



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:51 PM UTC

PDB ID : 4LY1 / pdb_00004ly1
Title : Structure of Human HDAC2 in complex with inhibitor 4-(acetylamino)-N-[2-amino-5-(thiophen-2-yl)phenyl]benzamide
Authors : Fong, R.; Lupardus, P.J.
Deposited on : 2013-07-30
Resolution : 1.57 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

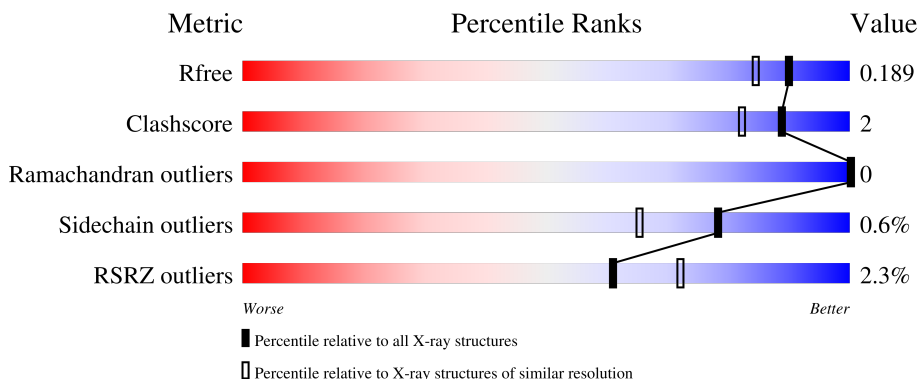
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

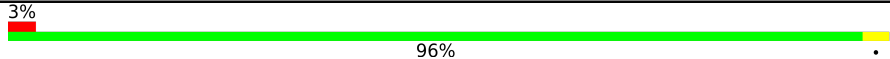
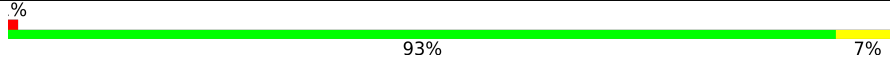
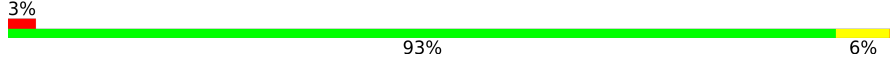
The reported resolution of this entry is 1.57 Å.

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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	369	 3% 96% .
1	B	369	 % 93% 7% .
1	C	369	 3% 93% 6% ..

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10080 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 Histone deacetylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	13	0
			2996	1916	506	549	25			
1	B	367	Total	C	N	O	S	0	9	0
			2982	1908	500	548	26			
1	C	366	Total	C	N	O	S	0	9	0
			2980	1904	504	546	26			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

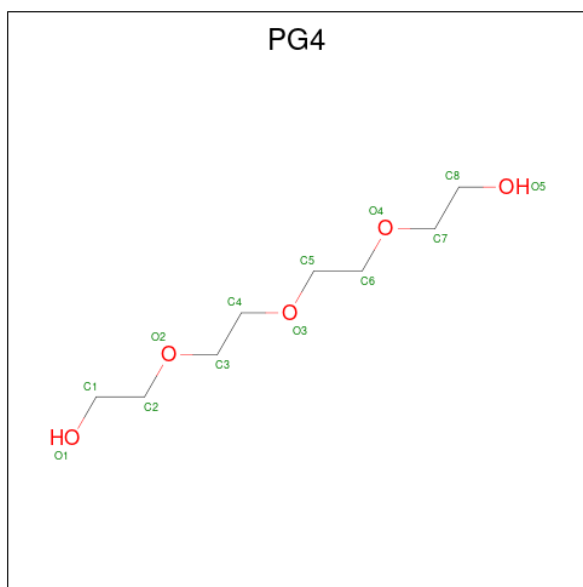
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

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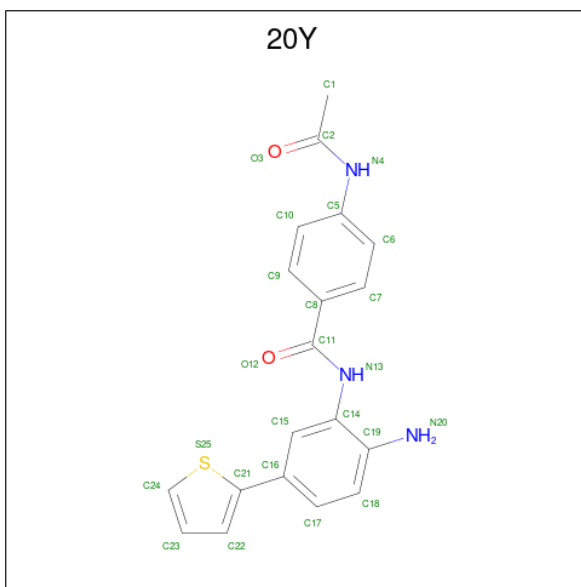
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



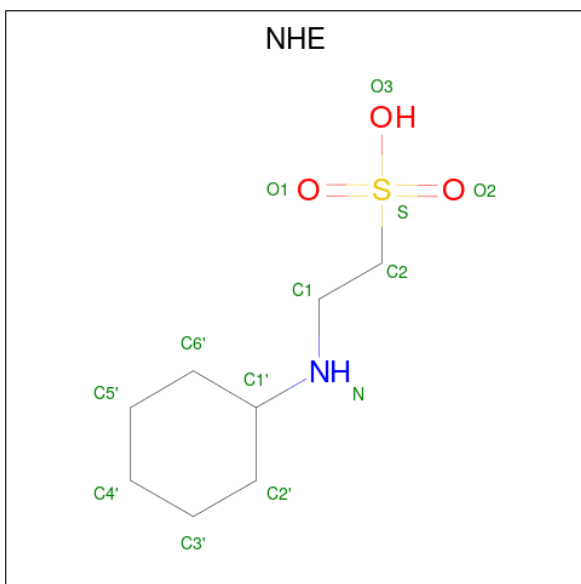
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		
5	A	1	Total	C	O	0	0
			13	8	5		
5	A	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			13	8	5		
5	B	1	Total	C	O	0	0
			13	8	5		
5	C	1	Total	C	O	0	0
			13	8	5		
5	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is 4-(acetylamino)-N-[2-amino-5-(thiophen-2-yl)phenyl]benzamide (CCD ID: 20Y) (formula: $C_{19}H_{17}N_3O_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	1
			50	38	6	4	2		
6	B	1	Total	C	N	O	S	0	1
			50	38	6	4	2		
6	C	1	Total	C	N	O	S	0	1
			50	38	6	4	2		

