



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 08:57 pm BST

PDB ID : 6HTH  
Title : Crystal structure of Schistosoma mansoni HDAC8 complexed with a benzohydroxamate inhibitor 5  
Authors : Shaik, T.B.; Marek, M.; Romier, C.  
Deposited on : 2018-10-04  
Resolution : 1.95 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](mailto: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.

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

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

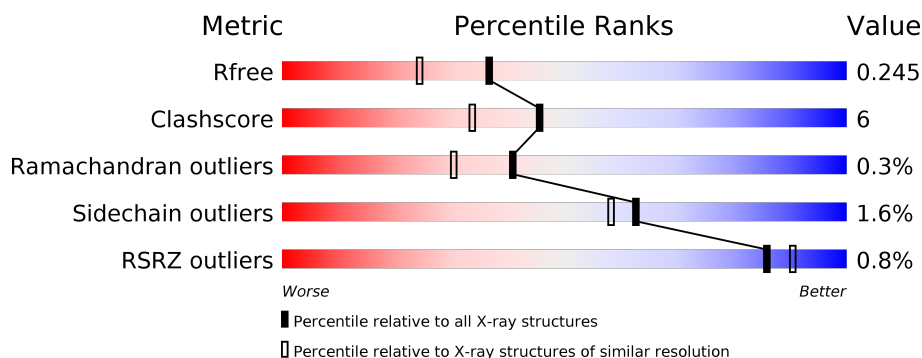
# 1 Overall quality at a glance

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))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	447	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 74%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>74%</span> <span>11%</span> <span>•</span> <span>14%</span> </div> </div>
1	B	447	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 13%, green 77%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>77%</span> <span>13%</span> <span>•</span> <span>8%</span> </div> </div>
1	C	447	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 12%, green 78%, grey 9%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>78%</span> <span>12%</span> <span>•</span> <span>9%</span> </div> </div>
1	D	447	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, orange 0%, yellow 10%, green 76%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>76%</span> <span>10%</span> <span>•</span> <span>14%</span> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	B	506	-	-	X	-
5	GOL	C	506	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13533 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
1	A	386	Total	C	N	O	S	0	5	0
			3100	1997	523	564	16			
1	B	410	Total	C	N	O	S	0	7	0
			3323	2143	558	606	16			
1	C	407	Total	C	N	O	S	0	6	0
			3280	2116	548	599	17			
1	D	384	Total	C	N	O	S	0	1	0
			3057	1972	513	558	14			

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

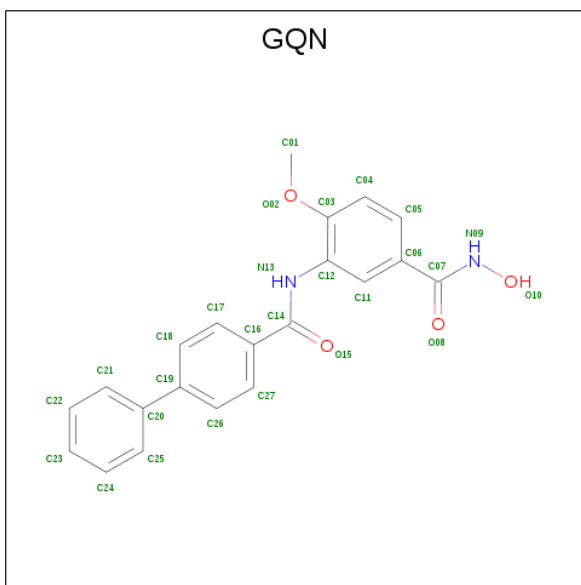
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

- Molecule 4 is 4-methoxy- {N}-oxidanyl-3-[(4-phenylphenyl)carbonylamino]benzamide (three-letter code: GQN) (formula: C<sub>21</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>).



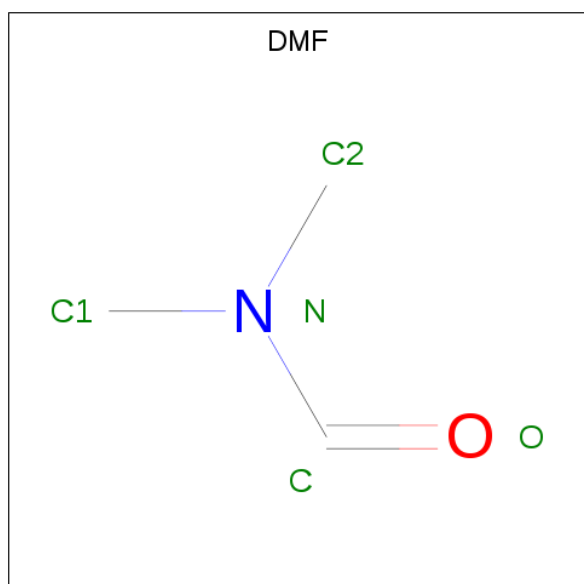
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			27	21	2	4		
4	B	1	Total	C	N	O	0	0
			27	21	2	4		
4	C	1	Total	C	N	O	0	0
			27	21	2	4		
4	D	1	Total	C	N	O	0	0
			27	21	2	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 6 is DIMETHYLFORMAMIDE (three-letter code: DMF) (formula:  $C_3H_7NO$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O 5 3 1 1	0	0
6	B	1	Total C N O 5 3 1 1	0	0
6	B	1	Total C N O 5 3 1 1	0	0
6	B	1	Total C N O 5 3 1 1	0	0
6	B	1	Total C N O 5 3 1 1	0	0
6	B	1	Total C N O 5 3 1 1	0	0
6	B	1	Total C N O 5 3 1 1	0	0
6	B	1	Total C N O 5 3 1 1	0	0
6	B	1	Total C N O 5 3 1 1	0	0
6	B	1	Total C N O 5 3 1 1	0	0
6	C	1	Total C N O 5 3 1 1	0	0
6	C	1	Total C N O 5 3 1 1	0	0
6	C	1	Total C N O 5 3 1 1	0	0
6	C	1	Total C N O 5 3 1 1	0	0
6	C	1	Total C N O 5 3 1 1	0	0
6	D	1	Total C N O 5 3 1 1	0	0
6	D	1	Total C N O 5 3 1 1	0	0
6	D	1	Total C N O 5 3 1 1	0	0
6	D	1	Total C N O 5 3 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	116	Total O 116 116	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	111	Total 111	O 111	0	0
7	C	128	Total 128	O 128	0	0
7	D	125	Total 125	O 125	0	0

