wwPDB X-ray Structure Validation Summary Report (i)

Jan 15, 2024 – 02:24 pm GMT

PDB ID	:	6HTI
Title	:	Crystal structure of Schistosoma mansoni HDAC8 complexed with a benzohydroxamate inhibitor 6
Authors	:	Shaik, T.B.; Marek, M.; Romier, C.
Deposited on	:	2018-10-04
Resolution	:	1.69 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

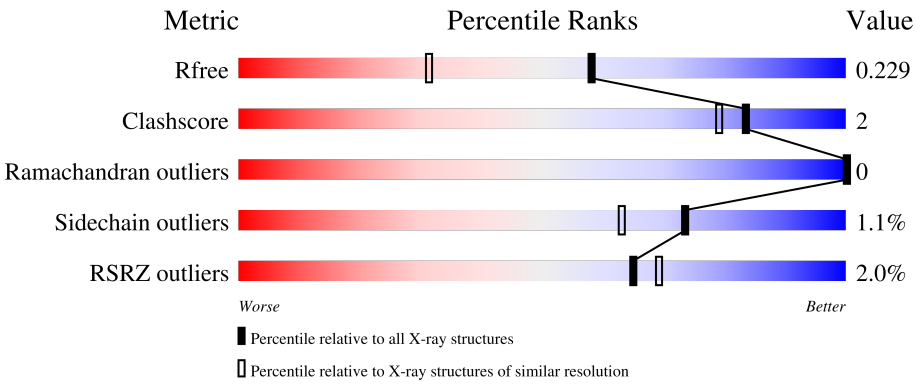
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.69 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 <=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	447	2% 83% 6% 11%
1	B	447	% 88% • 8%
1	C	447	2% 85% 7% 8%
1	D	447	2% 84% 5% 11%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13614 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	399	3199	2066	532	586	15	0	1	0
1	B	412	3298	2125	550	607	16	0	3	0
1	C	412	3300	2127	552	605	16	0	2	0
1	D	399	3202	2067	532	587	16	0	2	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP A5H660
A	441	GLY	-	expression tag	UNP A5H660
A	442	SER	-	expression tag	UNP A5H660
A	443	LEU	-	expression tag	UNP A5H660
A	444	VAL	-	expression tag	UNP A5H660
A	445	PRO	-	expression tag	UNP A5H660
A	446	ARG	-	expression tag	UNP A5H660
B	0	HIS	-	expression tag	UNP A5H660
B	441	GLY	-	expression tag	UNP A5H660
B	442	SER	-	expression tag	UNP A5H660
B	443	LEU	-	expression tag	UNP A5H660
B	444	VAL	-	expression tag	UNP A5H660
B	445	PRO	-	expression tag	UNP A5H660
B	446	ARG	-	expression tag	UNP A5H660
C	0	HIS	-	expression tag	UNP A5H660
C	441	GLY	-	expression tag	UNP A5H660
C	442	SER	-	expression tag	UNP A5H660
C	443	LEU	-	expression tag	UNP A5H660
C	444	VAL	-	expression tag	UNP A5H660
C	445	PRO	-	expression tag	UNP A5H660
C	446	ARG	-	expression tag	UNP A5H660

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP A5H660
D	441	GLY	-	expression tag	UNP A5H660
D	442	SER	-	expression tag	UNP A5H660
D	443	LEU	-	expression tag	UNP A5H660
D	444	VAL	-	expression tag	UNP A5H660
D	445	PRO	-	expression tag	UNP A5H660
D	446	ARG	-	expression tag	UNP A5H660

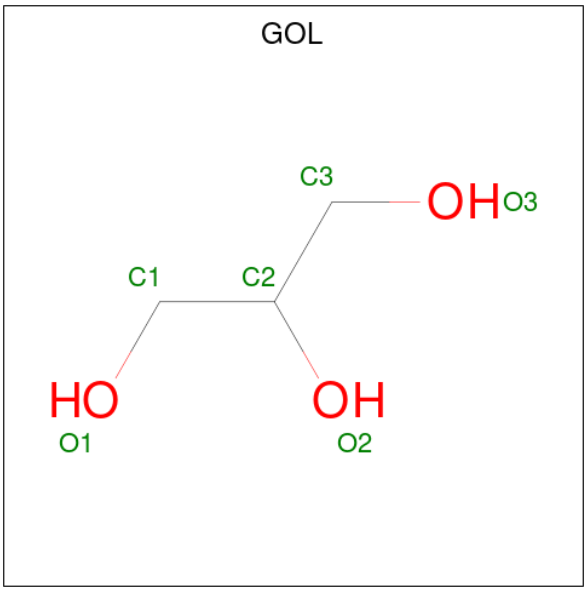
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