- Molecule 7 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (CCD ID: NHE) (formula: C₈H₁₇NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	299	Total	O	0	0
			299	299		
8	B	322	Total	O	0	0
			322	322		
8	C	225	Total	O	0	0
			225	225		

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.

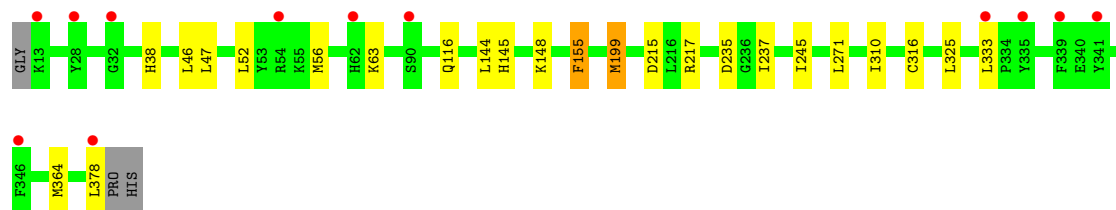
- Molecule 1: Histone deacetylase 2



- Molecule 1: Histone deacetylase 2



- Molecule 1: Histone deacetylase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.03Å 97.49Å 138.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.57 – 1.57 33.57 – 1.57	Depositor EDS
% Data completeness (in resolution range)	99.9 (33.57-1.57) 99.7 (33.57-1.57)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 1.57Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.169 , 0.187 0.169 , 0.189	Depositor DCC
R_{free} test set	8703 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	15.9	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10080	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NHE, PG4, NA, CA, 20Y

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	0.81	2/3096 (0.1%)	1.04	5/4179 (0.1%)
1	B	0.83	2/3087 (0.1%)	1.03	3/4169 (0.1%)
1	C	0.81	3/3079 (0.1%)	1.05	6/4156 (0.1%)
All	All	0.82	7/9262 (0.1%)	1.04	14/12504 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	199	MET	SD-CE	-8.04	1.59	1.79
1	A	103	GLU	CA-C	6.58	1.56	1.52
1	B	103	GLU	CA-C	6.20	1.55	1.52
1	A	136	MET	SD-CE	-6.08	1.64	1.79
1	B	89	MET	SD-CE	-5.45	1.66	1.79
1	C	38[A]	HIS	ND1-CE1	5.22	1.37	1.32
1	C	38[B]	HIS	ND1-CE1	5.22	1.37	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	38[A]	HIS	CB-CG-CD2	-7.50	121.45	131.20
1	C	38[B]	HIS	CB-CG-CD2	-7.50	121.45	131.20
1	B	310	ILE	N-CA-C	7.05	117.82	110.62
1	C	310	ILE	N-CA-C	6.94	117.70	110.62
1	A	104	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	71	LYS	N-CA-C	-5.80	105.46	112.54
1	A	179	ASP	CA-CB-CG	5.75	118.35	112.60
1	C	155	PHE	CA-CB-CG	5.75	119.55	113.80
1	A	245	ILE	N-CA-C	5.55	118.97	113.53
1	C	145	HIS	N-CA-C	5.42	119.52	113.01
1	B	145	HIS	N-CA-C	5.24	119.30	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	GLU	CB-CG-CD	5.22	121.48	112.60
1	C	235	ASP	CA-CB-CG	5.11	117.70	112.60
1	A	340	GLU	CB-CG-CD	5.05	121.19	112.60

There are no chirality outliers.

There are no planarity outliers.

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	2996	0	2906	3	0
1	B	2982	0	2881	18	0
1	C	2980	0	2877	10	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	39	0	54	1	0
5	B	39	0	54	2	0
5	C	26	0	36	0	0
6	A	50	0	34	1	0
6	B	50	0	34	0	0
6	C	50	0	34	0	0
7	B	13	0	17	4	0
8	A	299	0	0	1	0
8	B	322	0	0	4	0
8	C	225	0	0	1	0
All	All	10080	0	8927	34	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 2.