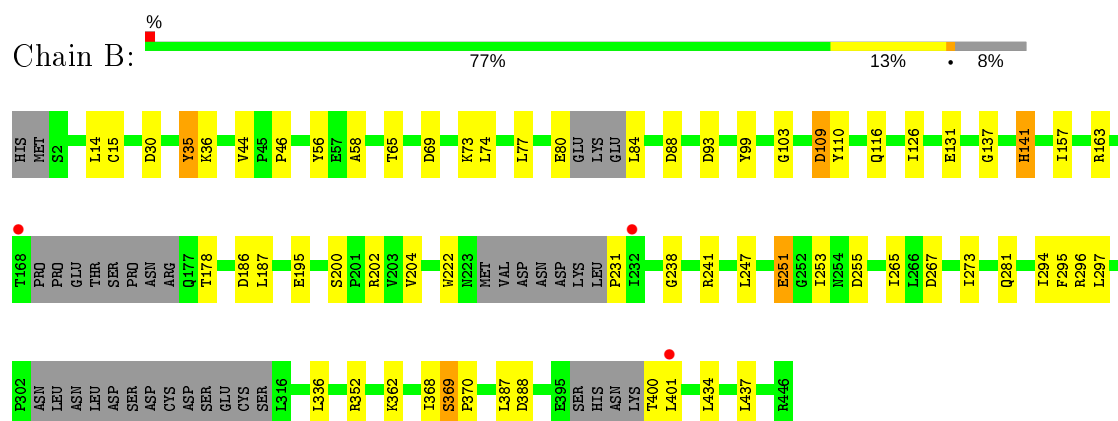
### 3 Residue-property plots [i](#)

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

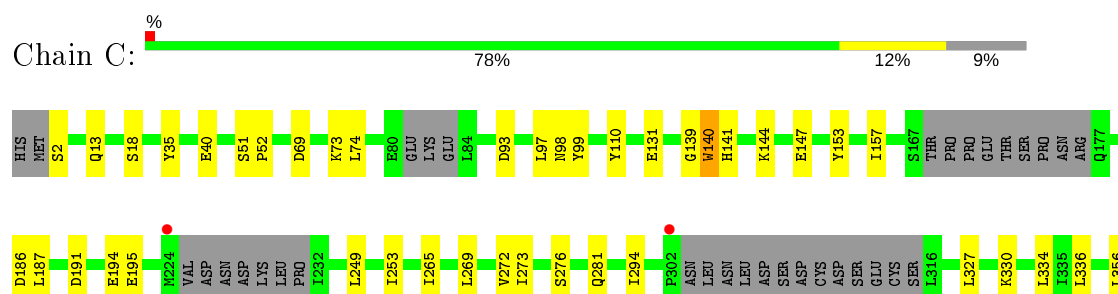
- Molecule 1: Histone deacetylase

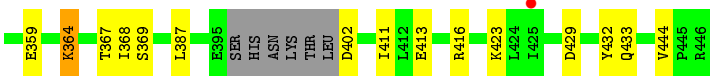


- Molecule 1: Histone deacetylase

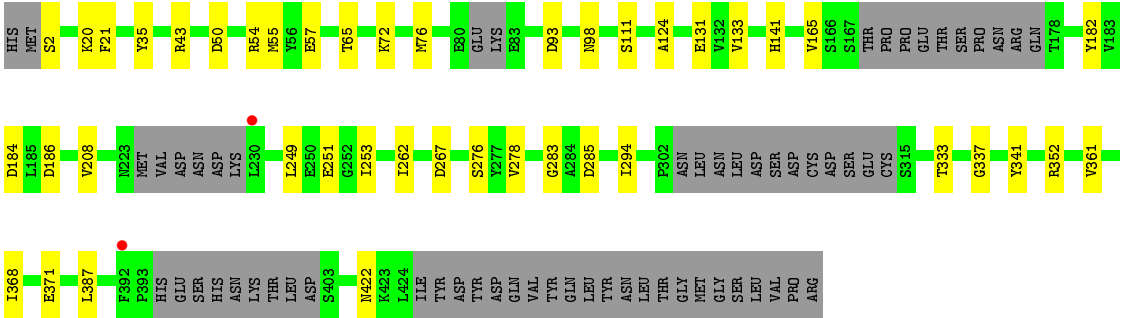


- Molecule 1: Histone deacetylase





• Molecule 1: Histone deacetylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.52Å 70.56Å 98.23Å 78.36° 75.84° 85.74°	Depositor
Resolution (Å)	46.76 – 1.95 46.76 – 1.95	Depositor EDS
% Data completeness (in resolution range)	95.6 (46.76-1.95) 95.6 (46.76-1.95)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.73 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.210 , 0.257 0.195 , 0.245	Depositor DCC
$R_{free}$ test set	6284 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.2	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 37.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.160 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13533	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GQN, ZN, K, DMF, GOL

