



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5ABH / pdb_00005abh
Title : Structure of GH84 with ligand
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Deposited on : 2015-08-05
Resolution : 1.95 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

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

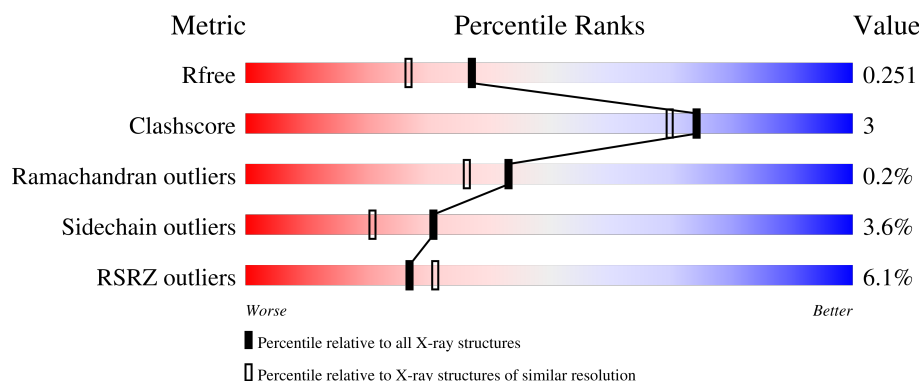
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	726	5% 83% 10% 7%
1	B	726	6% 83% 8% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11667 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 O-GLCNACASE BT_4395.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	677	Total	C	N	O	S	0	4	0
			5515	3529	932	1034	20			
1	B	669	Total	C	N	O	S	0	1	0
			5446	3487	921	1020	18			

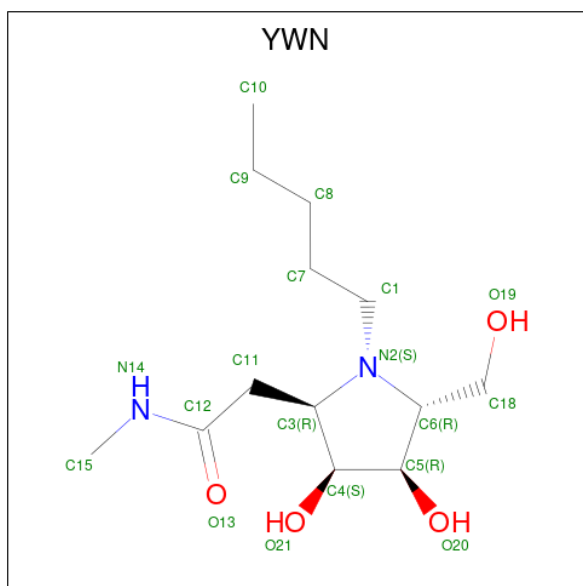
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	expression tag	UNP Q89ZI2
A	-8	GLY	-	expression tag	UNP Q89ZI2
A	-7	SER	-	expression tag	UNP Q89ZI2
A	-6	SER	-	expression tag	UNP Q89ZI2
A	-5	HIS	-	expression tag	UNP Q89ZI2
A	-4	HIS	-	expression tag	UNP Q89ZI2
A	-3	HIS	-	expression tag	UNP Q89ZI2
A	-2	HIS	-	expression tag	UNP Q89ZI2
A	-1	HIS	-	expression tag	UNP Q89ZI2
A	0	HIS	-	expression tag	UNP Q89ZI2
B	-9	MET	-	expression tag	UNP Q89ZI2
B	-8	GLY	-	expression tag	UNP Q89ZI2
B	-7	SER	-	expression tag	UNP Q89ZI2
B	-6	SER	-	expression tag	UNP Q89ZI2
B	-5	HIS	-	expression tag	UNP Q89ZI2
B	-4	HIS	-	expression tag	UNP Q89ZI2
B	-3	HIS	-	expression tag	UNP Q89ZI2
B	-2	HIS	-	expression tag	UNP Q89ZI2
B	-1	HIS	-	expression tag	UNP Q89ZI2
B	0	HIS	-	expression tag	UNP Q89ZI2

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0

- Molecule 3 is 2-[(2R,3S,4R,5R)-5-(hydroxymethyl)-3,4-bis(oxidanyl)-1-pentyl-pyrrolidin-2-yl]-N-methyl-ethanamide (CCD ID: YWN) (formula: $C_{13}H_{26}N_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 19 13 2 4	0	0
3	B	1	Total C N O 19 13 2 4	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		