All (34) 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:B:63:LYS:HZ1	7:B:404:NHE:H2'1	1.45	0.81
1:B:205:LYS:HD2	1:B:278[B]:CYS:SG	2.23	0.78
1:B:341:TYR:HA	5:B:405:PG4:H51	1.66	0.77
1:B:17[A]:CYS:SG	8:B:799:HOH:O	2.46	0.65
1:B:56:MET:HB3	1:B:325:LEU:HD21	1.81	0.63
1:C:56:MET:HB3	1:C:325:LEU:HD21	1.84	0.60
1:A:56:MET:HB3	1:A:325:LEU:HD21	1.87	0.57
1:B:205:LYS:CD	1:B:278[B]:CYS:SG	2.92	0.55
1:B:245:ILE:HG12	1:B:364:MET:CE	2.40	0.52
1:B:245:ILE:HG22	1:B:368:LYS:HE2	1.94	0.48
1:C:46:LEU:HD11	1:C:333:LEU:HD22	1.96	0.48
1:C:148:LYS:HE3	8:C:702:HOH:O	2.14	0.48
1:B:23:ASP:OD1	7:B:404:NHE:HC22	2.13	0.47
1:C:47:LEU:HB2	1:C:52:LEU:HD12	1.94	0.47
1:B:15:LYS:HG2	8:B:799:HOH:O	2.15	0.47
1:B:148:LYS:HE3	8:B:644:HOH:O	2.14	0.47
1:C:271:LEU:HD11	1:C:316:CYS:HB2	1.96	0.47
1:C:215:ASP:OD1	1:C:217[A]:ARG:HG2	2.15	0.47
1:B:63:LYS:HZ1	7:B:404:NHE:C2'	2.23	0.46
1:B:17[B]:CYS:HB2	1:B:59:TYR:HE2	1.81	0.46
1:A:245:ILE:HG12	1:A:364:MET:HE3	2.00	0.44
1:A:243:GLY:O	8:A:795:HOH:O	2.21	0.43
1:B:66:ALA:HB2	1:B:82:ARG:HH11	1.83	0.43
5:A:404:PG4:H32	5:A:404:PG4:H51	1.79	0.43
7:B:404:NHE:H4'1	5:B:407:PG4:H71	2.00	0.43
1:C:245:ILE:HG21	1:C:364[B]:MET:HE3	2.00	0.43
1:B:94:LYS:HA	1:B:94:LYS:HD2	1.91	0.42
1:B:40[B]:ILE:HD11	8:B:546:HOH:O	2.20	0.42
1:C:144:LEU:HD12	1:C:144:LEU:N	2.34	0.42
1:C:199:MET:HE1	1:C:378:LEU:HD21	2.02	0.41
1:B:245:ILE:HG22	1:B:368:LYS:CE	2.51	0.41
6:A:407[B]:20Y:H4	6:A:407[B]:20Y:O3	2.20	0.41
1:C:63:LYS:HB3	1:C:116:GLN:HB3	2.03	0.40
1:B:17[B]:CYS:HB2	1:B:59:TYR:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	373/369 (101%)	367 (98%)	6 (2%)	0	100	100
1	B	372/369 (101%)	366 (98%)	6 (2%)	0	100	100
1	C	370/369 (100%)	365 (99%)	5 (1%)	0	100	100
All	All	1115/1107 (101%)	1098 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	324/318 (102%)	323 (100%)	1 (0%)	86	79
1	B	323/318 (102%)	320 (99%)	3 (1%)	70	52
1	C	321/318 (101%)	319 (99%)	2 (1%)	78	65
All	All	968/954 (102%)	962 (99%)	6 (1%)	78	65

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	GLU
1	B	15	LYS
1	B	155	PHE
1	B	288	LYS
1	C	155	PHE

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Mol	Chain	Res	Type
1	C	237	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	369	GLN
1	B	95	GLN
1	C	172	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 9 are monoatomic - leaving 15 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	$\# Z > 2$
5	PG4	B	405	-	12,12,12	0.48	0	11,11,11	0.42	0
6	20Y	A	407[A]	2	27,27,27	0.78	0	37,37,37	1.01	1 (2%)
5	PG4	C	404	-	12,12,12	0.48	0	11,11,11	0.35	0
5	PG4	C	405	-	12,12,12	0.46	0	11,11,11	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	20Y	A	407[B]	2	27,27,27	0.75	0	37,37,37	0.94	2 (5%)
6	20Y	B	408[B]	2	27,27,27	0.76	0	37,37,37	0.96	1 (2%)
6	20Y	C	406[A]	2	27,27,27	0.83	0	37,37,37	0.95	2 (5%)
7	NHE	B	404	-	13,13,13	0.90	1 (7%)	16,17,17	2.19	5 (31%)
5	PG4	A	405	-	12,12,12	0.48	0	11,11,11	0.37	0
5	PG4	B	406	-	12,12,12	0.47	0	11,11,11	0.30	0
6	20Y	B	408[A]	2	27,27,27	0.73	0	37,37,37	0.96	2 (5%)
6	20Y	C	406[B]	2	27,27,27	0.86	0	37,37,37	1.38	6 (16%)
5	PG4	B	407	-	12,12,12	0.43	0	11,11,11	0.39	0
5	PG4	A	404	-	12,12,12	0.54	0	11,11,11	0.51	0
5	PG4	A	406	-	12,12,12	0.51	0	11,11,11	0.38	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
5	PG4	B	405	-	-	5/10/10/10	-
6	20Y	A	407[A]	2	-	0/16/16/16	0/3/3/3
5	PG4	C	404	-	-	2/10/10/10	-
5	PG4	C	405	-	-	2/10/10/10	-
6	20Y	A	407[B]	2	-	1/16/16/16	0/3/3/3
6	20Y	B	408[B]	2	-	2/16/16/16	0/3/3/3
6	20Y	C	406[A]	2	-	0/16/16/16	0/3/3/3
7	NHE	B	404	-	-	1/7/15/15	0/1/1/1
5	PG4	A	405	-	-	2/10/10/10	-
5	PG4	B	406	-	-	1/10/10/10	-
6	20Y	B	408[A]	2	-	0/16/16/16	0/3/3/3
6	20Y	C	406[B]	2	-	2/16/16/16	0/3/3/3
5	PG4	B	407	-	-	1/10/10/10	-
5	PG4	A	404	-	-	7/10/10/10	-
5	PG4	A	406	-	-	3/10/10/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	404	NHE	C1'-N	-2.20	1.42	1.48