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	0.77	1/3201 (0.0%)	0.77	2/4350 (0.0%)
1	B	0.77	2/3427 (0.1%)	0.76	1/4659 (0.0%)
1	C	0.79	1/3389 (0.0%)	0.77	1/4608 (0.0%)
1	D	0.74	0/3145	0.78	2/4277 (0.0%)
All	All	0.77	4/13162 (0.0%)	0.77	6/17894 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	194	GLU	CD-OE2	6.39	1.32	1.25
1	A	203	VAL	CB-CG2	5.81	1.65	1.52
1	B	44	VAL	CB-CG1	5.35	1.64	1.52
1	B	35	TYR	CE2-CZ	5.14	1.45	1.38

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	ASP	CB-CG-OD1	7.13	124.72	118.30
1	D	55	MET	CG-SD-CE	6.22	110.15	100.20
1	D	285	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	30	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	247	LEU	CB-CG-CD2	-5.05	102.41	111.00

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	3100	0	3021	38	0
1	B	3323	0	3228	58	0
1	C	3280	0	3186	43	0
1	D	3057	0	2968	25	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	27	0	0	1	0
4	B	27	0	0	0	0
4	C	27	0	0	0	0
4	D	27	0	0	1	0
5	A	24	0	32	6	0
5	B	36	0	48	12	0
5	C	12	0	16	7	0
5	D	6	0	8	0	0
6	A	5	0	7	0	0
6	B	45	0	63	3	0
6	C	25	0	35	5	0
6	D	20	0	28	3	0
7	A	116	0	0	9	4
7	B	111	0	0	11	3
7	C	128	0	0	8	1
7	D	125	0	0	5	0
All	All	13533	0	12640	165	4

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 165 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:94:SER:HA	5:A:506:GOL:H31	1.49	0.93
1:B:195:GLU:OE1	7:B:601:HOH:O	1.96	0.83
1:B:241:ARG:NH1	7:B:602:HOH:O	2.08	0.83
1:D:2:SER:N	1:D:131:GLU:OE1	2.14	0.80
1:C:40:GLU:OE2	7:C:601:HOH:O	2.01	0.79

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:622:HOH:O	7:C:601:HOH:O[1_565]	1.98	0.22
7:A:699:HOH:O	7:B:606:HOH:O[1_455]	2.01	0.19
7:A:649:HOH:O	7:B:606:HOH:O[1_455]	2.05	0.15
7:A:649:HOH:O	7:B:609:HOH:O[1_455]	2.07	0.13

## 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	381/447 (85%)	368 (97%)	12 (3%)	1 (0%)	41	30
1	B	405/447 (91%)	396 (98%)	8 (2%)	1 (0%)	47	38
1	C	401/447 (90%)	392 (98%)	8 (2%)	1 (0%)	47	38
1	D	373/447 (83%)	368 (99%)	4 (1%)	1 (0%)	41	30
All	All	1560/1788 (87%)	1524 (98%)	32 (2%)	4 (0%)	41	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	99	TYR
1	A	337	GLY
1	B	99	TYR

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Mol	Chain	Res	Type
1	D	337	GLY

### 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	338/392 (86%)	331 (98%)	7 (2%)	53	46
1	B	362/392 (92%)	356 (98%)	6 (2%)	60	55
1	C	358/392 (91%)	354 (99%)	4 (1%)	73	71
1	D	332/392 (85%)	327 (98%)	5 (2%)	65	60
All	All	1390/1568 (89%)	1368 (98%)	22 (2%)	62	58