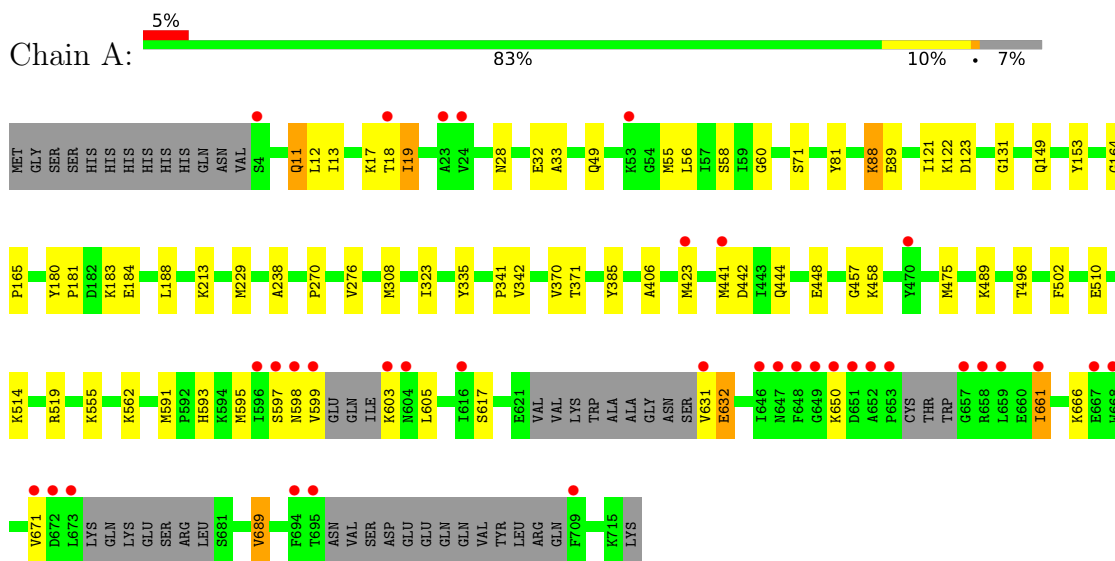
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	352	Total	O	0	0
			352	352		
6	B	306	Total	O	0	0
			306	306		

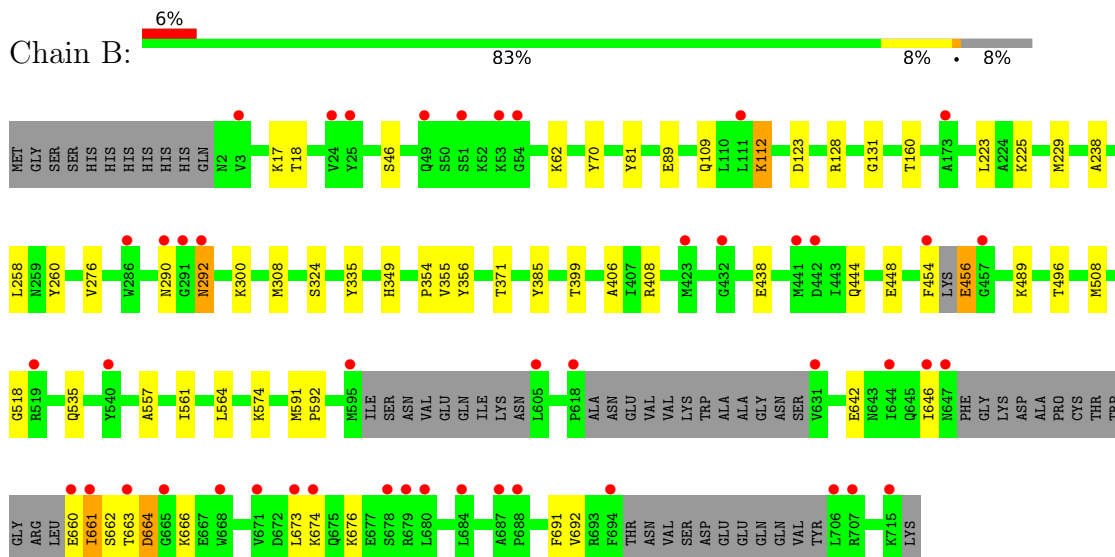
3 Residue-property plots [i](#)

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: O-GLCNACASE BT_4395



• Molecule 1: O-GLCNACASE BT_4395



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	51.41Å 161.31Å 223.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	130.74 – 1.95 130.74 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (130.74-1.95) 100.0 (130.74-1.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, R_{free}	0.212 , 0.252 0.217 , 0.251	Depositor DCC
R_{free} test set	6816 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.801	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11667	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.0175e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, EDO, YWN, CA