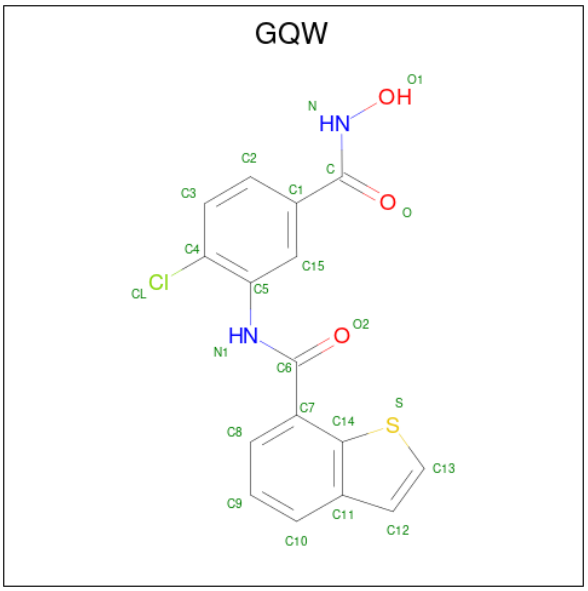
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
3	A	2	2	2	0	0
3	B	2	2	2	0	0
3	C	2	2	2	0	0
3	D	2	2	2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	C	1	6	3	3	0	0
4	D	1	6	3	3	0	0

- Molecule 5 is {N}-[2-chloranyl-5-(oxidanylcarbamoyl)phenyl]-1-benzothiophene-7-carboxamide (three-letter code: GQW) (formula: $C_{16}H_{11}ClN_2O_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
5	A	1	23	16	1	2	3	1	0	0
5	B	1	23	16	1	2	3	1	0	0
5	C	1	23	16	1	2	3	1	0	0
5	D	1	23	16	1	2	3	1	0	0

- Molecule 6 is water.

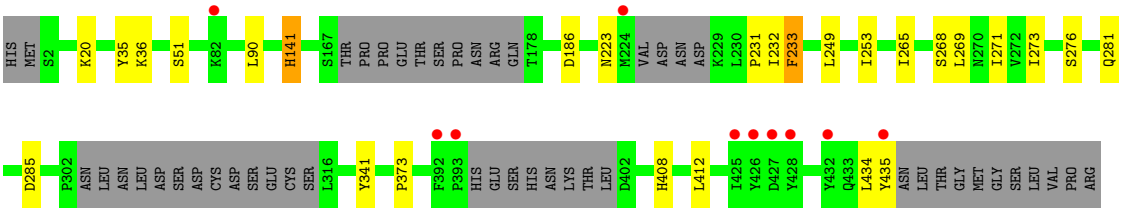
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	120	120	120	0	0
6	B	141	141	141	0	0
6	C	138	138	138	0	0
6	D	88	88	88	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

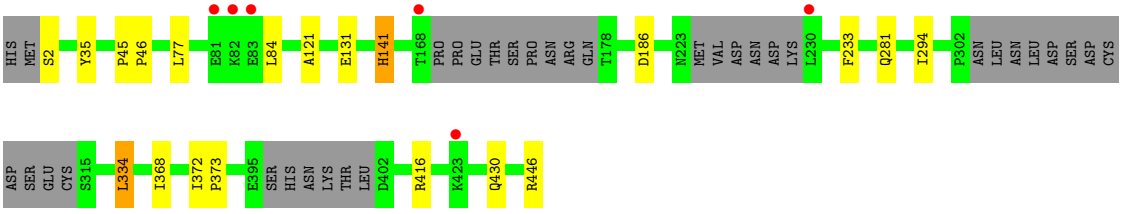
- Molecule 1: Histone deacetylase

Chain A:



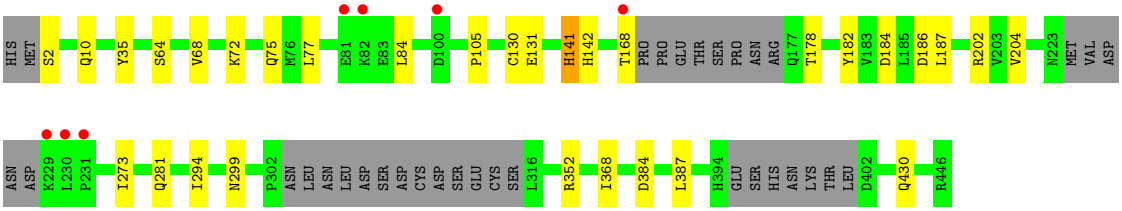
- Molecule 1: Histone deacetylase

Chain B:



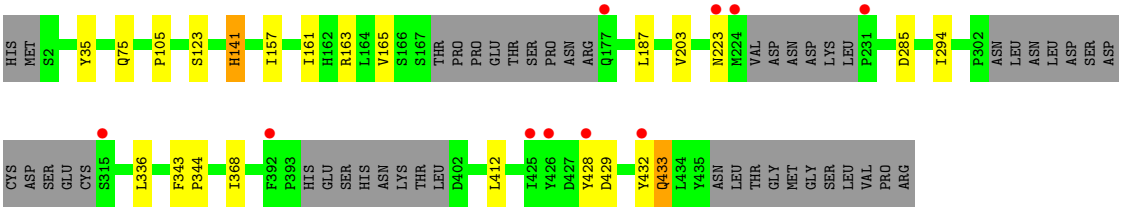
- Molecule 1: Histone deacetylase

Chain C:



- Molecule 1: Histone deacetylase

Chain D:


HIS
MET
S2
Y35
Q75
P105
S123
H141
I157
I161
H162
R163
L164
V165
S166
S167
THR
PRO
PRO
GLU
THR
SER
PRO
ASN
ARG
Q177
L187
V203
N223
M224
VAL
ASP
ASN
ASP
LYS
LEU
P231
D285
I294
P302
ASN
LEU
ASN
LEU
ASP
SER
ASP
CYS
ASP
SER
GLU
CYS
S315
L336
F343
P344
I368
F392
P393
HIS
GLU
SER
HIS
ASN
LYS
THR
LEU
D402
L412
I425
Y426
D427
Y428
D429
Y432
Q433
L434
Y435
ASN
LEU
THR
GLY
MET
GLY
SER
LEU
VAL
PRO
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	70.73Å 70.73Å 98.35Å 75.70° 78.01° 85.80°	Depositor
Resolution (Å)	48.12 – 1.69 48.13 – 1.69	Depositor EDS
% Data completeness (in resolution range)	94.3 (48.12-1.69) 94.4 (48.13-1.69)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 1.69Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.197 , 0.229 0.197 , 0.229	Depositor DCC
R_{free} test set	9490 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 33.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.100 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13614	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.43% 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: GQW, GOL, K, ZN

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	0.40	0/3292	0.54	1/4477 (0.0%)
1	B	0.41	0/3399	0.56	1/4624 (0.0%)
1	C	0.40	0/3398	0.57	1/4621 (0.0%)
1	D	0.38	0/3298	0.53	0/4484
All	All	0.40	0/13387	0.55	3/18206 (0.0%)

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	D	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	384	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	334	LEU	CA-CB-CG	5.39	127.70	115.30
1	A	90	LEU	CA-CB-CG	5.08	126.99	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	223	ASN	Peptide

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	3199	0	3100	20	0
1	B	3298	0	3197	13	0
1	C	3300	0	3201	19	0
1	D	3202	0	3101	11	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	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	A	23	0	0	1	0
5	B	23	0	0	0	0
5	C	23	0	0	1	0
5	D	23	0	0	0	0
6	A	120	0	0	0	0
6	B	141	0	0	0	0
6	C	138	0	0	0	0
6	D	88	0	0	0	0
All	All	13614	0	12631	61	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.

The worst 5 of 61 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:35:TYR:CE1	1:C:368:ILE:HG23	2.27	0.69
1:A:232:ILE:HG12	1:A:233:PHE:H	1.60	0.67
1:C:2:SER:N	1:C:131:GLU:OE1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:LEU:HD21	1:A:435:TYR:CE1	2.36	0.60
1:B:77:LEU:HD13	1:B:84:LEU:HG	1.83	0.60

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	390/447 (87%)	385 (99%)	5 (1%)	0	100	100
1	B	405/447 (91%)	400 (99%)	5 (1%)	0	100	100
1	C	404/447 (90%)	399 (99%)	5 (1%)	0	100	100
1	D	391/447 (88%)	386 (99%)	5 (1%)	0	100	100
All	All	1590/1788 (89%)	1570 (99%)	20 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	347/392 (88%)	343 (99%)	4 (1%)	71	59
1	B	360/392 (92%)	357 (99%)	3 (1%)	81	74
1	C	359/392 (92%)	355 (99%)	4 (1%)	73	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	348/392 (89%)	344 (99%)	4 (1%)	73	63
All	All	1414/1568 (90%)	1399 (99%)	15 (1%)	73	63

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	10	GLN
1	D	428	TYR
1	C	141	HIS
1	D	433	GLN
1	D	141	HIS

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 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	GQW	C	501	2	22,25,25	0.35	0	28,35,35	1.16	3 (10%)
5	GQW	B	501	2	22,25,25	0.37	0	28,35,35	1.29	4 (14%)
5	GQW	D	501	2	22,25,25	0.33	0	28,35,35	1.31	4 (14%)
5	GQW	A	505	2	22,25,25	0.36	0	28,35,35	1.25	4 (14%)
4	GOL	A	504	-	5,5,5	0.28	0	5,5,5	0.51	0
4	GOL	C	505	-	5,5,5	0.35	0	5,5,5	1.28	1 (20%)
4	GOL	B	505	-	5,5,5	0.29	0	5,5,5	0.33	0
4	GOL	D	505	-	5,5,5	0.43	0	5,5,5	0.40	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	GQW	C	501	2	-	2/14/14/14	0/3/3/3
5	GQW	B	501	2	-	2/14/14/14	0/3/3/3
5	GQW	D	501	2	-	2/14/14/14	0/3/3/3
5	GQW	A	505	2	-	2/14/14/14	0/3/3/3
4	GOL	A	504	-	-	0/4/4/4	-
4	GOL	C	505	-	-	2/4/4/4	-
4	GOL	B	505	-	-	4/4/4/4	-
4	GOL	D	505	-	-	0/4/4/4	-

