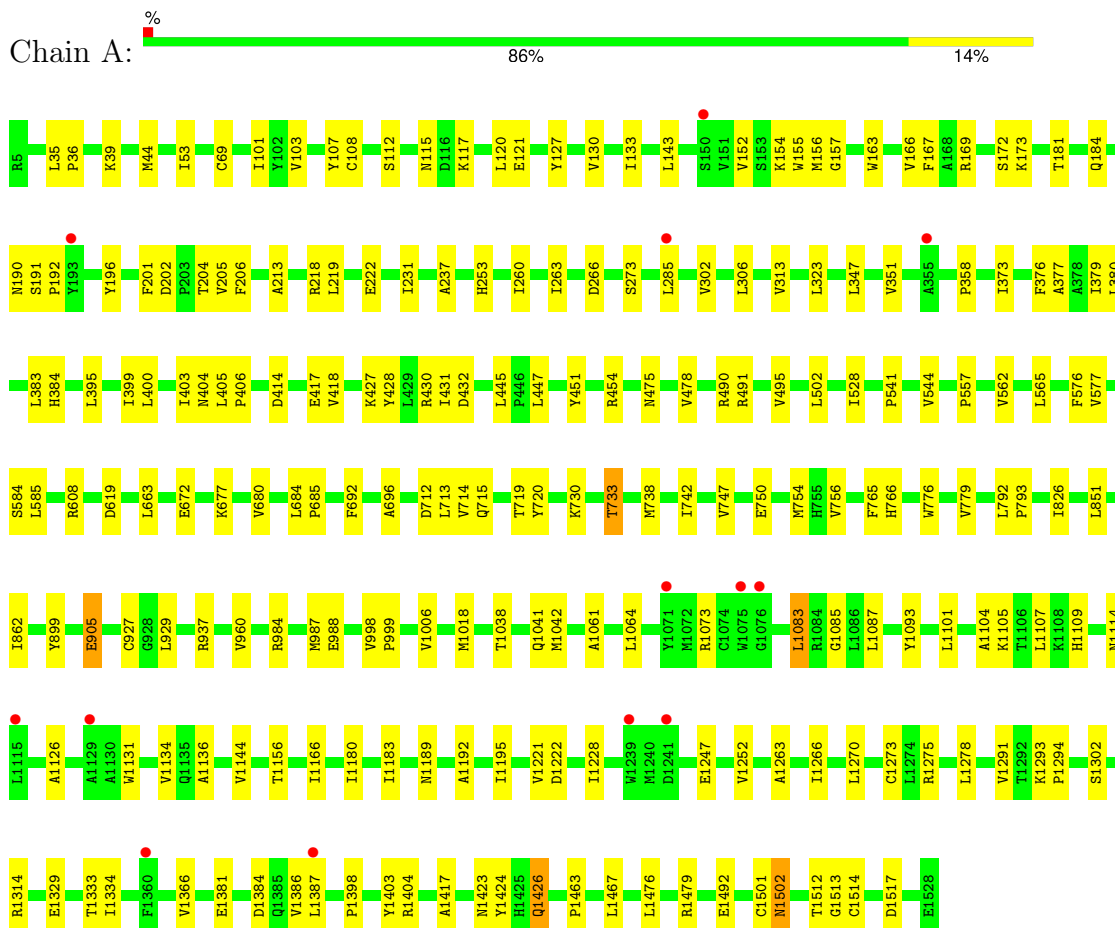


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	10	1	4		
2	B	1	Total	C	N	O	0	0
			15	10	1	4		

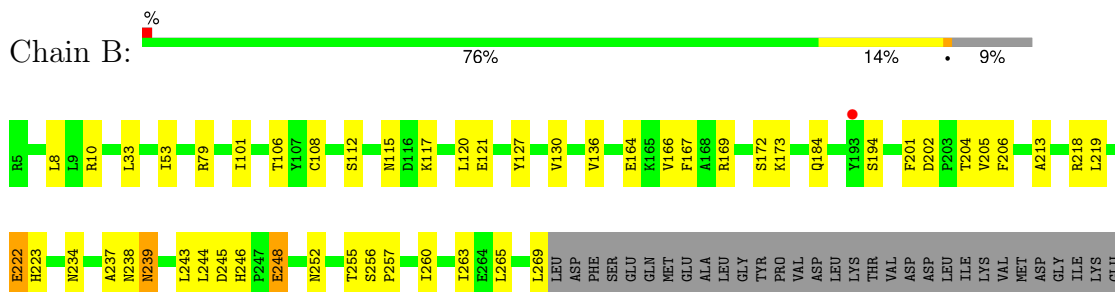
3 Residue-property plots

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: Glycogen debranching enzyme