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	0.74	1/5649 (0.0%)	0.85	5/7650 (0.1%)
1	B	0.79	0/5579	0.87	5/7555 (0.1%)
All	All	0.77	1/11228 (0.0%)	0.86	10/15205 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	5
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	442	ASP	CB-CG	5.10	1.64	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	292	ASN	N-CA-C	6.98	122.28	107.70
1	A	689	VAL	CB-CA-C	-5.87	101.76	110.33
1	A	180	TYR	CA-C-N	-5.79	114.79	120.52
1	A	180	TYR	C-N-CA	-5.79	114.79	120.52
1	B	444	GLN	CA-C-N	-5.71	112.71	119.84
1	B	444	GLN	C-N-CA	-5.71	112.71	119.84
1	B	489	LYS	CA-C-N	-5.53	113.33	119.19
1	B	489	LYS	C-N-CA	-5.53	113.33	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	489	LYS	CA-C-N	-5.52	113.34	119.19
1	A	489	LYS	C-N-CA	-5.52	113.34	119.19

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	270	PRO	Peptide
1	B	46	SER	Peptide
1	B	646	ILE	Peptide
1	B	663	THR	Peptide
1	B	673	LEU	Peptide
1	B	674	LYS	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5515	0	5431	41	0
1	B	5446	0	5363	26	0
2	A	1	0	0	0	0
3	A	19	0	26	0	0
3	B	19	0	26	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
5	B	1	0	0	1	0
6	A	352	0	0	3	0
6	B	306	0	0	3	0
All	All	11667	0	10858	68	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (68) 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:423[A]:MET:HE1	1:A:441[A]:MET:HG3	1.65	0.78
1:A:423[A]:MET:CE	1:A:441[A]:MET:HG3	2.18	0.74
5:B:1716:CA:CA	6:B:2034:HOH:O	1.67	0.71
1:B:454:PHE:C	1:B:456:GLU:O	2.36	0.68
1:B:223:LEU:CD1	1:B:260:TYR:HE2	2.08	0.67
1:A:11:GLN:HG2	1:A:122:LYS:HB2	1.76	0.67
1:B:355:VAL:O	1:B:399:THR:HG23	1.95	0.66
1:A:423[A]:MET:HE2	1:A:441[A]:MET:H	1.62	0.64
1:A:597:SER:HB3	1:A:631:VAL:HA	1.83	0.61
1:A:598:ASN:HB3	1:A:599:VAL:HG23	1.85	0.58
1:B:70:TYR:OH	1:B:89:GLU:OE2	2.19	0.57
1:B:109:GLN:O	1:B:112:LYS:HE2	2.05	0.56
1:B:223:LEU:HD11	1:B:260:TYR:CE2	2.44	0.54
1:A:457:GLY:HA2	6:A:2250:HOH:O	2.07	0.53
1:A:444[B]:GLN:NE2	1:A:448:GLU:OE1	2.41	0.53
1:A:597:SER:CB	1:A:631:VAL:HA	2.39	0.53
1:B:661:ILE:HG23	1:B:662:SER:N	2.24	0.52
1:B:661:ILE:HD12	1:B:692:VAL:HG13	1.91	0.52
1:B:81:TYR:CE2	1:B:123:ASP:HB3	2.45	0.51
1:B:662:SER:HB3	1:B:691:PHE:HB2	1.93	0.51
1:A:181:PRO:HG2	1:A:184:GLU:OE1	2.11	0.50
1:A:661:ILE:HD12	1:A:671:VAL:HG21	1.93	0.50
1:B:128:ARG:HD2	6:B:2050:HOH:O	2.12	0.50
1:A:555:LYS:NZ	6:A:2194:HOH:O	2.47	0.48
1:A:18:THR:O	1:A:19:ILE:HD12	2.14	0.48
1:A:385:TYR:CD1	1:A:406:ALA:HB2	2.50	0.47
1:A:597:SER:OG	1:A:632:GLU:N	2.47	0.47
1:A:238:ALA:HA	1:A:276:VAL:O	2.13	0.47
1:A:188:LEU:HD13	1:A:229:MET:HE1	1.95	0.47
1:B:223:LEU:CD1	1:B:260:TYR:CE2	2.91	0.47
1:A:131:GLY:O	1:A:370:VAL:HA	2.15	0.46
1:B:308:MET:HA	1:B:335:TYR:O	2.15	0.46
1:A:28:ASN:HB2	1:A:56:LEU:HD11	1.98	0.46
1:B:81:TYR:CZ	1:B:123:ASP:HB3	2.50	0.46
1:A:308:MET:HA	1:A:335:TYR:O	2.16	0.46
1:B:131:GLY:HA3	1:B:160:THR:O	2.17	0.45
1:A:595:MET:SD	1:A:595:MET:O	2.75	0.45
1:A:605:LEU:HD13	1:A:617:SER:O	2.17	0.45
1:B:354:PRO:HB2	1:B:399:THR:HG22	1.98	0.45
1:A:11:GLN:O	1:A:11:GLN:HG3	2.16	0.44
1:B:661:ILE:CD1	1:B:692:VAL:HG13	2.48	0.44
1:B:238:ALA:HA	1:B:276:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:ALA:HB1	1:B:561:ILE:HB	1.99	0.44
1:A:12:LEU:HD13	1:A:121:ILE:HG12	1.99	0.44
1:A:562[A]:LYS:HD3	6:A:2281:HOH:O	2.16	0.44
1:A:81:TYR:CZ	1:A:123:ASP:HB3	2.54	0.43
1:A:164:GLY:N	1:A:165:PRO:CD	2.81	0.43
1:A:441[A]:MET:HE2	1:A:441[A]:MET:HB3	1.89	0.43
1:A:475:MET:HE3	1:A:502:PHE:CE1	2.54	0.43
1:A:88:LYS:HD2	1:A:89:GLU:HB3	2.01	0.43
1:B:356:TYR:HB3	1:B:399:THR:HG21	2.00	0.43
1:B:385:TYR:CD1	1:B:406:ALA:HB2	2.54	0.43
1:B:508:MET:HE2	1:B:535:GLN:HG3	2.01	0.43
1:A:423[A]:MET:O	1:A:423[A]:MET:HG3	2.19	0.42
1:B:225:LYS:O	1:B:229:MET:HG2	2.19	0.42
1:B:349:HIS:HE1	6:B:2078:HOH:O	2.02	0.42
1:A:12:LEU:HD13	1:A:121:ILE:CG1	2.49	0.42
1:A:33:ALA:HB2	1:A:60:GLY:HA2	2.02	0.42
1:A:510:GLU:O	1:A:514:LYS:HG3	2.19	0.42
1:A:591:MET:HG3	1:A:593:HIS:O	2.20	0.41
1:B:223:LEU:HD12	1:B:260:TYR:HE2	1.85	0.41
1:A:599:VAL:C	1:A:603:LYS:HB2	2.44	0.41
1:A:28:ASN:HB3	1:A:58:SER:HA	2.01	0.41
1:A:81:TYR:CE2	1:A:123:ASP:HB3	2.56	0.41
1:A:341:PRO:O	1:A:342:VAL:C	2.64	0.41
1:A:149:GLN:HB3	1:A:153:TYR:CZ	2.56	0.41
1:A:12:LEU:HD12	1:A:13:ILE:N	2.37	0.40
1:B:591:MET:SD	1:B:592:PRO:HD2	2.61	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	669/726 (92%)	640 (96%)	29 (4%)	0	100	100
1	B	658/726 (91%)	628 (95%)	28 (4%)	2 (0%)	36	28
All	All	1327/1452 (91%)	1268 (96%)	57 (4%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	518	GLY
1	B	664	ASP