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	501	GQW	C5-N1-C6	4.10	138.17	126.93
5	D	501	GQW	C5-N1-C6	4.06	138.05	126.93
5	A	505	GQW	C5-N1-C6	4.03	137.99	126.93
5	C	501	GQW	C5-N1-C6	3.37	136.17	126.93
5	D	501	GQW	C4-C5-N1	2.86	123.77	119.24

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	505	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	C	505	GOL	O2-C2-C3-O3
5	A	505	GQW	C4-C5-N1-C6
5	B	501	GQW	C4-C5-N1-C6
5	C	501	GQW	C4-C5-N1-C6

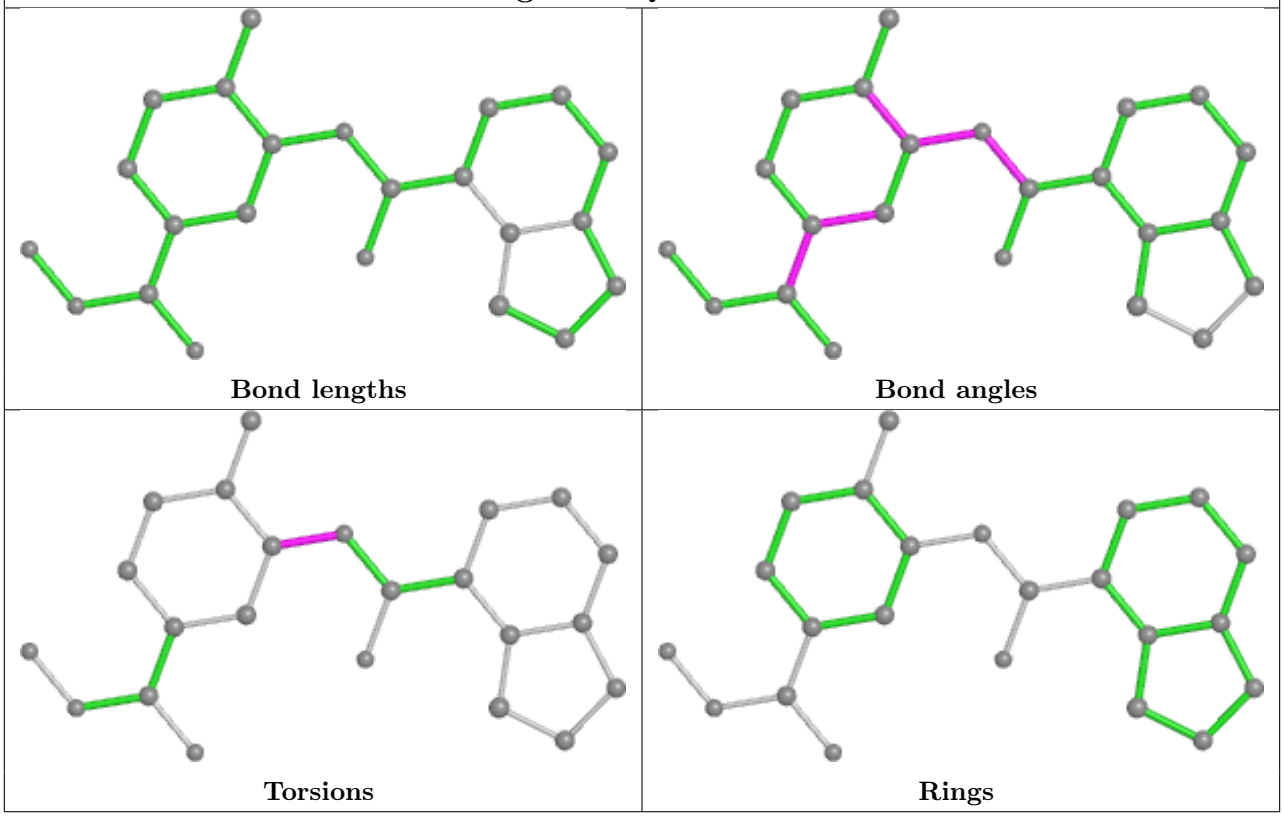
There are no ring outliers.