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	141	HIS
1	B	369	SER
1	D	276	SER
1	B	200	SER
1	B	251	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	13	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 48 ligands modelled in this entry, 12 are monoatomic - leaving 36 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	$\# Z  > 2$
6	DMF	B	519	-	4,4,4	0.40	0	4,4,4	0.28	0
6	DMF	B	517	-	4,4,4	0.36	0	4,4,4	0.44	0
5	GOL	B	507	-	5,5,5	0.27	0	5,5,5	0.41	0
6	DMF	C	508	-	4,4,4	0.22	0	4,4,4	0.82	0
5	GOL	A	505	-	5,5,5	0.68	0	5,5,5	0.65	0
5	GOL	C	505	-	5,5,5	0.30	0	5,5,5	0.44	0
6	DMF	B	515	-	4,4,4	0.44	0	4,4,4	0.62	0
5	GOL	B	505	-	5,5,5	0.35	0	5,5,5	0.37	0
6	DMF	B	511	-	4,4,4	0.32	0	4,4,4	0.64	0
6	DMF	C	510	-	4,4,4	0.36	0	4,4,4	0.47	0
4	GQN	A	504	2	29,29,29	0.71	1 (3%)	39,39,39	1.97	8 (20%)
4	GQN	C	504	2	29,29,29	0.86	2 (6%)	39,39,39	1.71	8 (20%)
5	GOL	B	509	-	5,5,5	0.58	0	5,5,5	0.47	0
5	GOL	A	507	-	5,5,5	0.69	0	5,5,5	0.70	0
6	DMF	A	509	-	4,4,4	0.23	0	4,4,4	0.28	0
6	DMF	B	513	-	4,4,4	0.38	0	4,4,4	0.34	0
5	GOL	A	508	-	5,5,5	0.34	0	5,5,5	0.53	0
4	GQN	B	504	2	29,29,29	0.72	1 (3%)	39,39,39	1.64	6 (15%)
6	DMF	C	511	-	4,4,4	0.35	0	4,4,4	0.59	0
6	DMF	C	507	-	4,4,4	0.43	0	4,4,4	0.62	0
6	DMF	C	509	-	4,4,4	0.18	0	4,4,4	0.65	0
5	GOL	B	510	-	5,5,5	0.40	0	5,5,5	0.44	0
6	DMF	B	516	5	4,4,4	0.46	0	4,4,4	0.24	0
6	DMF	B	514	-	4,4,4	0.32	0	4,4,4	0.56	0
5	GOL	C	506	-	5,5,5	0.23	0	5,5,5	1.33	0
5	GOL	B	508	-	5,5,5	0.35	0	5,5,5	0.85	0
6	DMF	B	518	-	4,4,4	0.46	0	4,4,4	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	GOL	B	506	-	5,5,5	0.54	0	5,5,5	1.52	0
6	DMF	B	512	-	4,4,4	0.38	0	4,4,4	0.95	0
6	DMF	D	509	-	4,4,4	0.44	0	4,4,4	0.52	0
4	GQN	D	504	2	29,29,29	0.66	0	39,39,39	1.57	6 (15%)
5	GOL	A	506	6	5,5,5	0.27	0	5,5,5	1.00	1 (20%)
6	DMF	D	508	-	4,4,4	0.43	0	4,4,4	1.07	0
6	DMF	D	506	-	4,4,4	0.28	0	4,4,4	0.63	0
6	DMF	D	507	-	4,4,4	0.34	0	4,4,4	0.69	0
5	GOL	D	505	-	5,5,5	0.46	0	5,5,5	1.41	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
6	DMF	B	519	-	-	2/2/2/2	-
6	DMF	B	517	-	-	0/2/2/2	-
5	GOL	B	507	-	-	3/4/4/4	-
6	DMF	C	508	-	-	0/2/2/2	-
5	GOL	A	505	-	-	2/4/4/4	-
5	GOL	C	505	-	-	4/4/4/4	-
6	DMF	B	515	-	-	2/2/2/2	-
5	GOL	B	505	-	-	2/4/4/4	-
6	DMF	B	511	-	-	0/2/2/2	-
6	DMF	C	510	-	-	2/2/2/2	-
4	GQN	A	504	2	-	8/20/20/20	0/3/3/3
4	GQN	C	504	2	-	0/20/20/20	0/3/3/3
5	GOL	B	509	-	-	2/4/4/4	-
5	GOL	A	507	-	-	2/4/4/4	-
6	DMF	A	509	-	-	2/2/2/2	-
6	DMF	B	513	-	-	0/2/2/2	-
5	GOL	A	508	-	-	2/4/4/4	-
4	GQN	B	504	2	-	4/20/20/20	0/3/3/3
6	DMF	C	511	-	-	2/2/2/2	-
6	DMF	C	507	-	-	0/2/2/2	-
6	DMF	C	509	-	-	0/2/2/2	-
5	GOL	B	510	-	-	2/4/4/4	-
6	DMF	B	516	5	-	0/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DMF	B	514	-	-	2/2/2/2	-
5	GOL	C	506	-	-	3/4/4/4	-
5	GOL	B	508	-	-	4/4/4/4	-
6	DMF	B	518	-	-	0/2/2/2	-
5	GOL	B	506	-	-	1/4/4/4	-
6	DMF	B	512	-	-	0/2/2/2	-
6	DMF	D	509	-	-	0/2/2/2	-
4	GQN	D	504	2	-	0/20/20/20	0/3/3/3
5	GOL	A	506	6	-	2/4/4/4	-
6	DMF	D	508	-	-	0/2/2/2	-
6	DMF	D	506	-	-	2/2/2/2	-
6	DMF	D	507	-	-	0/2/2/2	-
5	GOL	D	505	-	-	4/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	504	GQN	C07-N09	2.38	1.35	1.32
4	A	504	GQN	C12-N13	-2.27	1.37	1.41
4	B	504	GQN	C12-N13	-2.16	1.37	1.41
4	C	504	GQN	C12-N13	-2.07	1.37	1.41

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	504	GQN	O02-C03-C12	6.80	123.15	114.80
4	A	504	GQN	O02-C03-C12	6.66	122.98	114.80
4	D	504	GQN	O02-C03-C12	5.58	121.65	114.80
4	C	504	GQN	O02-C03-C12	5.21	121.20	114.80
4	B	504	GQN	O02-C03-C04	-4.44	116.76	124.37