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	598/639 (94%)	578 (97%)	20 (3%)	33	24
1	B	591/639 (92%)	568 (96%)	23 (4%)	28	18
All	All	1189/1278 (93%)	1146 (96%)	43 (4%)	31	21

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	17	LYS
1	A	19	ILE
1	A	32	GLU
1	A	49	GLN
1	A	55	MET
1	A	71	SER
1	A	88	LYS
1	A	183	LYS
1	A	213	LYS
1	A	323	ILE
1	A	371	THR
1	A	458	LYS
1	A	496	THR

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Mol	Chain	Res	Type
1	A	519	ARG
1	A	632	GLU
1	A	650	LYS
1	A	661	ILE
1	A	666	LYS
1	A	689	VAL
1	B	17	LYS
1	B	18	THR
1	B	62	LYS
1	B	112	LYS
1	B	258	LEU
1	B	290	ASN
1	B	292	ASN
1	B	300	LYS
1	B	324	SER
1	B	371	THR
1	B	408	ARG
1	B	438	GLU
1	B	448	GLU
1	B	456	GLU
1	B	496	THR
1	B	564	LEU
1	B	574	LYS
1	B	642	GLU
1	B	660	GLU
1	B	661	ILE
1	B	664	ASP
1	B	666	LYS
1	B	676	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	ASN
1	A	198	ASN
1	A	469	GLN
1	A	608	GLN
1	A	685	GLN
1	B	28	ASN
1	B	144	GLN
1	B	156	ASN
1	B	283	ASN