2 monomers are involved in 2 short contacts:

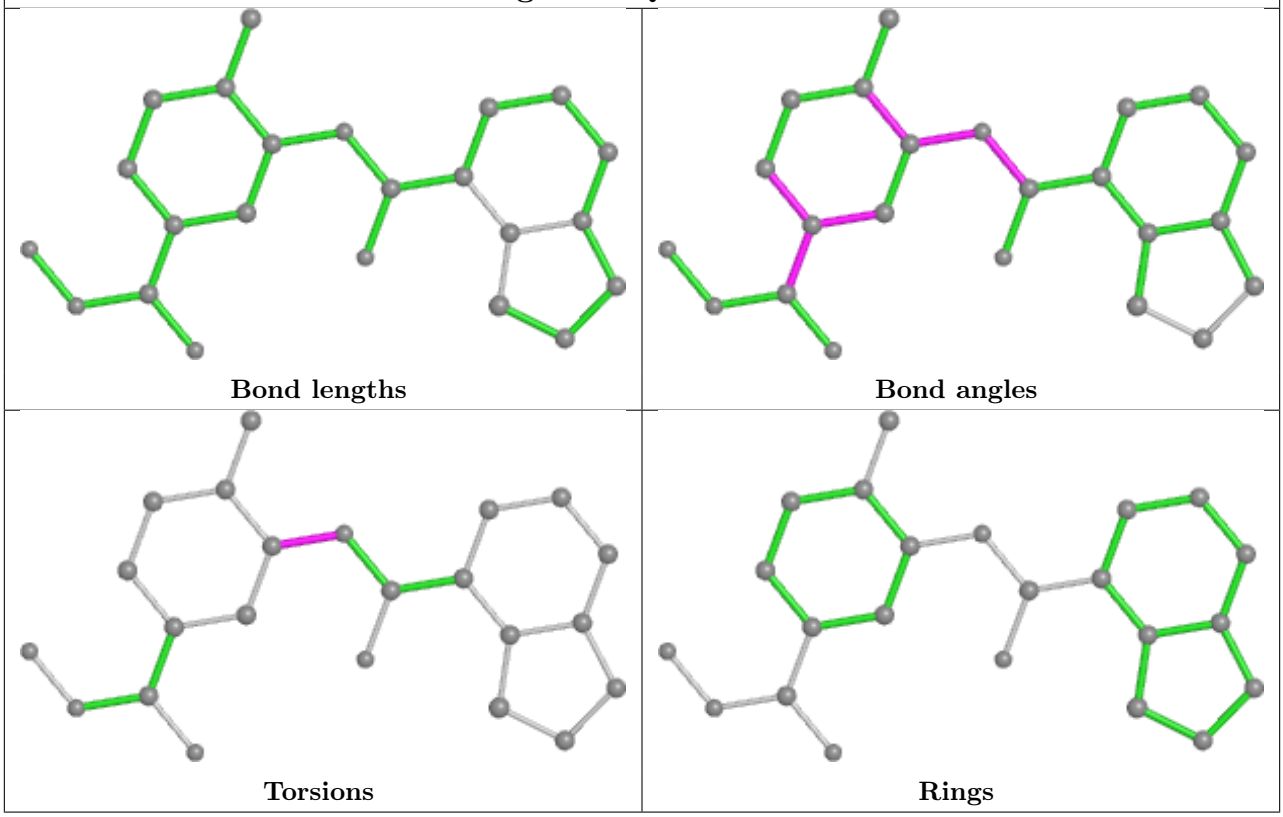
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	501	GQW	1	0
5	A	505	GQW	1	0

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 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.