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

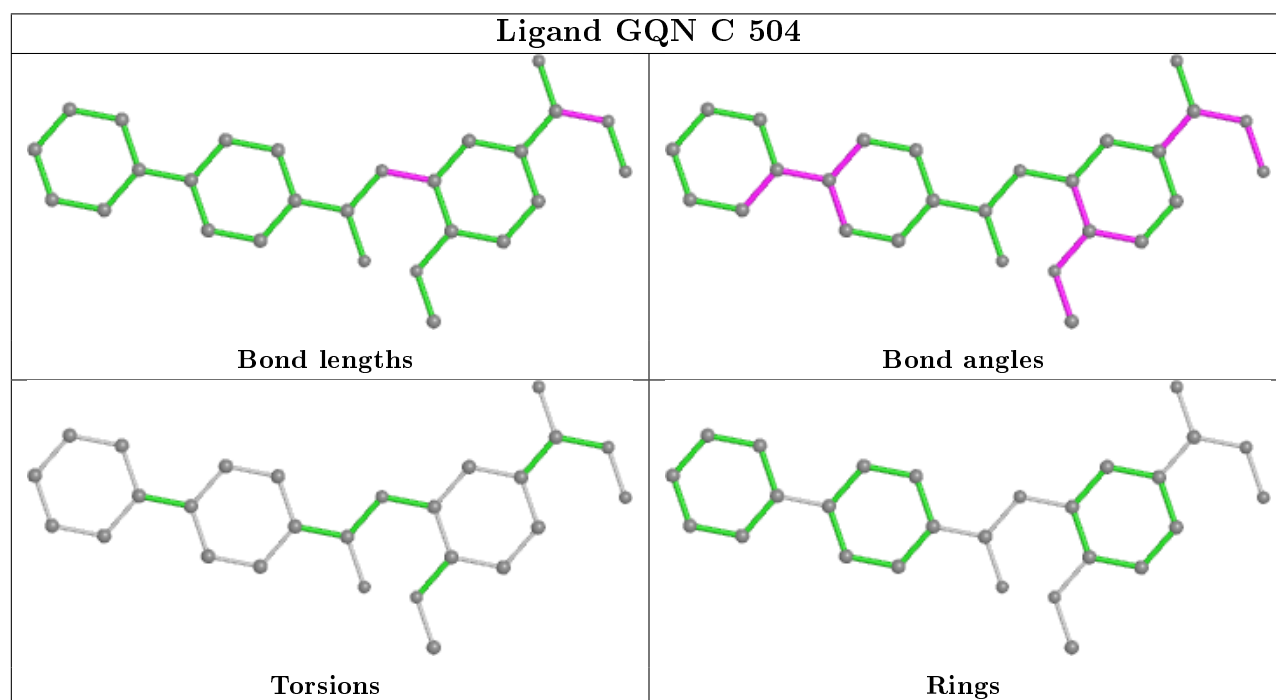
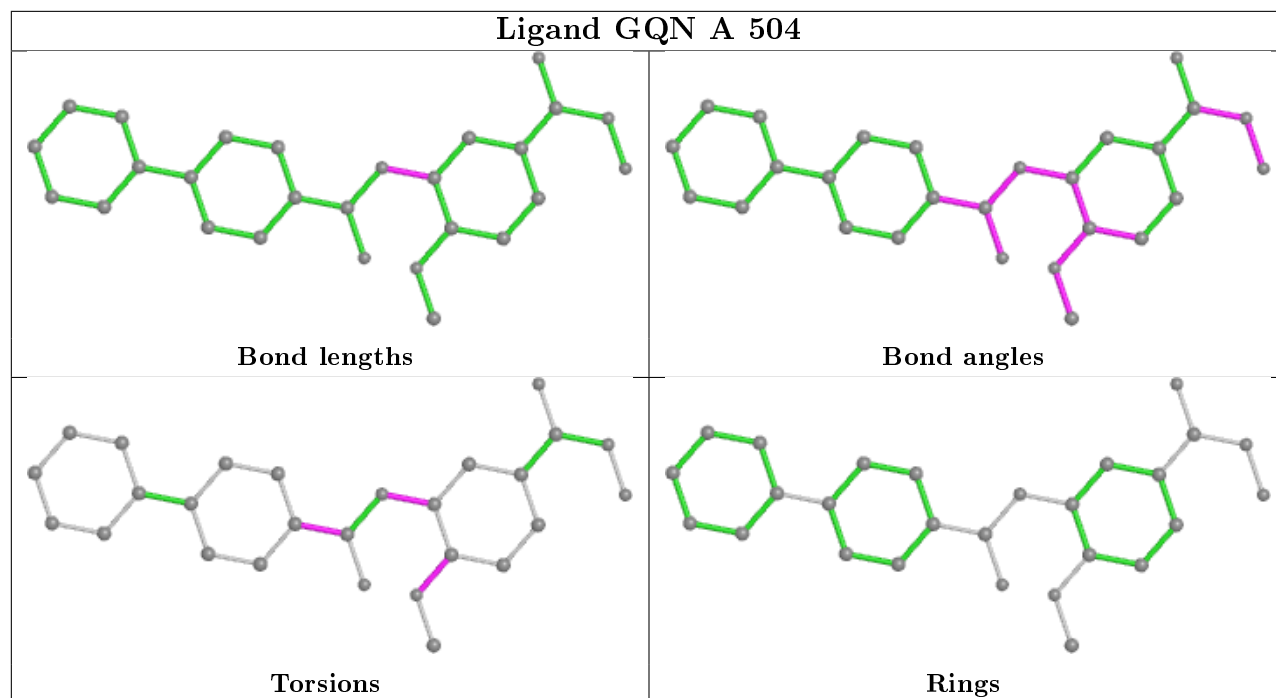
Mol	Chain	Res	Type	Atoms
5	A	505	GOL	C1-C2-C3-O3
5	C	505	GOL	O1-C1-C2-C3
5	C	505	GOL	C1-C2-C3-O3
5	A	508	GOL	C1-C2-C3-O3
5	B	509	GOL	O1-C1-C2-C3