• Molecule 1: Glycogen debranching enzyme



GLY	SER	LEU	GLY	GLY	ARG	GLY	SER	ASN	LYS	LYS	ILE	ASN	TYR	VAL	ASP	LYS	PHE	ALA	LYS	LEU	LYS	LEU	LYS	GLY	ARG	GLY	ASN	ASN	ASP	ASP	ASP	ASP	ASP	ASP	ASN	ASN	LEU	ALA	LYS	PHE	VAL	GLY	ARG	ASP	GLY	ASN	ASN	GLY	PHE
TRP	ILE	TRP	ASP	GLY	ASN	PRO	LEU	VAL	ASP	ASP	PHE	A481	S482	A487	Y488	R491	E492	V495	W496	G497	D498	C499	V500	K501	S511	L514	I528	P541	V544	V562	L565	F576	S584	L663	F664	T668	H669	D670	N671	V680	L684	P685	V690						
A691	F692	L713	R718	T719	K730	T733	M738	I742	E745	A746	V747	M754	H755	V756	F765	H766	W776	V779	L792	P793	E821	K1108	I822	I823	E824	G825	I826	L851	I862	Y899	G928	L929	V960	M969	N987	P994	L997	V998	P999										
V1006	T1029	T1038	Q1041	M1042	M1046	A1061	F1067	S1068	Y1071	M1072	R1073	C1074	R1077	S1082	L1083	R1084	G1085	L1086	L1087	L1101	A1104	L1107	K1108	H1109	M1114	D1117	A1118	G1119	A1126	R1127	D1128	W1131	V1134	Q1135	A1136	L1161	I1166	I1180											
I1183	I1195	K1196	Y1197	R1198	E1199	A1200	L1206	K1211	D1212	E1213	V1217	D1222	W1223	E1224	T1225	G1226	L1227	W1239	M1240	K1248	A1249	P1255	P1258	A1263	I1266	L1270	R1275	K1293	P1294	V1318	I1330	T1333	I1334	I1335	R1338	Q1355	F1356	R1357	P1358	N1359									
V1366	E1381	D1384	Q1385	V1386	L1387	R1388	V1391	G1392	M1393	R1394	T1395	L1396	D1397	P1398	S1399	D1400	Y1401	N1402	Y1403	E1411	T1418	S1419	E1429	W1432	C1433	Y1434	P1463	L1467	L1476	R1479	T1494	M1495	K1496	E1499	A1509	T1512	G1513	C1514	D1517	E1528									

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	159.08 Å 199.27 Å 254.21 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	127.11 – 3.24 127.11 – 3.24	Depositor EDS
% Data completeness (in resolution range)	56.7 (127.11-3.24) 56.7 (127.11-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.26 Å)	Xtriage
Refinement program	REFMAC 5.8.0431 (refmacat 0.4.105)	Depositor
R, R_{free}	0.235 , 0.274 0.241 , 0.277	Depositor DCC
R_{free} test set	1857 reflections (2.88%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 94.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	23473	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NBV

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	0.46	0/12574	0.86	1/17049 (0.0%)
1	B	0.46	0/11463	0.87	1/15542 (0.0%)
All	All	0.46	0/24037	0.87	2/32591 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	245	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	1222	ASP	CA-CB-CG	5.17	117.77	112.60

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	12264	0	11948	135	0
1	B	11179	0	10899	141	0
2	A	15	0	21	4	0
2	B	15	0	21	0	0
All	All	23473	0	22889	277	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 277 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:VAL:HG11	1:A:155:TRP:CE3	2.05	0.91
1:A:1038:THR:HG21	1:A:1512:THR:HG21	1.60	0.84
1:B:1038:THR:HG21	1:B:1512:THR:HG21	1.61	0.81
1:A:1424:TYR:OH	2:A:1601:NBV:H161	1.86	0.75
1:B:1400:ASP:O	1:B:1401:TYR:HB3	1.88	0.74

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	1522/1524 (100%)	1430 (94%)	89 (6%)	3 (0%)	43	72
1	B	1382/1524 (91%)	1269 (92%)	97 (7%)	16 (1%)	10	38
All	All	2904/3048 (95%)	2699 (93%)	186 (6%)	19 (1%)	18	50

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	482	SER
1	B	500	VAL
1	B	1334	ILE
1	B	1401	TYR
1	B	1496	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1343/1343 (100%)	1335 (99%)	8 (1%)	78	83
1	B	1225/1343 (91%)	1212 (99%)	13 (1%)	65	77
All	All	2568/2686 (96%)	2547 (99%)	21 (1%)	73	80