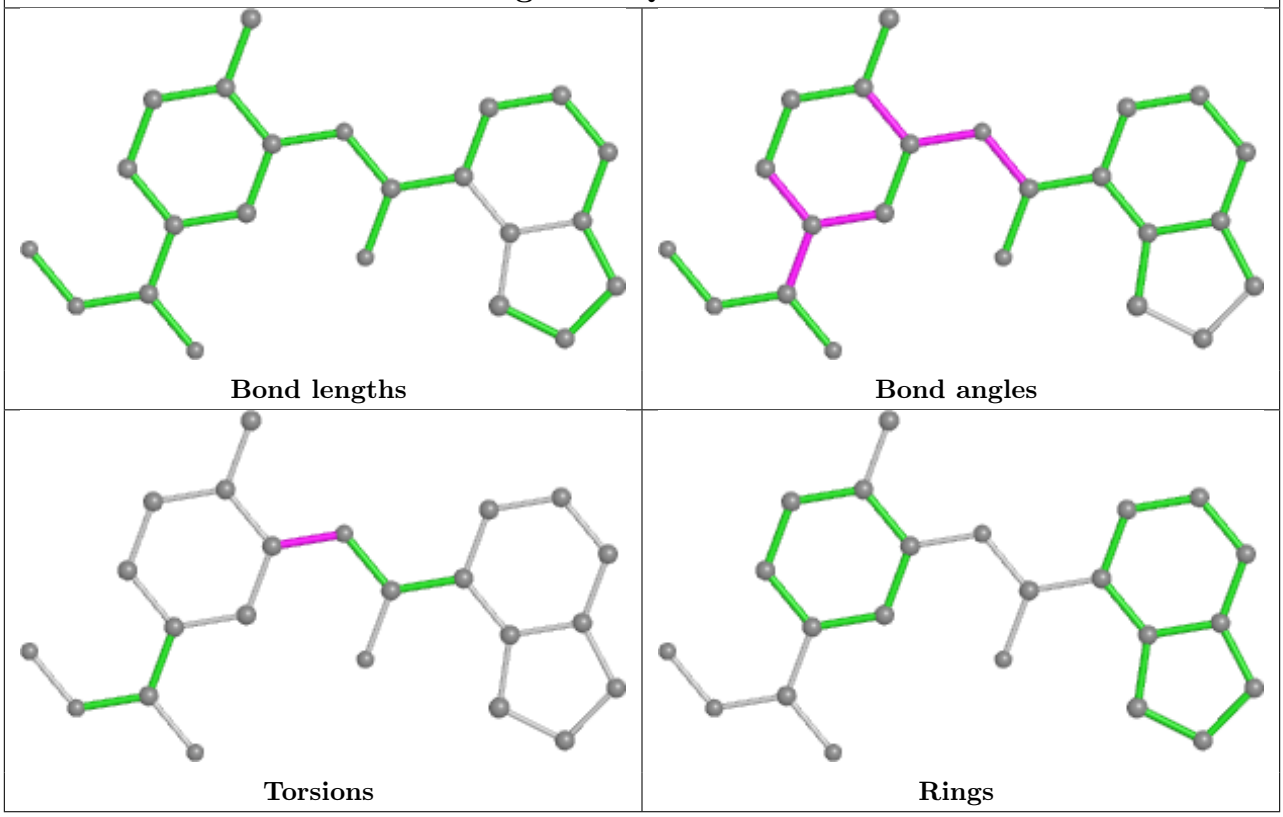
Ligand GQW C 501



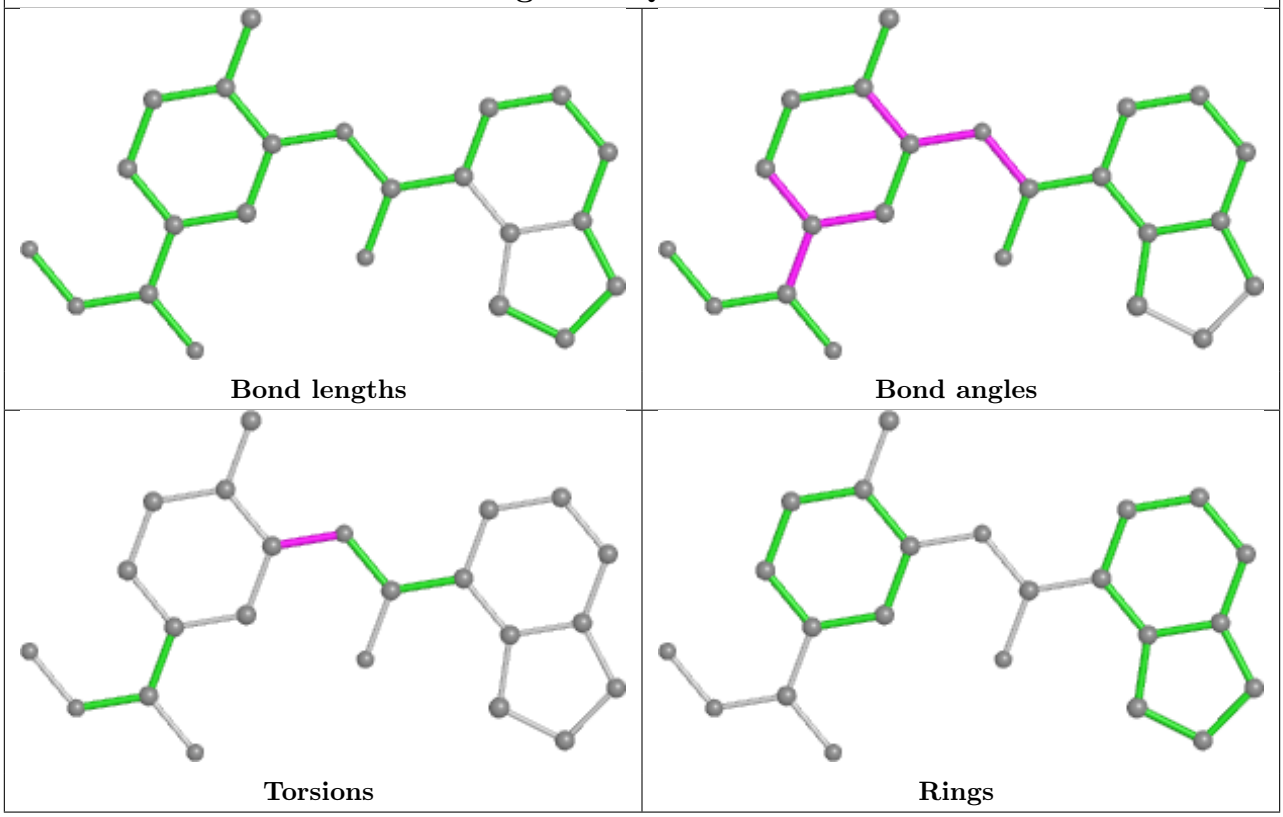
Ligand GQW B 501



Ligand GQW D 501



Ligand GQW A 505



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	399/447 (89%)	-0.31	10 (2%)	57	61	16, 26, 54, 90	0
1	B	412/447 (92%)	-0.47	6 (1%)	73	77	16, 24, 42, 86	0
1	C	412/447 (92%)	-0.43	7 (1%)	70	74	16, 23, 42, 86	0
1	D	399/447 (89%)	-0.31	10 (2%)	57	61	17, 25, 51, 75	0
All	All	1622/1788 (90%)	-0.38	33 (2%)	65	69	16, 24, 48, 90	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	425	ILE	8.4
1	A	425	ILE	7.3
1	D	392	PHE	5.8
1	D	428	TYR	5.5
1	D	426	TYR	5.3

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

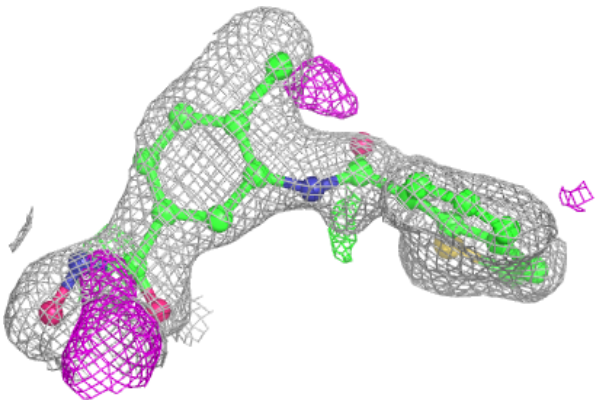
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

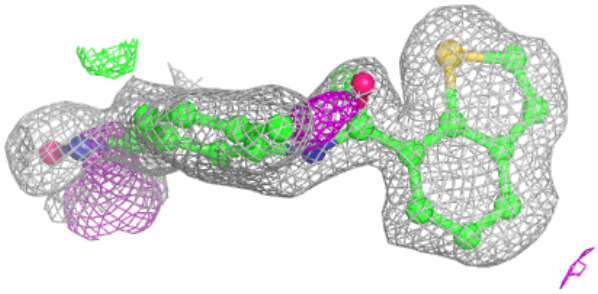
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GQW	D	501	23/23	0.81	0.14	34,50,59,60	0