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	404	NHE	O2-S-C2	4.96	114.22	106.73
7	B	404	NHE	C1-N-C1'	3.92	121.73	114.18
7	B	404	NHE	O2-S-O1	-3.64	101.99	113.82
6	C	406[B]	20Y	C15-C16-C21	-2.68	117.19	120.97
6	C	406[B]	20Y	C18-C17-C16	-2.51	118.12	120.80
6	C	406[B]	20Y	C19-C14-N13	2.47	123.75	119.30
7	B	404	NHE	C5'-C6'-C1'	2.34	115.30	111.09
6	C	406[B]	20Y	C1-C2-N4	2.25	118.33	114.95
6	A	407[A]	20Y	C1-C2-N4	2.23	118.30	114.95
6	A	407[B]	20Y	C1-C2-N4	2.22	118.30	114.95
7	B	404	NHE	C6'-C1'-C2'	2.22	114.63	110.80
6	C	406[A]	20Y	C1-C2-N4	2.17	118.21	114.95
6	C	406[B]	20Y	O12-C11-N13	-2.16	118.25	123.75
6	A	407[B]	20Y	O3-C2-C1	-2.16	118.21	122.05
6	B	408[A]	20Y	C23-C24-S25	-2.07	107.95	113.02
6	B	408[B]	20Y	C1-C2-N4	2.03	118.01	114.95
6	C	406[A]	20Y	C18-C19-C14	2.02	120.30	118.24
6	B	408[A]	20Y	C15-C16-C21	-2.02	118.12	120.97
6	C	406[B]	20Y	C18-C19-C14	2.00	120.28	118.24

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	405	PG4	O3-C5-C6-O4
5	A	406	PG4	O4-C7-C8-O5
5	A	404	PG4	C3-C4-O3-C5
5	A	404	PG4	O2-C3-C4-O3
5	C	405	PG4	O3-C5-C6-O4
5	B	405	PG4	O4-C7-C8-O5
5	A	406	PG4	O3-C5-C6-O4
5	A	404	PG4	O1-C1-C2-O2
7	B	404	NHE	C1-C2-S-O2
5	B	406	PG4	C1-C2-O2-C3
5	C	404	PG4	C1-C2-O2-C3
5	A	404	PG4	C1-C2-O2-C3
5	A	405	PG4	C6-C5-O3-C4
5	A	404	PG4	C8-C7-O4-C6
5	C	405	PG4	C1-C2-O2-C3
5	A	404	PG4	C5-C6-O4-C7
5	B	405	PG4	C5-C6-O4-C7

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Mol	Chain	Res	Type	Atoms
6	C	406[B]	20Y	C15-C16-C21-C22
5	C	404	PG4	O1-C1-C2-O2
5	B	405	PG4	C3-C4-O3-C5
5	B	407	PG4	C5-C6-O4-C7
5	B	405	PG4	C4-C3-O2-C2
5	A	405	PG4	O3-C5-C6-O4
6	B	408[B]	20Y	C6-C5-N4-C2
6	A	407[B]	20Y	C15-C16-C21-S25
6	B	408[B]	20Y	C10-C5-N4-C2
5	A	406	PG4	C6-C5-O3-C4
6	C	406[B]	20Y	C17-C16-C21-C22
5	A	404	PG4	O3-C5-C6-O4

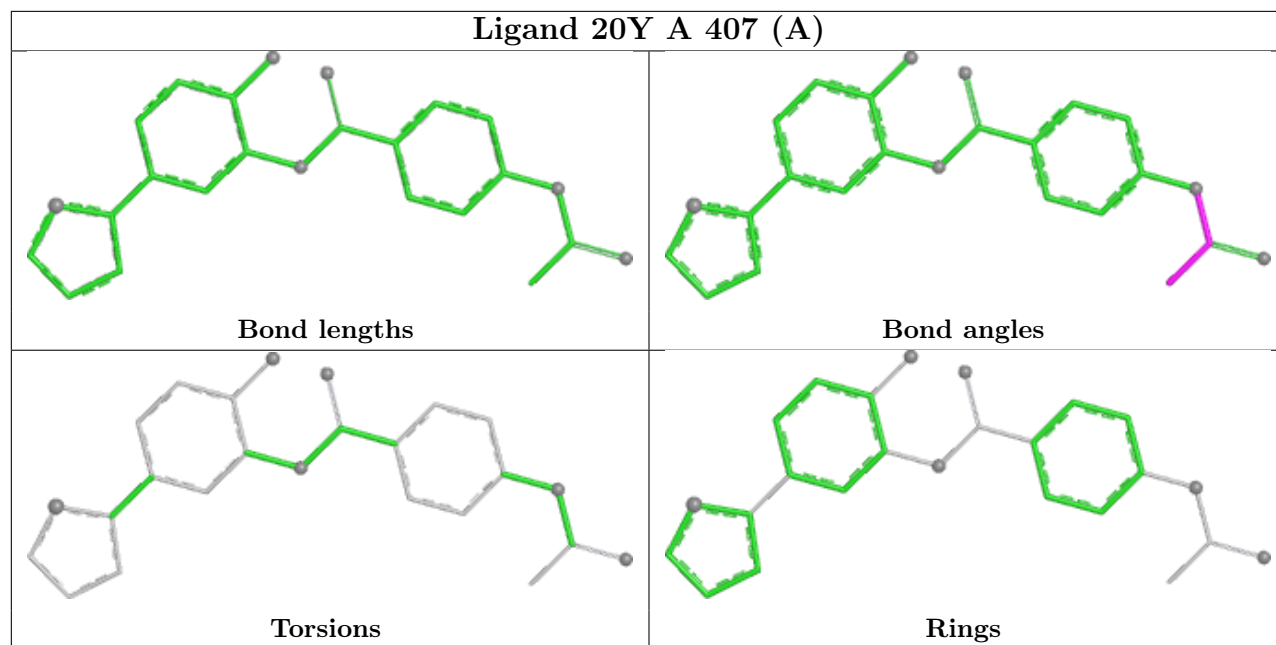
There are no ring outliers.

