



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 14, 2024 – 10:55 am GMT

PDB ID : 6RLW  
Title : Structure of the human 8-oxoguanine DNA Glycosylase hOGG1 in complex with inhibitor TH5487  
Authors : Masuyer, G.; Stenmark, P.  
Deposited on : 2019-05-03  
Resolution : 2.00 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.

The types of validation reports are described at

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

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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 : 1.8.4, 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

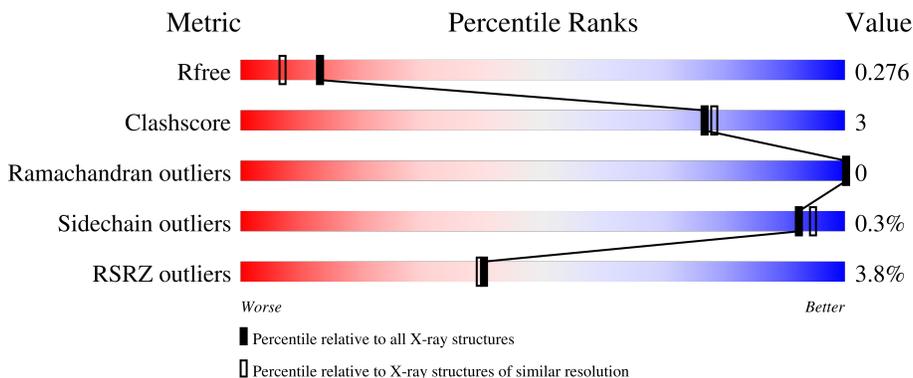
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	AAA	337	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 0%, orange 1%, yellow 2, green 84%, grey 93%);"></div> <div style="margin-left: 10px;"> <p>84%</p> <p>9%</p> <p>7%</p> </div> </div>
1	BBB	337	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 0%, orange 3%, yellow 3, green 85%, grey 92%);"></div> <div style="margin-left: 10px;"> <p>85%</p> <p>7%</p> <p>8%</p> </div> </div>
1	CCC	337	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 0%, orange 3%, yellow 3, green 84%, grey 90%);"></div> <div style="margin-left: 10px;"> <p>84%</p> <p>6%</p> <p>10%</p> </div> </div>
1	DDD	337	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 0%, orange 7%, yellow 7, green 84%, grey 91%);"></div> <div style="margin-left: 10px;"> <p>84%</p> <p>7%</p> <p>10%</p> </div> </div>
1	EEE	337	<div style="display: flex; align-items: center;"> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 0%, orange 3%, yellow 3, green 85%, grey 92%);"></div> <div style="margin-left: 10px;"> <p>85%</p> <p>7%</p> <p>7%</p> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13184 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 N-glycosylase/DNA lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	314	Total 2496	C 1583	N 451	O 450	S 12	0	0	0
1	BBB	310	Total 2463	C 1564	N 443	O 444	S 12	0	0	0
1	CCC	303	Total 2415	C 1537	N 432	O 434	S 12	0	0	0
1	DDD	304	Total 2413	C 1534	N 432	O 435	S 12	0	0	0
1	EEE	312	Total 2491	C 1580	N 450	O 449	S 12	0	1	0

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-9	MET	-	initiating methionine	UNP O15527
AAA	-8	GLY	-	expression tag	UNP O15527
AAA	-7	SER	-	expression tag	UNP O15527
AAA	-6	SER	-	expression tag	UNP O15527
AAA	-5	HIS	-	expression tag	UNP O15527
AAA	-4	HIS	-	expression tag	UNP O15527
AAA	-3	HIS	-	expression tag	UNP O15527
AAA	-2	HIS	-	expression tag	UNP O15527
AAA	-1	HIS	-	expression tag	UNP O15527
AAA	0	HIS	-	expression tag	UNP O15527
AAA	1	SER	-	expression tag	UNP O15527
AAA	2	SER	-	expression tag	UNP O15527
AAA	3	GLY	-	expression tag	UNP O15527
AAA	4	LEU	-	expression tag	UNP O15527
AAA	5	VAL	-	expression tag	UNP O15527
AAA	6	PRO	-	expression tag	UNP O15527
AAA	7	ARG	-	expression tag	UNP O15527
AAA	8	GLY	-	expression tag	UNP O15527
AAA	9	SER	-	expression tag	UNP O15527