5	GQW	C	501	23/23	0.88	0.13	26,39,50,53	0
5	GQW	A	505	23/23	0.88	0.12	35,52,62,65	0
4	GOL	B	505	6/6	0.89	0.10	26,38,39,39	0
5	GQW	B	501	23/23	0.89	0.11	27,38,47,56	0
4	GOL	A	504	6/6	0.93	0.07	25,31,33,33	0
4	GOL	C	505	6/6	0.93	0.09	25,32,39,39	0
4	GOL	D	505	6/6	0.94	0.10	25,30,31,32	0
3	K	C	503	1/1	1.00	0.04	18,18,18,18	0
3	K	C	504	1/1	1.00	0.05	21,21,21,21	0
3	K	D	503	1/1	1.00	0.05	18,18,18,18	0
3	K	D	504	1/1	1.00	0.06	20,20,20,20	0
2	ZN	A	501	1/1	1.00	0.02	31,31,31,31	0
2	ZN	B	502	1/1	1.00	0.01	29,29,29,29	0
2	ZN	C	502	1/1	1.00	0.02	29,29,29,29	0
2	ZN	D	502	1/1	1.00	0.02	29,29,29,29	0
3	K	A	502	1/1	1.00	0.07	20,20,20,20	0
3	K	A	503	1/1	1.00	0.08	22,22,22,22	0
3	K	B	503	1/1	1.00	0.06	17,17,17,17	0
3	K	B	504	1/1	1.00	0.05	23,23,23,23	0

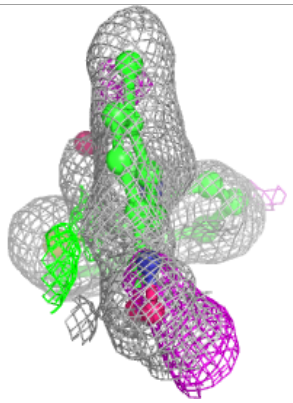
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GQW D 501:

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

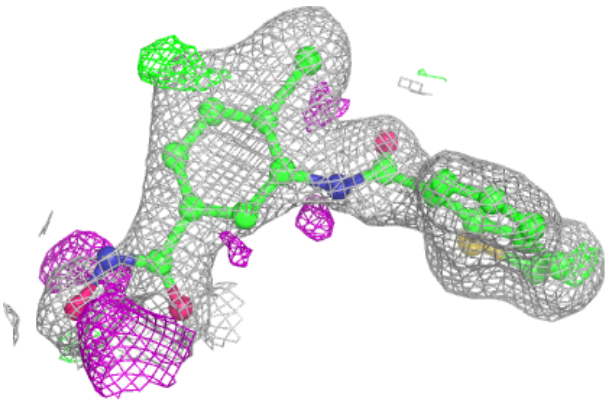


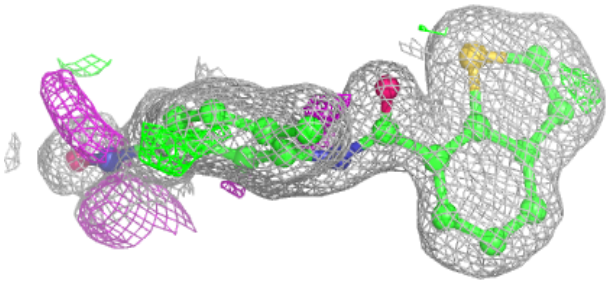


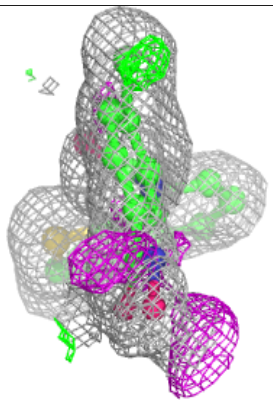


Electron density around GQW C 501:

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

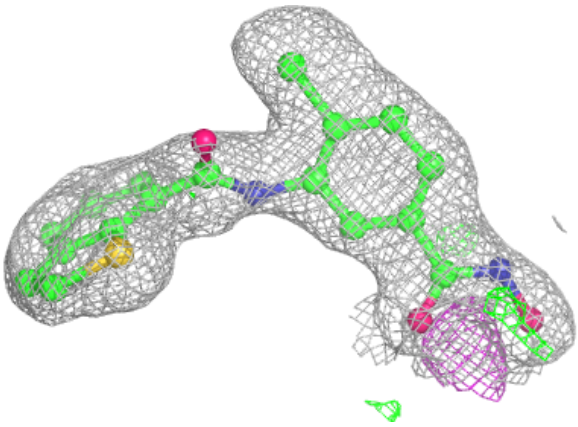


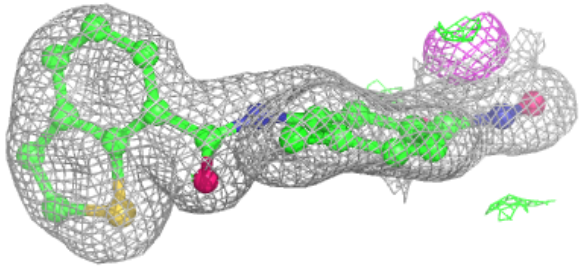


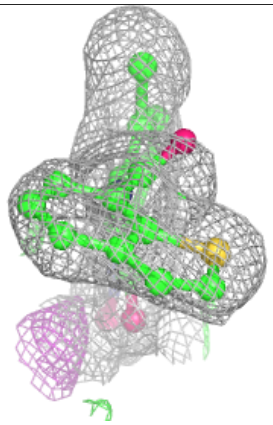


Electron density around GQW A 505:

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

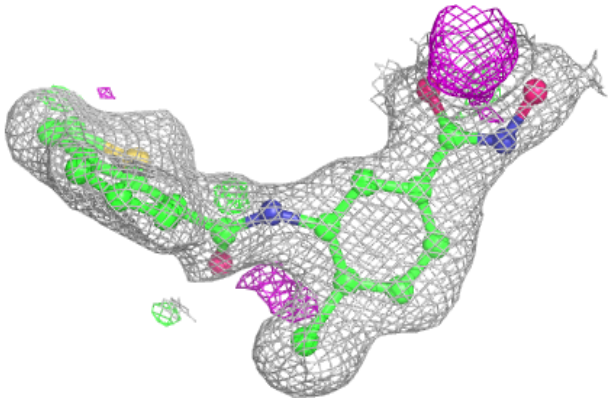


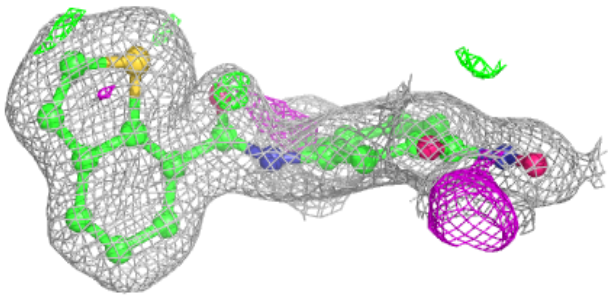


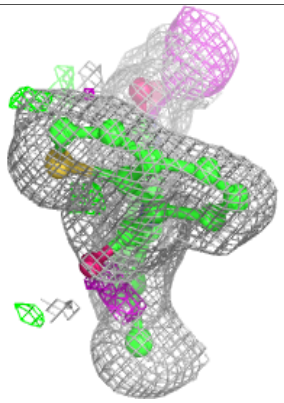


Electron density around GQW B 501:

$2mF_o$-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.