5 monomers are involved in 7 short contacts:

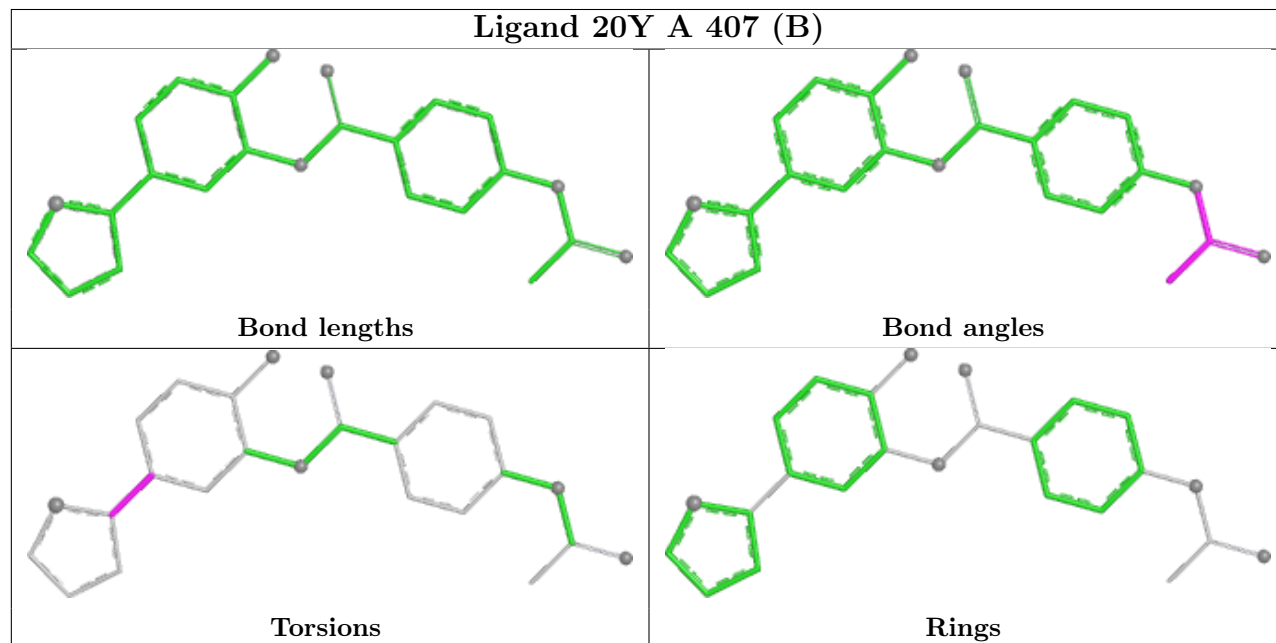
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	405	PG4	1	0
6	A	407[B]	20Y	1	0
7	B	404	NHE	4	0
5	B	407	PG4	1	0
5	A	404	PG4	1	0

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.

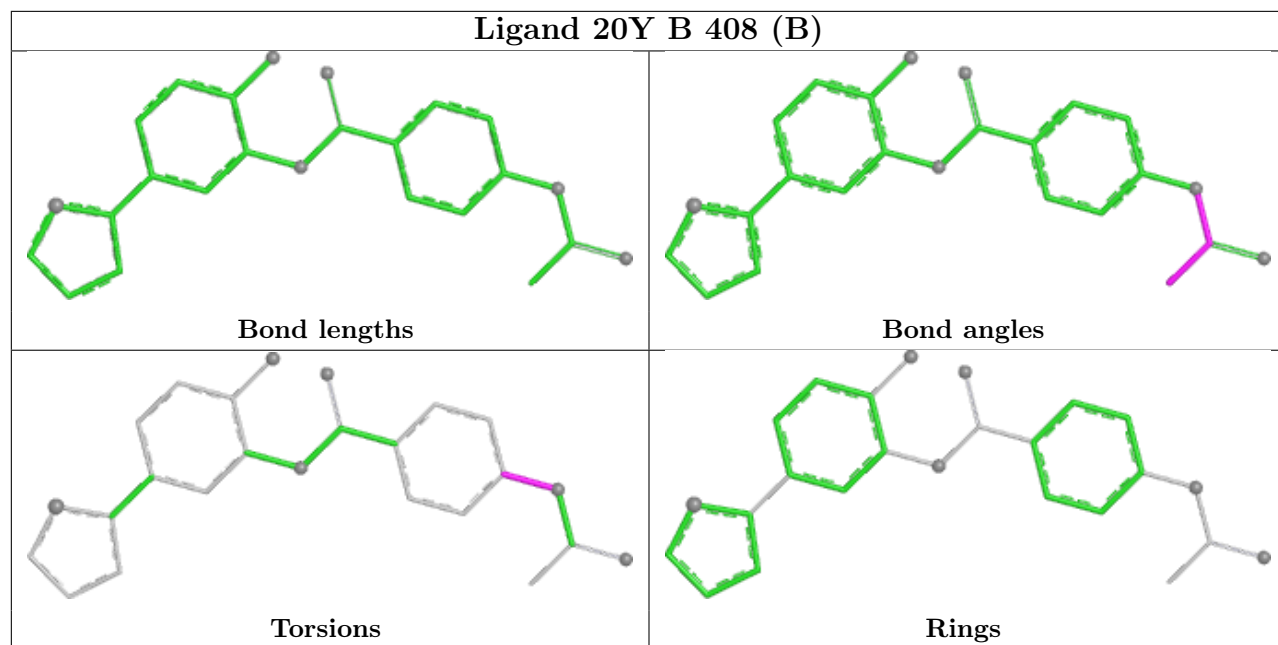
Ligand 20Y A 407 (A)