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1073	ARG
1	B	1166	ILE
1	B	1394	ARG
1	B	1217	VAL
1	B	1161	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	224	ASN
1	B	404	ASN
1	B	1449	ASN
1	B	866	GLN
1	B	1359	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NBV	B	1601	-	15,15,15	0.29	0	19,20,20	0.75	0
2	NBV	A	1601	-	15,15,15	0.34	0	19,20,20	1.22	3 (15%)

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	NBV	B	1601	-	-	3/6/26/26	0/1/1/1
2	NBV	A	1601	-	-	2/6/26/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1601	NBV	C12-C11-N1	-2.48	107.47	112.51
2	A	1601	NBV	C7-C8-C9	-2.45	107.25	110.17
2	A	1601	NBV	C12-C11-C10	-2.04	109.85	112.93

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1601	NBV	C10-C11-C12-O9

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Mol	Chain	Res	Type	Atoms
2	B	1601	NBV	N1-C13-C14-C15
2	B	1601	NBV	C13-C14-C15-C16
2	A	1601	NBV	C14-C13-N1-C7
2	A	1601	NBV	C14-C13-N1-C11

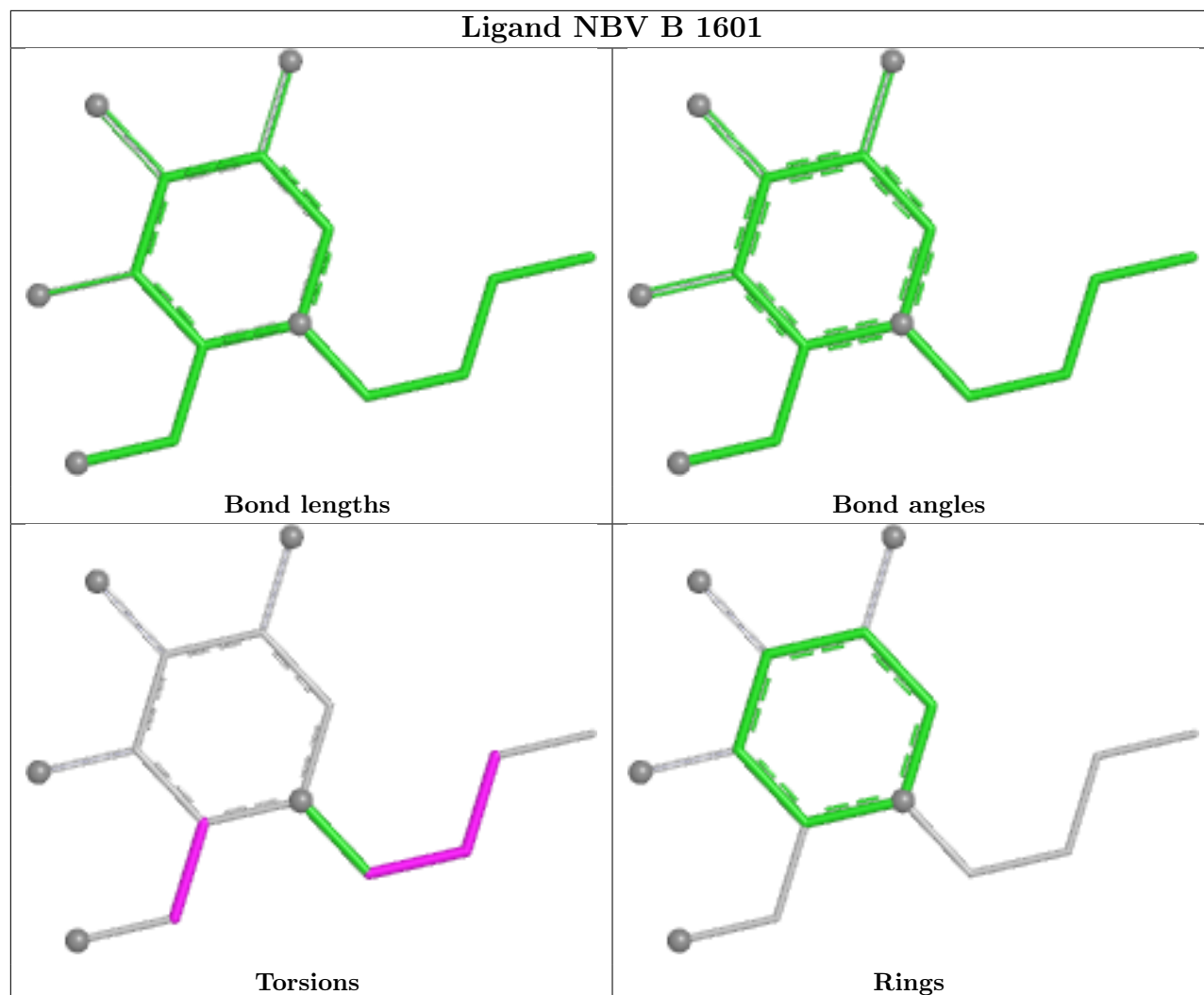
There are no ring outliers.