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Mol	Chain	Res	Type
1	B	290	ASN
1	B	349	HIS
1	B	433	HIS
1	B	459	ASN
1	B	583	HIS
1	B	608	GLN
1	B	685	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 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	YWN	B	1717	-	19,19,19	0.73	0	22,25,25	0.98	2 (9%)
3	YWN	A	1717	-	19,19,19	0.80	1 (5%)	22,25,25	0.95	2 (9%)
4	EDO	A	1718	-	3,3,3	0.56	0	2,2,2	0.45	0
4	EDO	B	1718	-	3,3,3	0.50	0	2,2,2	0.50	0

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	YWN	B	1717	-	-	1/13/33/33	0/1/1/1
3	YWN	A	1717	-	-	4/13/33/33	0/1/1/1
4	EDO	A	1718	-	-	0/1/1/1	-
4	EDO	B	1718	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1717	YWN	C4-C3	-2.24	1.50	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1717	YWN	C7-C1-N2	2.78	119.70	113.10
3	A	1717	YWN	C1-N2-C6	2.43	119.05	114.05
3	B	1717	YWN	C4-C3-N2	2.15	107.86	104.58
3	B	1717	YWN	C1-N2-C6	-2.14	109.66	114.05

There are no chirality outliers.

All (6) torsion outliers are listed below:

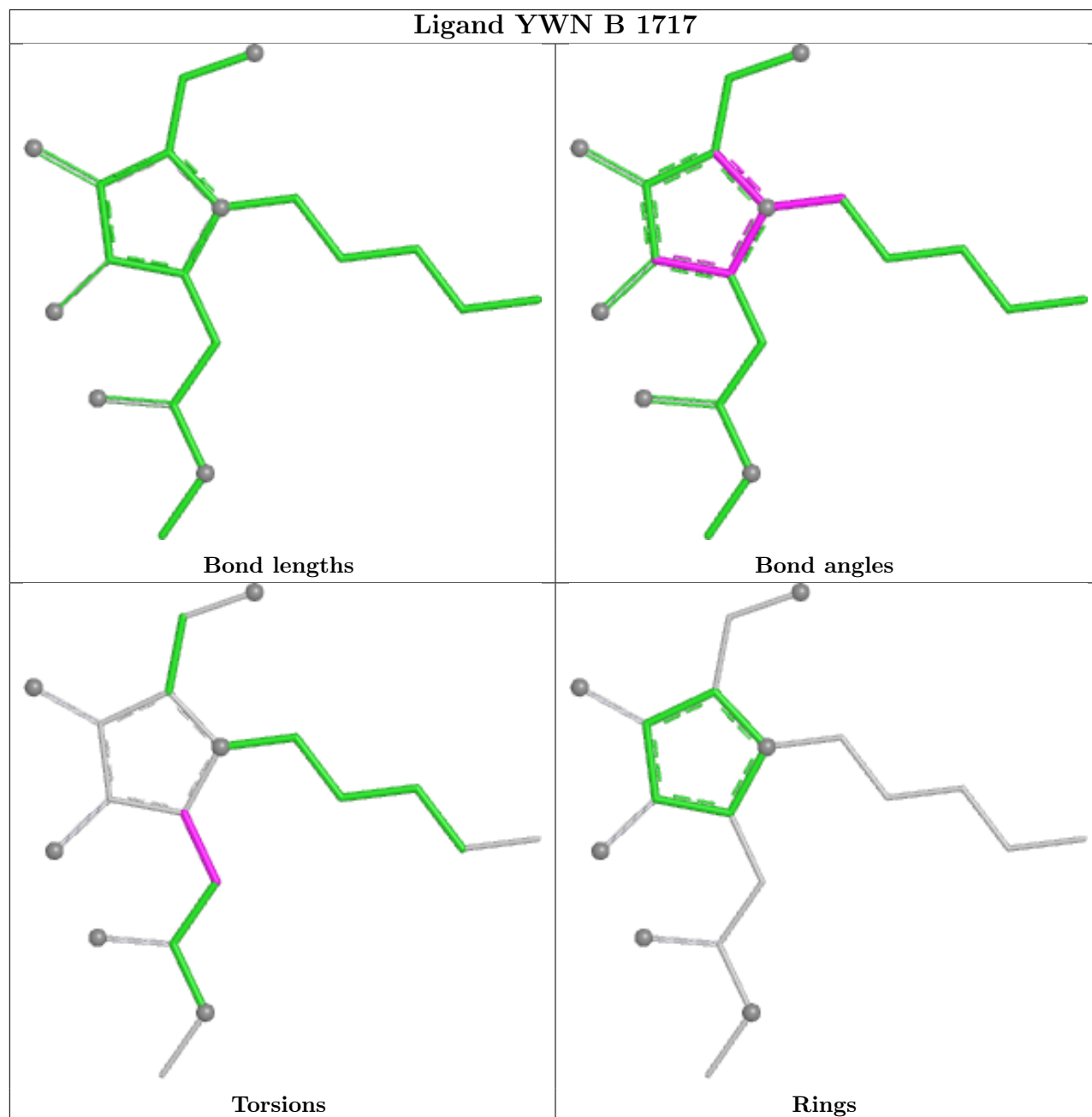
Mol	Chain	Res	Type	Atoms
3	A	1717	YWN	C7-C1-N2-C3
3	A	1717	YWN	C7-C1-N2-C6
3	A	1717	YWN	C12-C11-C3-N2
3	B	1717	YWN	C12-C11-C3-N2
3	A	1717	YWN	C1-C7-C8-C9
4	B	1718	EDO	O1-C1-C2-O2