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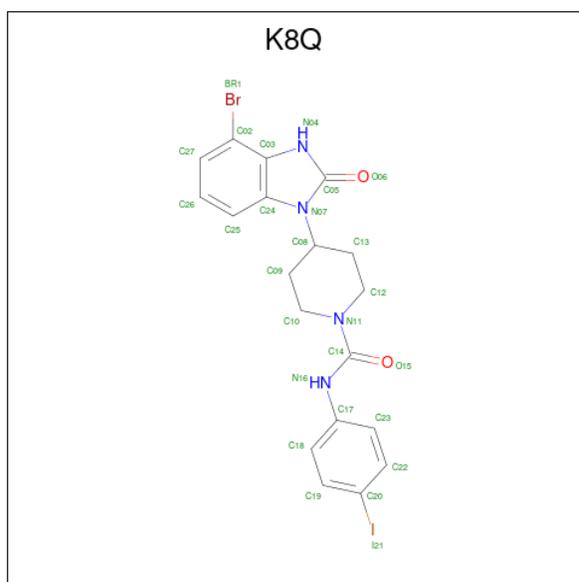
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	10	HIS	-	expression tag	UNP O15527
BBB	-9	MET	-	initiating methionine	UNP O15527
BBB	-8	GLY	-	expression tag	UNP O15527
BBB	-7	SER	-	expression tag	UNP O15527
BBB	-6	SER	-	expression tag	UNP O15527
BBB	-5	HIS	-	expression tag	UNP O15527
BBB	-4	HIS	-	expression tag	UNP O15527
BBB	-3	HIS	-	expression tag	UNP O15527
BBB	-2	HIS	-	expression tag	UNP O15527
BBB	-1	HIS	-	expression tag	UNP O15527
BBB	0	HIS	-	expression tag	UNP O15527
BBB	1	SER	-	expression tag	UNP O15527
BBB	2	SER	-	expression tag	UNP O15527
BBB	3	GLY	-	expression tag	UNP O15527
BBB	4	LEU	-	expression tag	UNP O15527
BBB	5	VAL	-	expression tag	UNP O15527
BBB	6	PRO	-	expression tag	UNP O15527
BBB	7	ARG	-	expression tag	UNP O15527
BBB	8	GLY	-	expression tag	UNP O15527
BBB	9	SER	-	expression tag	UNP O15527
BBB	10	HIS	-	expression tag	UNP O15527
CCC	-9	MET	-	initiating methionine	UNP O15527
CCC	-8	GLY	-	expression tag	UNP O15527
CCC	-7	SER	-	expression tag	UNP O15527
CCC	-6	SER	-	expression tag	UNP O15527
CCC	-5	HIS	-	expression tag	UNP O15527
CCC	-4	HIS	-	expression tag	UNP O15527
CCC	-3	HIS	-	expression tag	UNP O15527
CCC	-2	HIS	-	expression tag	UNP O15527
CCC	-1	HIS	-	expression tag	UNP O15527
CCC	0	HIS	-	expression tag	UNP O15527
CCC	1	SER	-	expression tag	UNP O15527
CCC	2	SER	-	expression tag	UNP O15527
CCC	3	GLY	-	expression tag	UNP O15527
CCC	4	LEU	-	expression tag	UNP O15527
CCC	5	VAL	-	expression tag	UNP O15527
CCC	6	PRO	-	expression tag	UNP O15527
CCC	7	ARG	-	expression tag	UNP O15527
CCC	8	GLY	-	expression tag	UNP O15527
CCC	9	SER	-	expression tag	UNP O15527
CCC	10	HIS	-	expression tag	UNP O15527
DDD	-9	MET	-	initiating methionine	UNP O15527