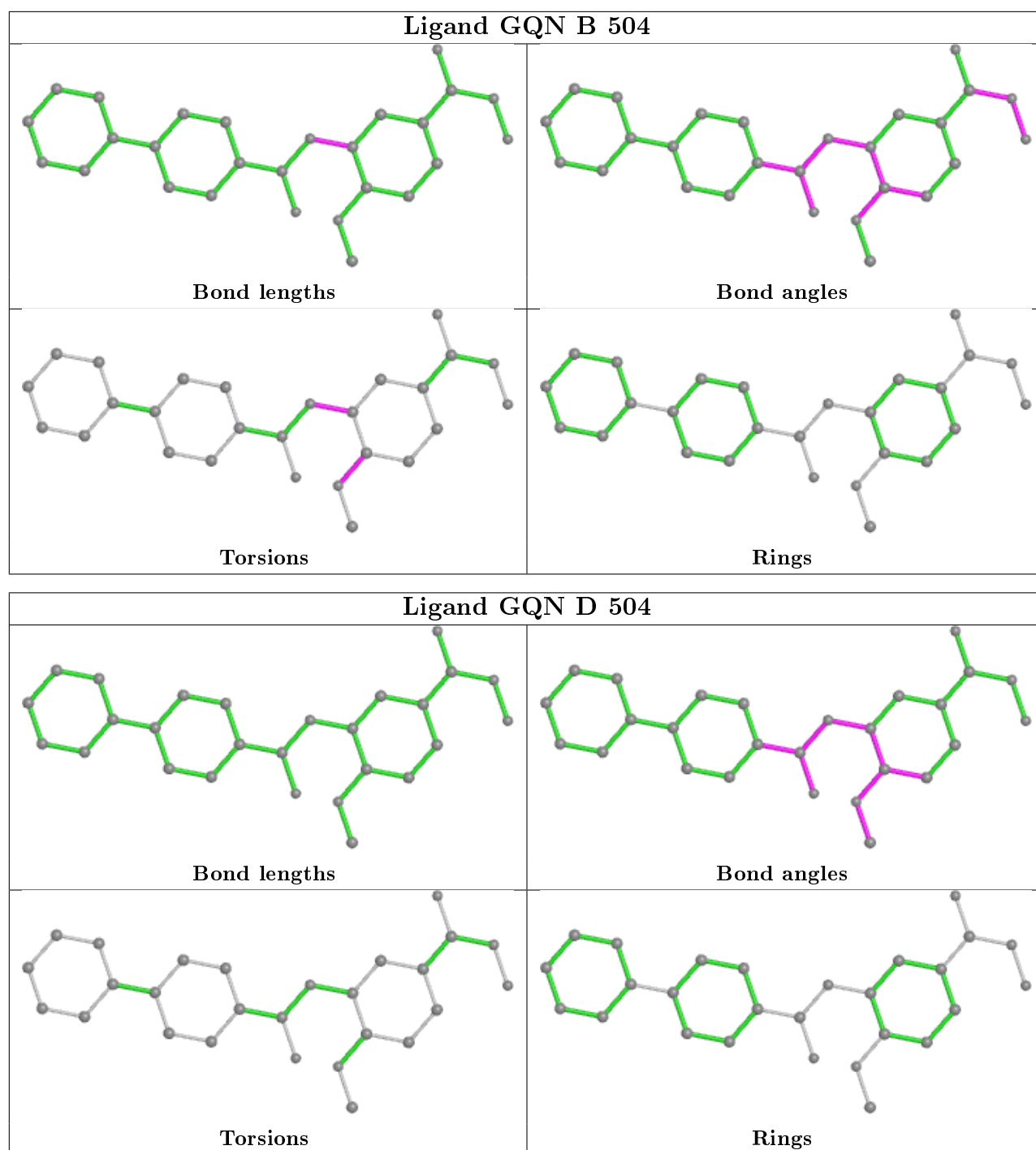
There are no ring outliers.

19 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	517	DMF	2	0
5	B	507	GOL	3	0
5	A	505	GOL	3	0
5	C	505	GOL	1	0
5	B	505	GOL	1	0
6	B	511	DMF	1	0
4	A	504	GQN	1	0
5	B	509	GOL	1	0
5	A	508	GOL	1	0
6	C	511	DMF	1	0
6	C	507	DMF	2	0
6	C	509	DMF	2	0
5	C	506	GOL	6	0
5	B	506	GOL	7	0
4	D	504	GQN	1	0
5	A	506	GOL	2	0
6	D	508	DMF	1	0
6	D	506	DMF	1	0
6	D	507	DMF	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.





## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	386/447 (86%)	-0.30	4 (1%) 82 87	9, 20, 46, 88	0
1	B	410/447 (91%)	-0.38	3 (0%) 87 92	7, 18, 42, 73	0
1	C	407/447 (91%)	-0.39	3 (0%) 87 92	7, 18, 43, 81	0
1	D	384/447 (85%)	-0.37	2 (0%) 91 94	7, 19, 44, 80	0
All	All	1587/1788 (88%)	-0.36	12 (0%) 86 90	7, 19, 44, 88	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	230	LEU	4.4
1	B	168	THR	3.6
1	C	224	MET	3.3
1	B	232	ILE	3.1
1	C	425	ILE	2.8

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	GQN	A	504	27/27	0.83	0.25	34,65,75,76	0
5	GOL	B	510	6/6	0.87	0.23	46,50,53,59	0
6	DMF	B	516	5/5	0.87	0.19	23,25,38,42	0
4	GQN	D	504	27/27	0.87	0.27	33,63,72,74	0
4	GQN	C	504	27/27	0.88	0.27	29,63,87,90	0
5	GOL	A	506	6/6	0.88	0.16	22,39,41,43	0
6	DMF	C	510	5/5	0.89	0.21	38,45,48,51	0
5	GOL	C	505	6/6	0.90	0.15	26,41,43,44	0
5	GOL	B	506	6/6	0.90	0.30	30,38,42,42	0
6	DMF	D	509	5/5	0.90	0.17	46,52,58,61	0
6	DMF	C	511	5/5	0.91	0.20	54,55,56,57	0
6	DMF	B	515	5/5	0.91	0.13	31,42,49,52	0
5	GOL	B	509	6/6	0.91	0.22	28,39,49,56	0
4	GQN	B	504	27/27	0.92	0.17	15,54,66,72	0
6	DMF	B	514	5/5	0.93	0.13	51,52,54,55	0
6	DMF	B	518	5/5	0.94	0.16	26,31,35,41	0
5	GOL	B	505	6/6	0.94	0.17	40,45,49,58	0
5	GOL	A	508	6/6	0.95	0.17	40,41,43,44	0
5	GOL	C	506	6/6	0.95	0.14	8,21,31,34	0
6	DMF	D	506	5/5	0.95	0.12	35,36,41,45	0
6	DMF	C	507	5/5	0.95	0.13	22,25,30,47	0
6	DMF	B	519	5/5	0.96	0.16	27,42,48,48	0
5	GOL	B	508	6/6	0.96	0.07	14,24,27,33	0
6	DMF	C	509	5/5	0.96	0.09	24,29,43,49	0
5	GOL	A	507	6/6	0.96	0.13	17,25,28,29	0
6	DMF	A	509	5/5	0.96	0.10	26,28,42,49	0
5	GOL	D	505	6/6	0.96	0.13	18,27,34,40	0
6	DMF	C	508	5/5	0.97	0.10	23,26,33,33	0
5	GOL	A	505	6/6	0.97	0.11	25,26,32,45	0
6	DMF	D	508	5/5	0.97	0.11	19,23,32,35	0
6	DMF	B	512	5/5	0.97	0.09	24,28,30,39	0
6	DMF	B	511	5/5	0.97	0.13	31,32,37,43	0
6	DMF	D	507	5/5	0.97	0.12	26,35,37,44	0
5	GOL	B	507	6/6	0.97	0.13	21,24,32,33	0
6	DMF	B	513	5/5	0.98	0.07	27,30,31,37	0
6	DMF	B	517	5/5	0.98	0.12	31,33,39,46	0
3	K	D	502	1/1	1.00	0.08	13,13,13,13	0
3	K	C	502	1/1	1.00	0.08	10,10,10,10	0
2	ZN	B	501	1/1	1.00	0.04	24,24,24,24	0
3	K	C	503	1/1	1.00	0.07	18,18,18,18	0
3	K	B	502	1/1	1.00	0.10	11,11,11,11	0
3	K	A	502	1/1	1.00	0.07	12,12,12,12	0
2	ZN	C	501	1/1	1.00	0.03	25,25,25,25	0