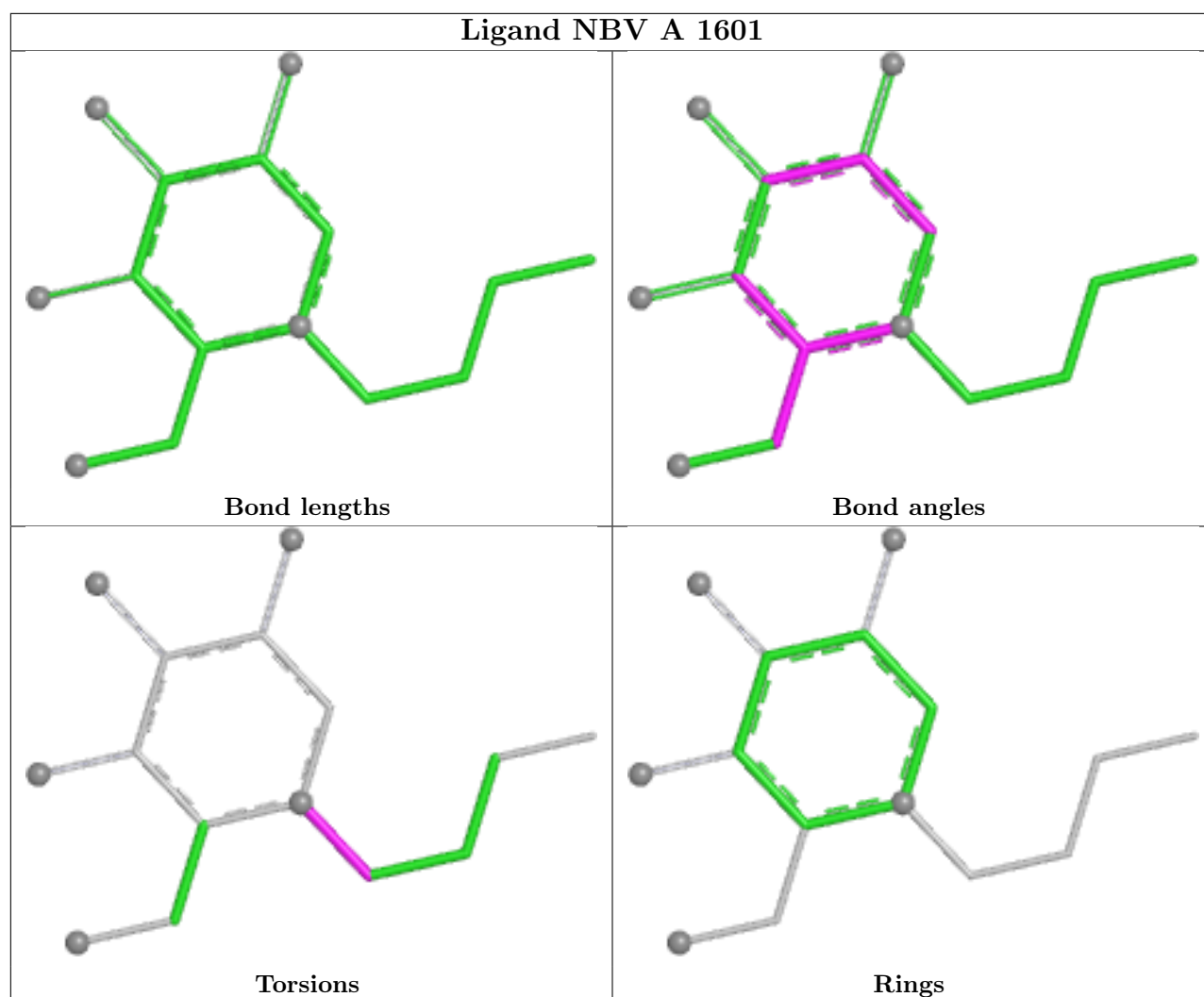
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1601	NBV	4	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 NBV B 1601