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	-8	GLY	-	expression tag	UNP O15527
DDD	-7	SER	-	expression tag	UNP O15527
DDD	-6	SER	-	expression tag	UNP O15527
DDD	-5	HIS	-	expression tag	UNP O15527
DDD	-4	HIS	-	expression tag	UNP O15527
DDD	-3	HIS	-	expression tag	UNP O15527
DDD	-2	HIS	-	expression tag	UNP O15527
DDD	-1	HIS	-	expression tag	UNP O15527
DDD	0	HIS	-	expression tag	UNP O15527
DDD	1	SER	-	expression tag	UNP O15527
DDD	2	SER	-	expression tag	UNP O15527
DDD	3	GLY	-	expression tag	UNP O15527
DDD	4	LEU	-	expression tag	UNP O15527
DDD	5	VAL	-	expression tag	UNP O15527
DDD	6	PRO	-	expression tag	UNP O15527
DDD	7	ARG	-	expression tag	UNP O15527
DDD	8	GLY	-	expression tag	UNP O15527
DDD	9	SER	-	expression tag	UNP O15527
DDD	10	HIS	-	expression tag	UNP O15527
EEE	-9	MET	-	initiating methionine	UNP O15527
EEE	-8	GLY	-	expression tag	UNP O15527
EEE	-7	SER	-	expression tag	UNP O15527
EEE	-6	SER	-	expression tag	UNP O15527
EEE	-5	HIS	-	expression tag	UNP O15527
EEE	-4	HIS	-	expression tag	UNP O15527
EEE	-3	HIS	-	expression tag	UNP O15527
EEE	-2	HIS	-	expression tag	UNP O15527
EEE	-1	HIS	-	expression tag	UNP O15527
EEE	0	HIS	-	expression tag	UNP O15527
EEE	1	SER	-	expression tag	UNP O15527
EEE	2	SER	-	expression tag	UNP O15527
EEE	3	GLY	-	expression tag	UNP O15527
EEE	4	LEU	-	expression tag	UNP O15527
EEE	5	VAL	-	expression tag	UNP O15527
EEE	6	PRO	-	expression tag	UNP O15527
EEE	7	ARG	-	expression tag	UNP O15527
EEE	8	GLY	-	expression tag	UNP O15527
EEE	9	SER	-	expression tag	UNP O15527
EEE	10	HIS	-	expression tag	UNP O15527

- Molecule 2 is 4-(4-bromanyl-2-oxidanylidene-3 {H}-benzimidazol-1-yl)- {N}-(4-iodophenyl) piperidine-1-carboxamide (three-letter code: K8Q) (formula: C<sub>19</sub>H<sub>18</sub>BrIN<sub>4</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	Br	C	I	N			O
2	AAA	1	27	1	19	1	4	2	0	0
2	BBB	1	27	1	19	1	4	2	0	0
2	CCC	1	27	1	19	1	4	2	0	0
2	DDD	1	27	1	19	1	4	2	0	0
2	EEE	1	27	1	19	1	4	2	0	0

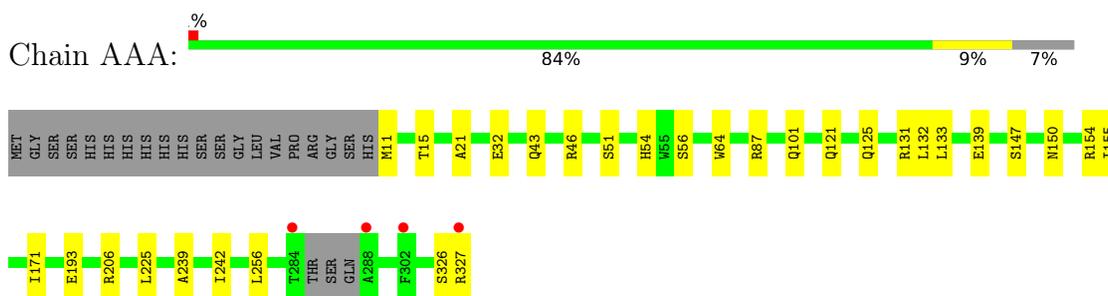
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	AAA	205	205	205	0	0
3	BBB	189	189	189	0	0
3	CCC	141	141	141	0	0
3	DDD	92	92	92	0	0
3	EEE	144	144	144	0	0

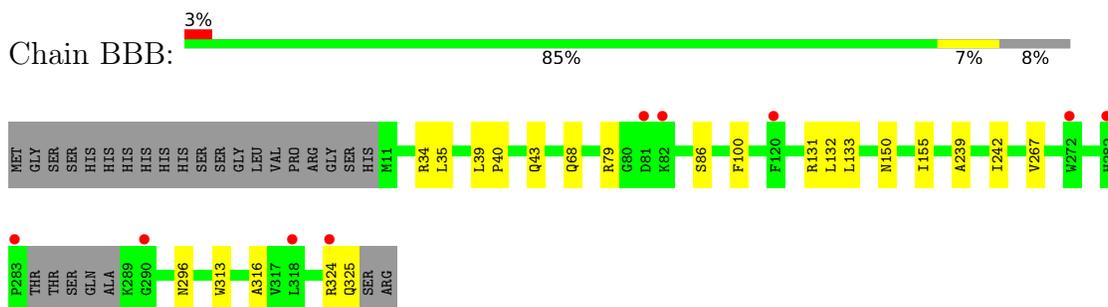
### 3 Residue-property plots [i](#)

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.