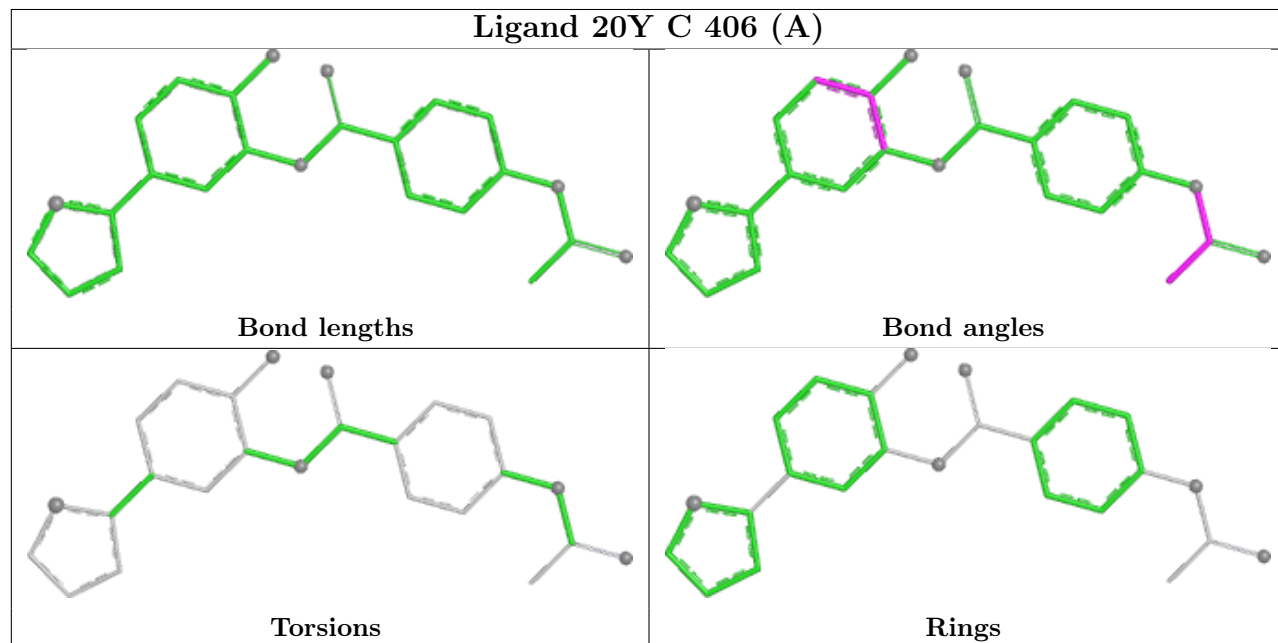
Ligand 20Y A 407 (B)

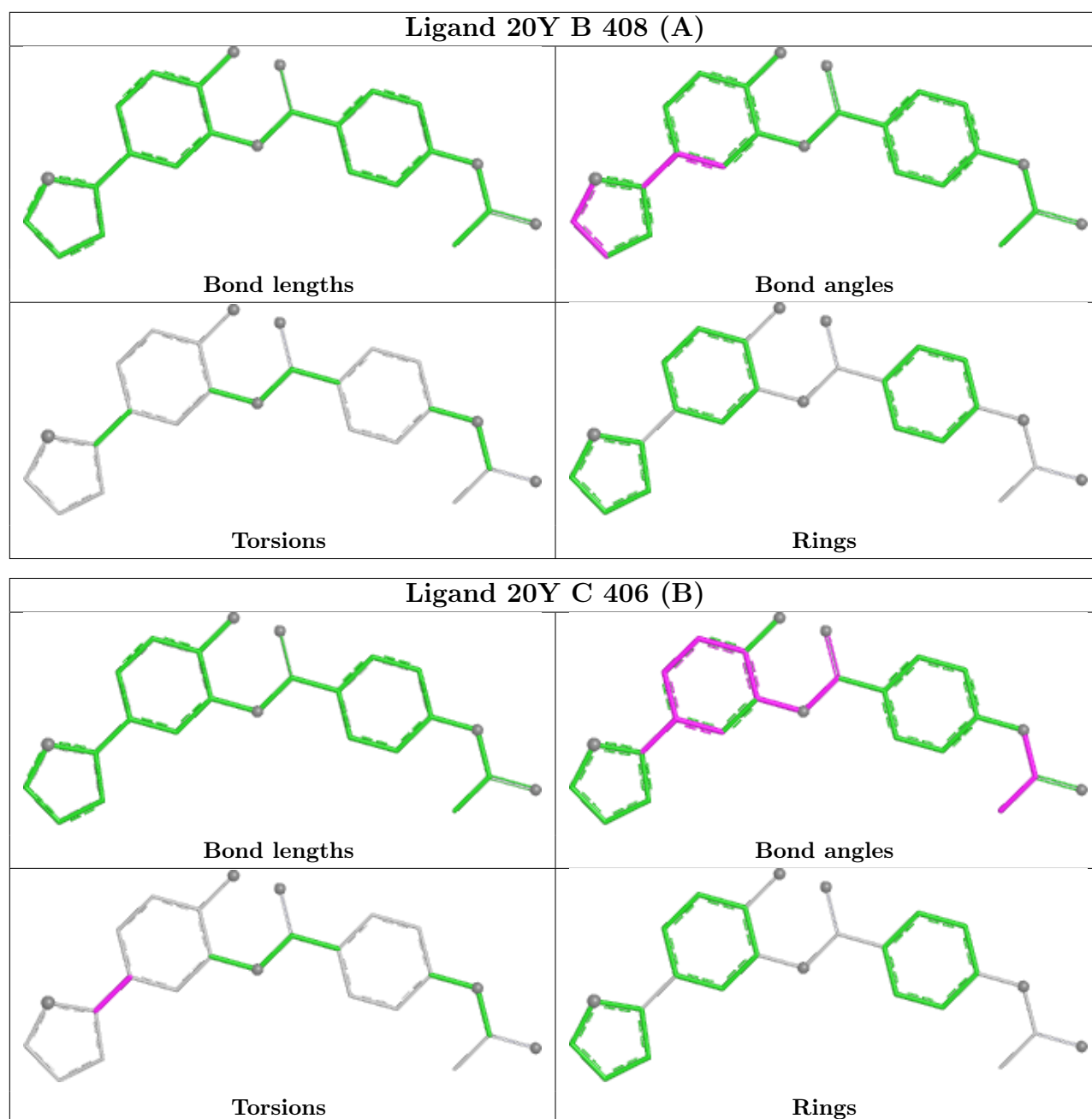


Ligand 20Y B 408 (B)