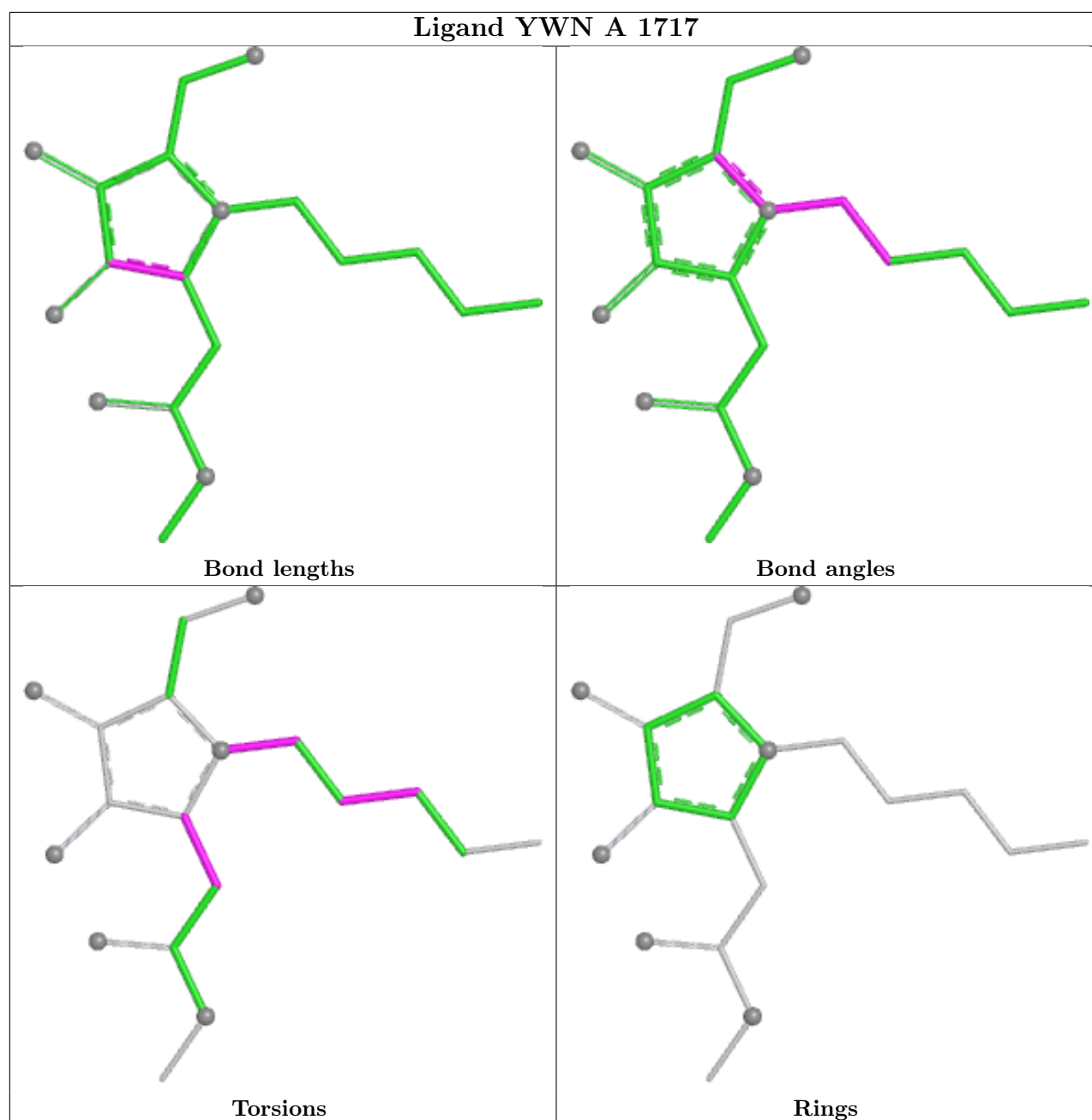
There are no ring outliers.