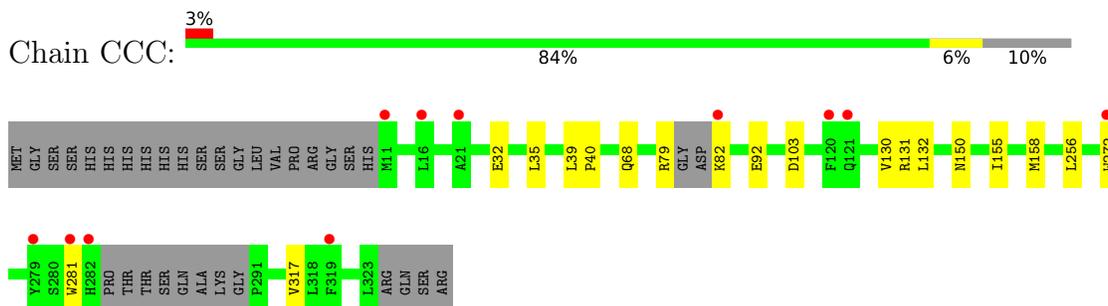
- Molecule 1: N-glycosylase/DNA lyase



- Molecule 1: N-glycosylase/DNA lyase

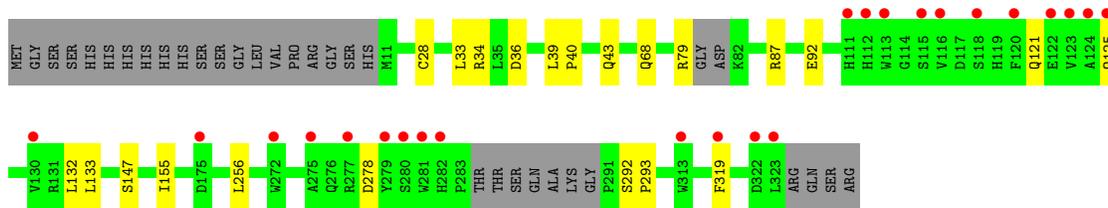


- Molecule 1: N-glycosylase/DNA lyase

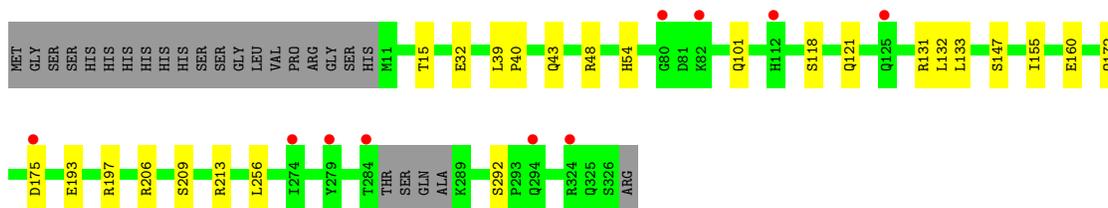
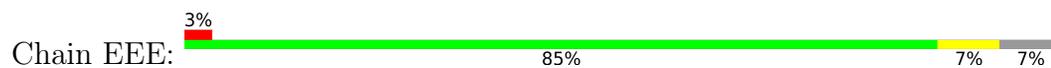


- Molecule 1: N-glycosylase/DNA lyase





• Molecule 1: N-glycosylase/DNA lyase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.37Å 86.37Å 432.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.84 – 2.00 84.69 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (84.84-2.00) 99.9 (84.69-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.93 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.223 , 0.274 0.230 , 0.276	Depositor DCC
$R_{free}$ test set	5560 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.3	Xtrriage
Anisotropy	0.242	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13184	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 65.98 % 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 6.5034e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: K8Q

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	AAA	0.64	0/2564	0.75	0/3486
1	BBB	0.64	0/2531	0.72	0/3443
1	CCC	0.65	0/2481	0.72	0/3373
1	DDD	0.65	0/2478	0.73	0/3369
1	EEE	0.64	0/2559	0.74	0/3479
All	All	0.64	0/12613	0.73	0/17150

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2496	0	2437	19	0
1	BBB	2463	0	2396	14	0
1	CCC	2415	0	2356	12	0
1	DDD	2413	0	2355	13	0
1	EEE	2491	0	2431	15	0
2	AAA	27	0	0	0	0
2	BBB	27	0	0	0	0
2	CCC	27	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	DDD	27	0	0	0	0
2	EEE	27	0	0	0	0
3	AAA	205	0	0	0	0
3	BBB	189	0	0	0	0
3	CCC	141	0	0	1	0
3	DDD	92	0	0	1	0
3	EEE	144	0	0	1	0
All	All	13184	0	11975	73	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.