Ligand 20Y C 406 (A)





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	368/369 (99%)	-0.09	10 (2%) 56 68	9, 17, 36, 53	13 (3%)
1	B	367/369 (99%)	-0.24	3 (0%) 82 87	8, 16, 34, 56	8 (2%)
1	C	366/369 (99%)	0.35	12 (3%) 49 62	14, 23, 41, 63	8 (2%)
All	All	1101/1107 (99%)	0.01	25 (2%) 61 72	8, 19, 38, 63	29 (2%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	379	PRO	4.5
1	B	379	PRO	3.8
1	A	12	GLY	3.5
1	C	378	LEU	3.4
1	C	341	TYR	2.9
1	A	208[A]	GLU	2.9
1	A	102	GLY	2.7
1	B	15	LYS	2.7
1	B	14	LYS	2.6
1	C	32	GLY	2.6
1	C	13	LYS	2.3
1	C	54	ARG	2.2
1	C	333	LEU	2.2
1	A	258	GLN	2.2
1	C	62[A]	HIS	2.2
1	A	369	GLN	2.2
1	C	346	PHE	2.2
1	C	335	TYR	2.1
1	A	90	SER	2.1
1	C	28	TYR	2.1
1	C	339	PHE	2.0
1	A	92	TYR	2.0
1	A	171	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	90	SER	2.0
1	A	95[A]	GLN	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
7	NHE	B	404	13/13	0.70	0.20	39,40,44,47	0
5	PG4	A	405	13/13	0.73	0.19	46,51,54,56	0
5	PG4	A	404	13/13	0.77	0.21	61,62,66,67	0
5	PG4	A	406	13/13	0.79	0.17	36,43,58,61	0
5	PG4	B	407	13/13	0.82	0.16	29,38,48,49	0
5	PG4	B	405	13/13	0.85	0.15	43,47,54,56	0
5	PG4	C	405	13/13	0.87	0.14	38,42,47,47	0
5	PG4	B	406	13/13	0.88	0.13	32,36,43,43	0
5	PG4	C	404	13/13	0.88	0.13	26,30,50,51	0
6	20Y	C	406[B]	25/25	0.94	0.10	6,12,26,29	25
6	20Y	C	406[A]	25/25	0.94	0.10	15,20,40,43	25
6	20Y	A	407[B]	25/25	0.96	0.05	10,13,24,27	25
6	20Y	A	407[A]	25/25	0.96	0.05	9,14,20,22	25
6	20Y	B	408[B]	25/25	0.98	0.05	9,12,23,26	25
6	20Y	B	408[A]	25/25	0.98	0.05	9,11,19,19	25
4	NA	C	403	1/1	0.99	0.04	11,11,11,11	0
2	ZN	C	401	1/1	0.99	0.03	16,16,16,16	0
3	CA	C	402	1/1	0.99	0.08	17,17,17,17	0
4	NA	A	403	1/1	0.99	0.06	13,13,13,13	0
3	CA	B	402	1/1	1.00	0.03	13,13,13,13	0
2	ZN	B	401	1/1	1.00	0.02	11,11,11,11	0

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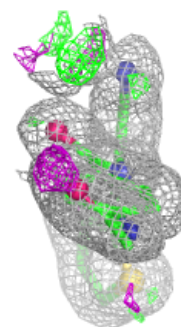
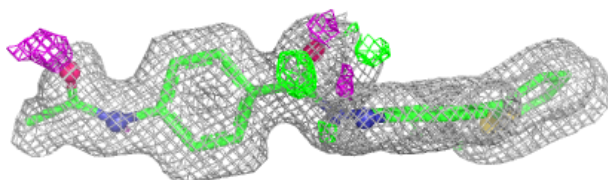
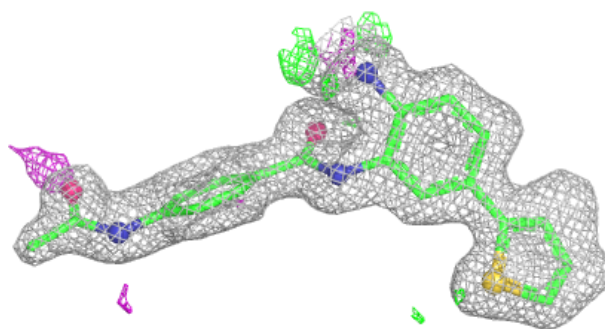
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	401	1/1	1.00	0.03	13,13,13,13	0
4	NA	B	403	1/1	1.00	0.10	12,12,12,12	0
3	CA	A	402	1/1	1.00	0.03	14,14,14,14	0

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.

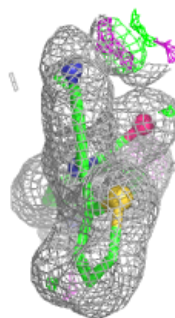
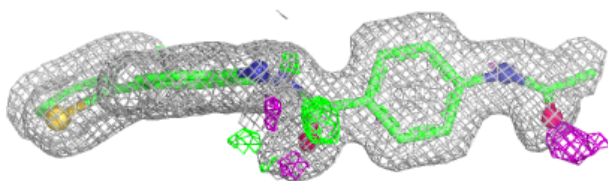
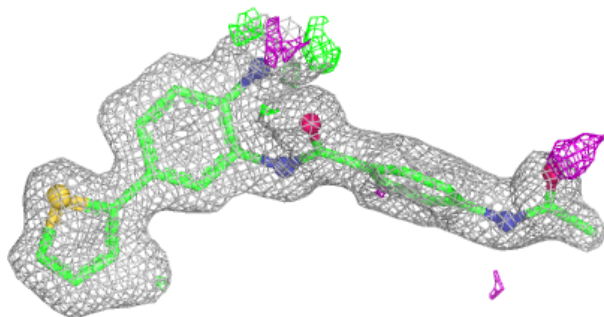
Electron density around 20Y C 406 (B):