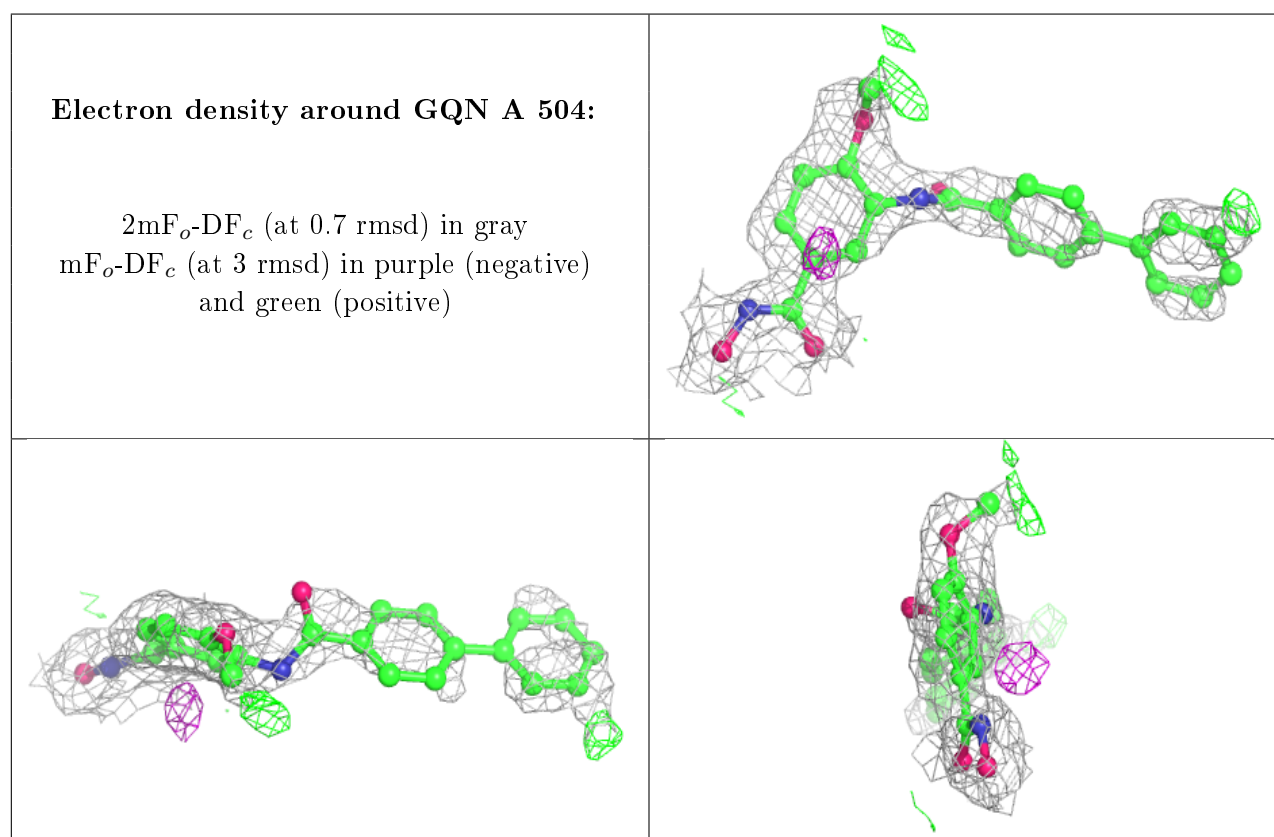
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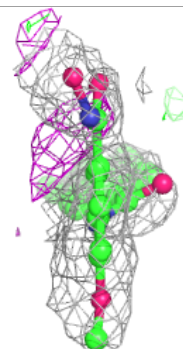
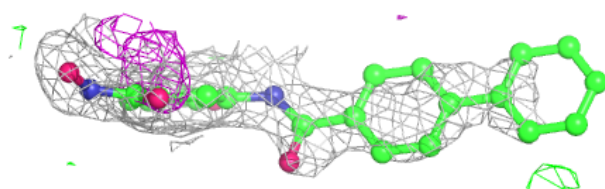
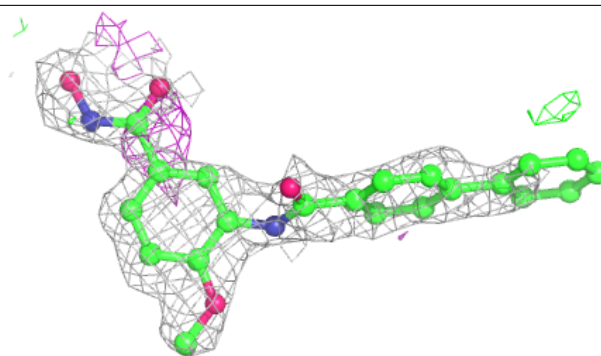
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	K	B	503	1/1	1.00	0.07	18,18,18,18	0
2	ZN	A	501	1/1	1.00	0.05	24,24,24,24	0
3	K	A	503	1/1	1.00	0.09	16,16,16,16	0
3	K	D	503	1/1	1.00	0.08	18,18,18,18	0
2	ZN	D	501	1/1	1.00	0.04	24,24,24,24	0

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.