The worst 5 of 73 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:BBB:100:PHE:O	1:BBB:131:ARG:HD3	1.80	0.81
1:BBB:43:GLN:HE22	1:BBB:133:LEU:H	1.28	0.79
1:AAA:43:GLN:HE22	1:AAA:133:LEU:H	1.37	0.72
1:EEE:43:GLN:HE22	1:EEE:133:LEU:H	1.39	0.69
1:EEE:132:LEU:HD21	1:EEE:256:LEU:HG	1.76	0.68

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	AAA	310/337 (92%)	297 (96%)	13 (4%)	0	100   100
1	BBB	306/337 (91%)	294 (96%)	12 (4%)	0	100   100
1	CCC	297/337 (88%)	289 (97%)	8 (3%)	0	100   100
1	DDD	298/337 (88%)	283 (95%)	15 (5%)	0	100   100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EEE	309/337 (92%)	293 (95%)	16 (5%)	0	100	100
All	All	1520/1685 (90%)	1456 (96%)	64 (4%)	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	AAA	264/284 (93%)	263 (100%)	1 (0%)	91	93
1	BBB	260/284 (92%)	260 (100%)	0	100	100
1	CCC	256/284 (90%)	256 (100%)	0	100	100
1	DDD	256/284 (90%)	254 (99%)	2 (1%)	81	86
1	EEE	264/284 (93%)	263 (100%)	1 (0%)	91	93
All	All	1300/1420 (92%)	1296 (100%)	4 (0%)	92	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	51	SER
1	DDD	278	ASP
1	DDD	319	PHE
1	EEE	292	SER

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](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	K8Q	EEE	401	-	30,30,30	0.67	1 (3%)	43,43,43	0.68	2 (4%)
2	K8Q	AAA	401	-	30,30,30	0.66	1 (3%)	43,43,43	0.68	1 (2%)
2	K8Q	BBB	401	-	30,30,30	0.72	1 (3%)	43,43,43	0.71	2 (4%)
2	K8Q	CCC	401	-	30,30,30	0.64	1 (3%)	43,43,43	0.65	1 (2%)
2	K8Q	DDD	401	-	30,30,30	0.66	1 (3%)	43,43,43	0.66	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	K8Q	EEE	401	-	-	2/12/22/22	0/4/4/4
2	K8Q	AAA	401	-	-	2/12/22/22	0/4/4/4
2	K8Q	BBB	401	-	-	0/12/22/22	0/4/4/4
2	K8Q	CCC	401	-	-	1/12/22/22	0/4/4/4
2	K8Q	DDD	401	-	-	0/12/22/22	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	401	K8Q	C03-C24	-3.19	1.36	1.46
2	BBB	401	K8Q	C03-C24	-3.19	1.36	1.46
2	EEE	401	K8Q	C03-C24	-3.08	1.36	1.46
2	CCC	401	K8Q	C03-C24	-3.05	1.36	1.46
2	AAA	401	K8Q	C03-C24	-2.87	1.37	1.46

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	401	K8Q	C24-C03-N04	2.44	109.30	106.48
2	BBB	401	K8Q	C24-C03-N04	2.30	109.14	106.48
2	DDD	401	K8Q	C24-C03-N04	2.23	109.06	106.48
2	EEE	401	K8Q	C10-N11-C14	-2.19	113.88	121.94
2	BBB	401	K8Q	C24-N07-C05	-2.19	107.66	109.25

There are no chirality outliers.