No monomer is involved in short contacts.

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, 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	677/726 (93%)	0.30	36 (5%) 32 37	16, 38, 78, 102	4 (0%)
1	B	669/726 (92%)	0.28	46 (6%) 23 26	20, 35, 76, 97	1 (0%)
All	All	1346/1452 (92%)	0.29	82 (6%) 27 31	16, 37, 77, 102	5 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	653	PRO	6.7
1	B	673	LEU	6.1
1	A	599	VAL	6.0
1	B	694	PHE	5.5
1	A	652	ALA	5.4
1	A	648	PHE	5.3
1	A	695	THR	4.8
1	B	668	TRP	4.6
1	A	657	GLY	4.6
1	B	286	TRP	4.6
1	B	290	ASN	4.5
1	A	631	VAL	4.4
1	B	540[A]	TYR	4.3
1	B	661	ILE	4.1
1	A	709	PHE	4.0
1	B	663	THR	3.7
1	B	687	ALA	3.6
1	A	649	GLY	3.6
1	A	598	ASN	3.5
1	B	605	LEU	3.4
1	B	647	ASN	3.4
1	B	291	GLY	3.3
1	A	694	PHE	3.3
1	B	441	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	646	ILE	3.2
1	A	668	TRP	3.2
1	B	595	MET	3.0
1	A	423[A]	MET	3.0
1	B	457	GLY	3.0
1	A	658	ARG	3.0
1	B	3	VAL	2.9
1	B	706	LEU	2.9
1	B	54	GLY	2.9
1	A	673	LEU	2.9
1	B	680	LEU	2.8
1	A	441[A]	MET	2.7
1	B	292	ASN	2.7
1	B	631	VAL	2.7
1	A	23	ALA	2.6
1	A	667	GLU	2.6
1	A	650	LYS	2.6
1	B	618	PRO	2.6
1	A	647	ASN	2.6
1	A	616	ILE	2.6
1	A	661	ILE	2.6
1	A	651	ASP	2.6
1	B	454	PHE	2.6
1	B	660	GLU	2.6
1	B	665	GLY	2.6
1	A	597	SER	2.6
1	A	4	SER	2.5
1	B	53	LYS	2.5
1	A	671	VAL	2.5
1	A	672	ASP	2.5
1	A	596	ILE	2.4
1	A	659	LEU	2.4
1	A	18	THR	2.4
1	A	24	VAL	2.4
1	B	25	TYR	2.4
1	B	707	ARG	2.4
1	B	24	VAL	2.4
1	A	470	TYR	2.3
1	A	603	LYS	2.3
1	A	53	LYS	2.3
1	B	674	LYS	2.3
1	B	679	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	671	VAL	2.3
1	B	51	SER	2.2
1	B	678	SER	2.2
1	B	688	PRO	2.2
1	B	715	LYS	2.2
1	B	646	ILE	2.2
1	B	519	ARG	2.2
1	B	111	LEU	2.2
1	B	684	LEU	2.2
1	B	644	ILE	2.1
1	B	49	GLN	2.1
1	B	432	GLY	2.1
1	B	423	MET	2.1
1	A	604	ASN	2.0
1	B	173	ALA	2.0
1	B	442	ASP	2.0

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](#)

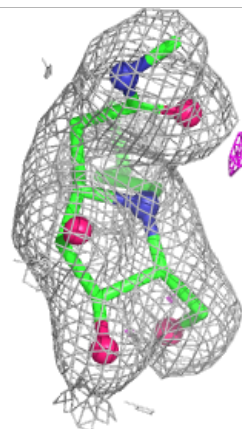
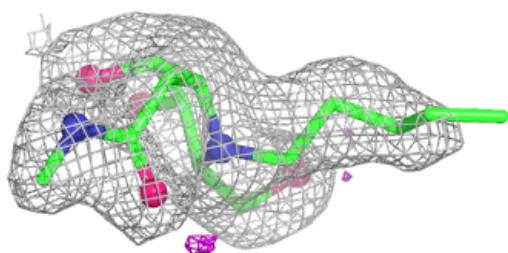
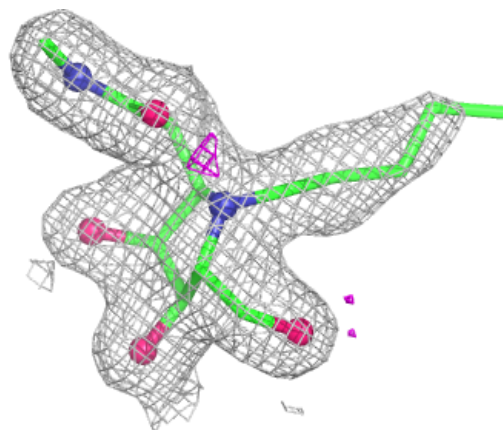
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