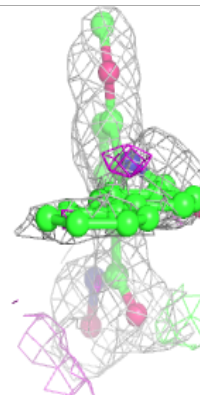
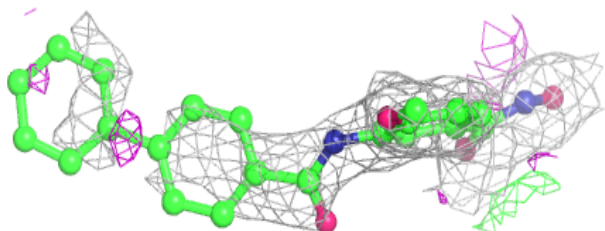
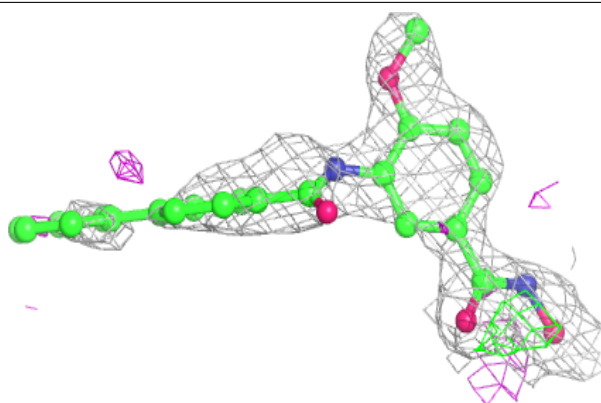


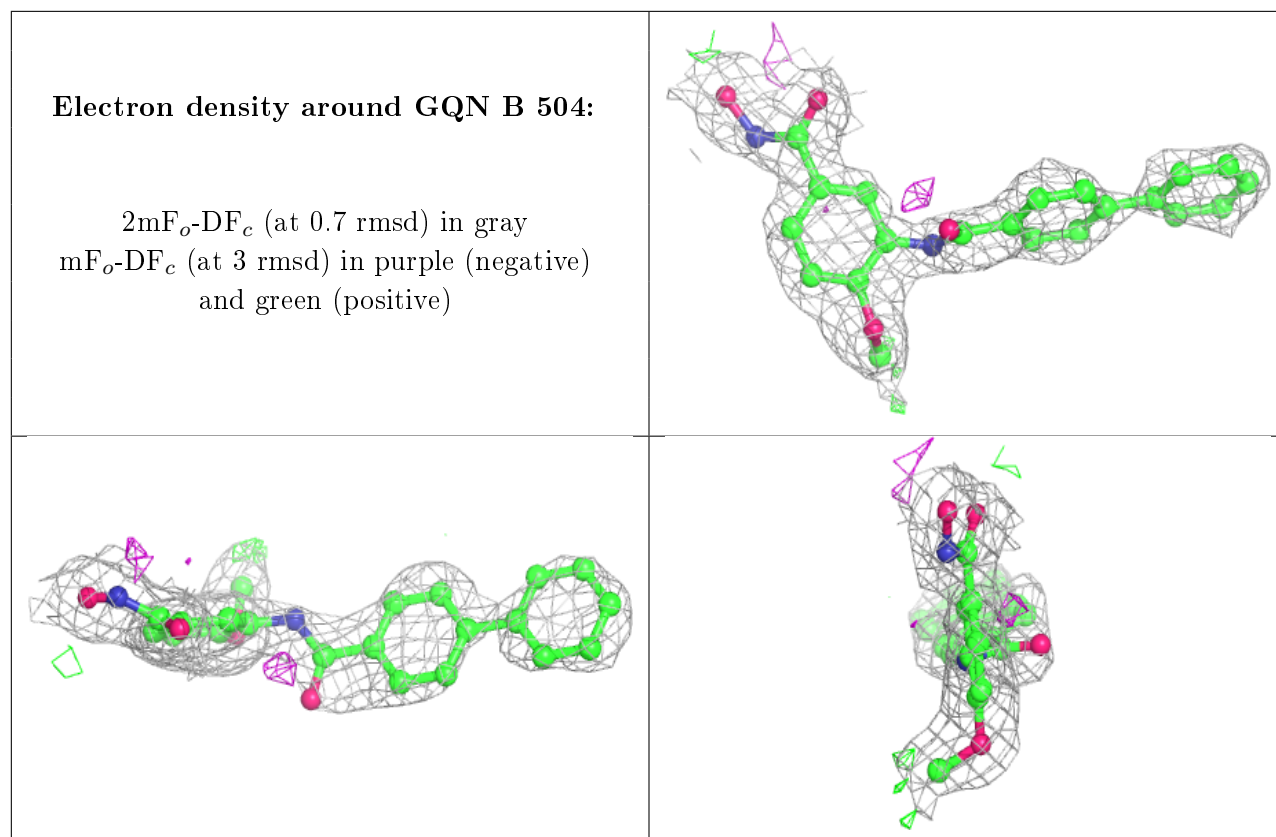
**Electron density around GQN D 504:**

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

**Electron density around GQN C 504:**

$2mF_o-DF_c$  (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.