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	1524/1524 (100%)	-0.10	13 (0%) 81 64	46, 92, 158, 204	0
1	B	1388/1524 (91%)	-0.09	17 (1%) 76 58	37, 75, 113, 167	0
All	All	2912/3048 (95%)	-0.09	30 (1%) 79 63	37, 82, 148, 204	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1075	TRP	3.3
1	B	1240	MET	3.3
1	B	1071	TYR	3.2
1	B	1239	TRP	3.2
1	B	388	TYR	3.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

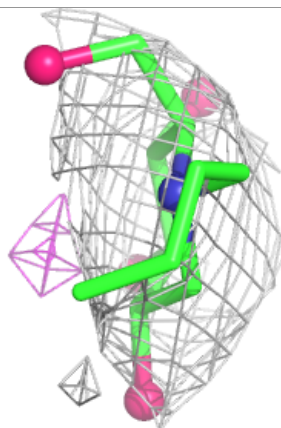
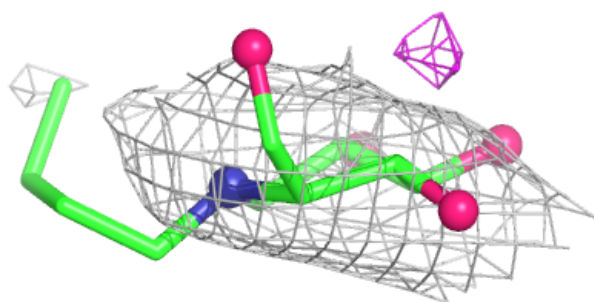
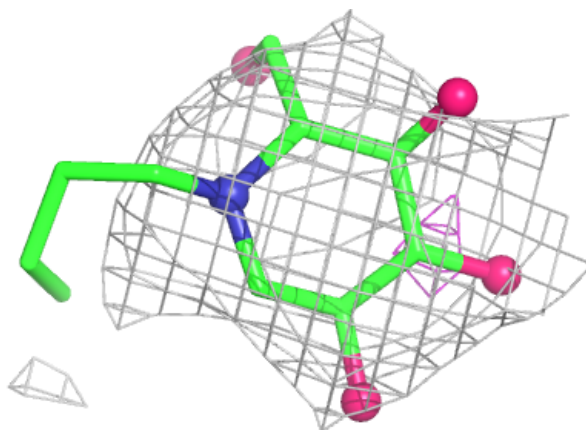
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NBV	A	1601	15/15	0.89	0.12	83,89,91,92	0
2	NBV	B	1601	15/15	0.96	0.11	75,82,86,88	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.

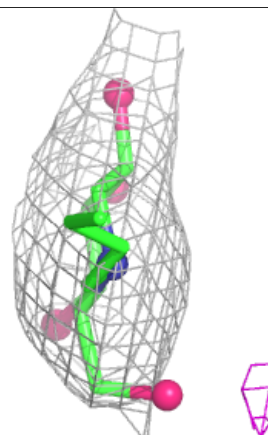
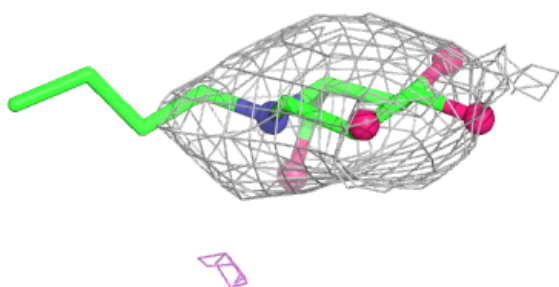
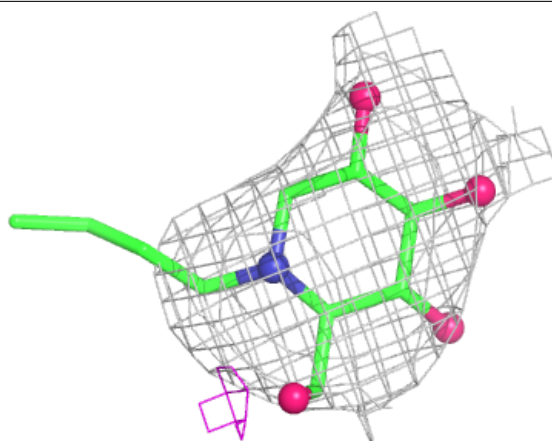
Electron density around NBV A 1601:

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 NBV B 1601:

$2mF_o-DF_c$ (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.