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

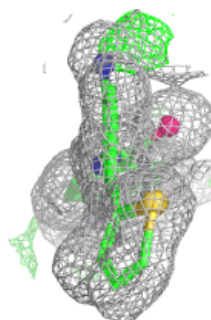
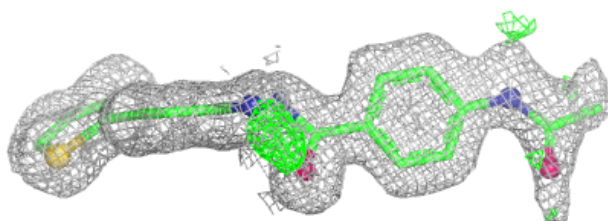
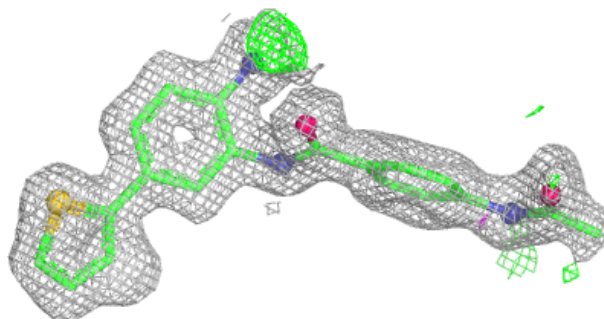


Electron density around 20Y C 406 (A):

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

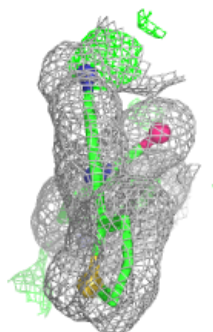
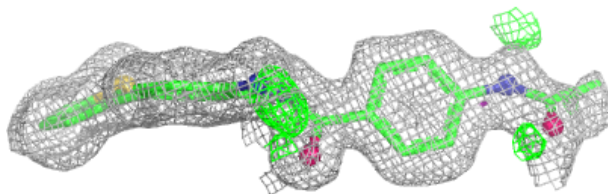
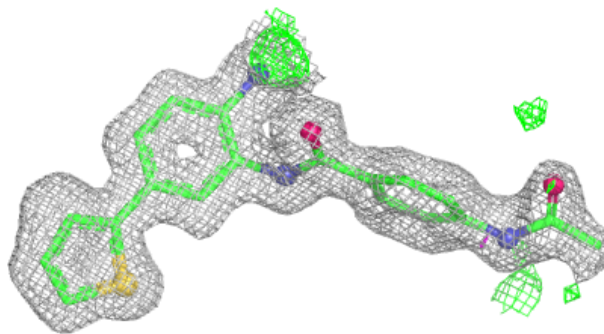
**Electron density around 20Y A 407 (B):**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

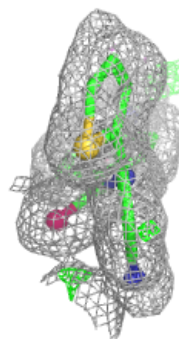
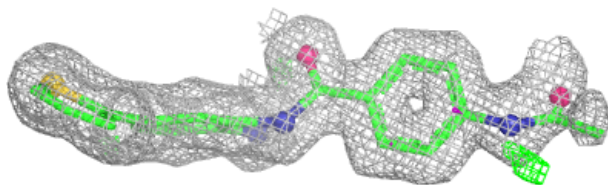
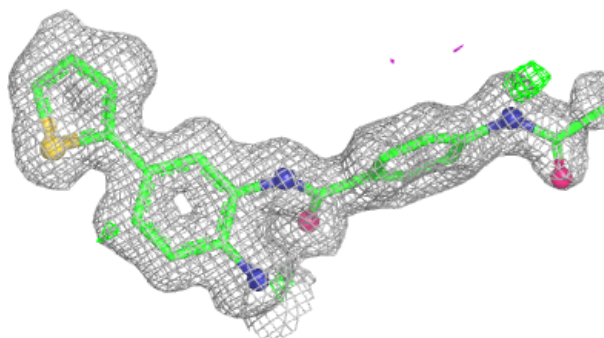


Electron density around 20Y A 407 (A):

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

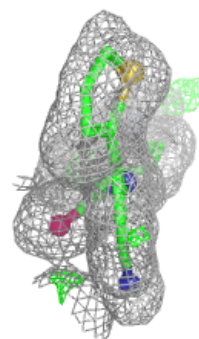
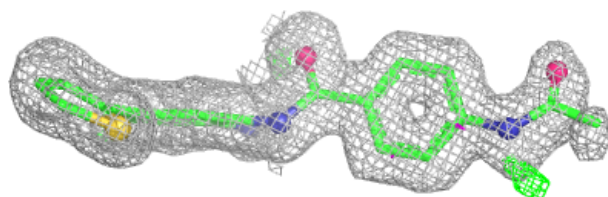
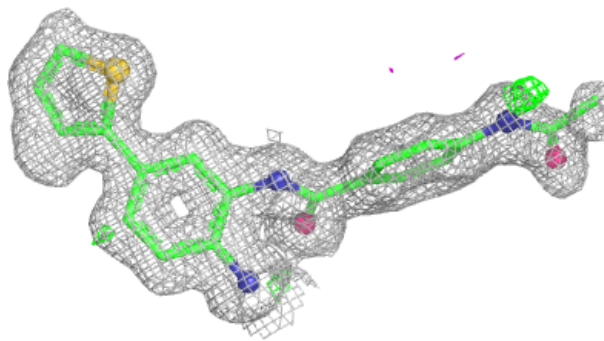
**Electron density around 20Y B 408 (B):**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 20Y B 408 (A):

$2mF_o-DF_c$ (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.