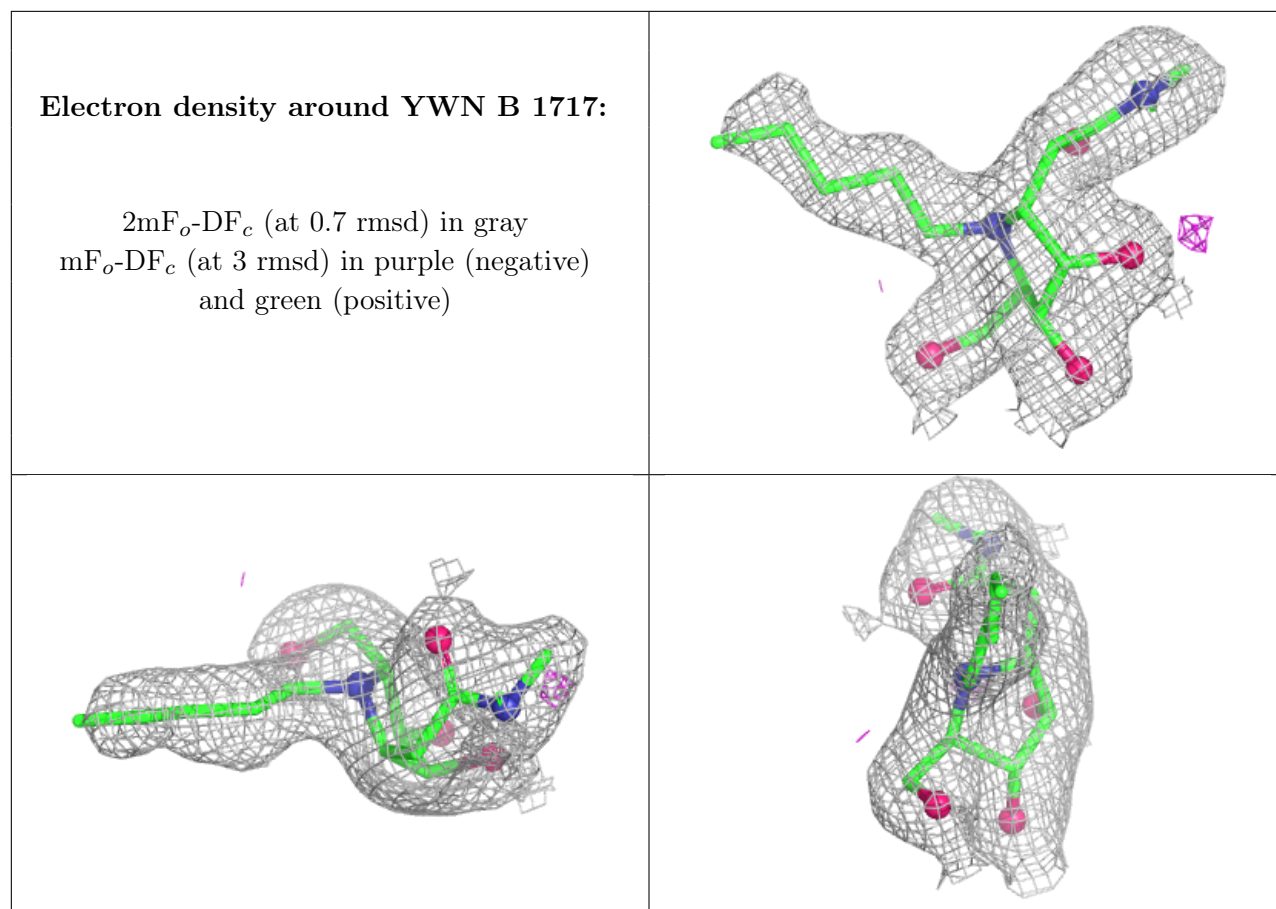
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	YWN	A	1717	19/19	0.94	0.11	26,36,51,59	0
4	EDO	A	1718	4/4	0.94	0.10	33,34,36,39	0
3	YWN	B	1717	19/19	0.95	0.10	29,36,50,54	0
2	CL	A	1716	1/1	0.95	0.12	69,69,69,69	0
4	EDO	B	1718	4/4	0.95	0.09	35,40,41,42	0
5	CA	B	1716	1/1	0.99	0.03	36,36,36,36	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 YWN A 1717:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.