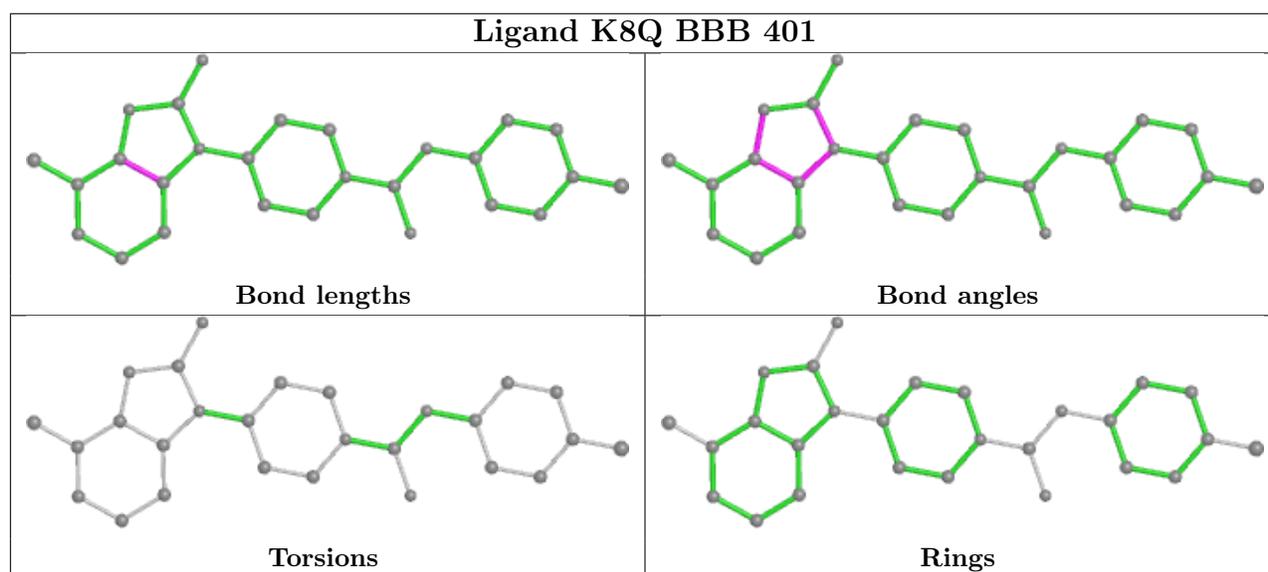
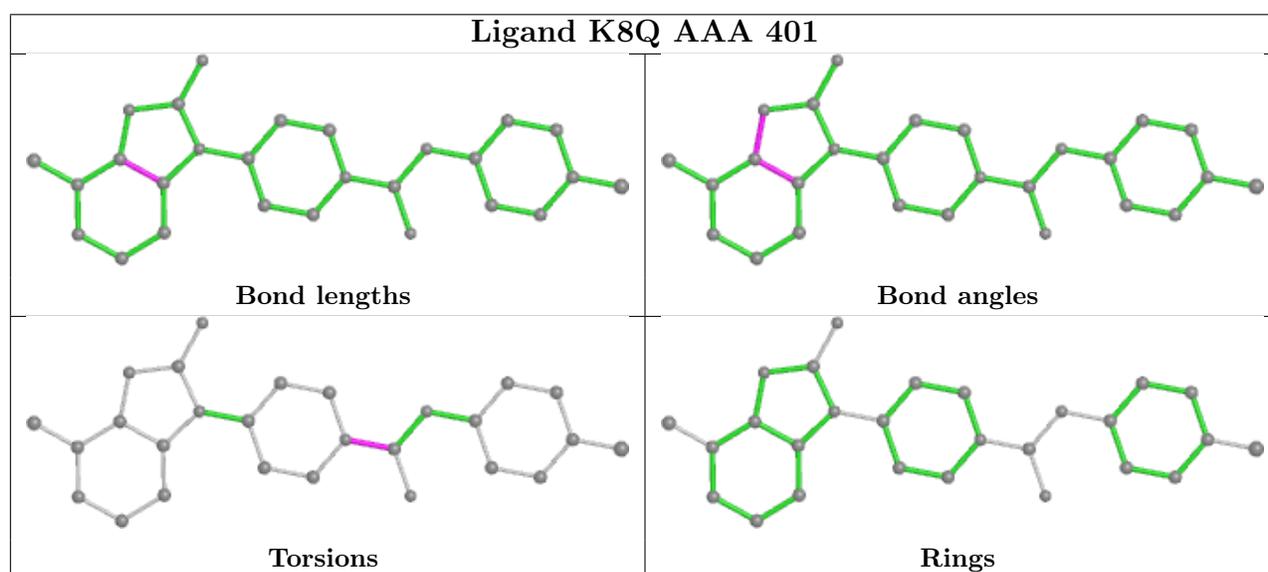
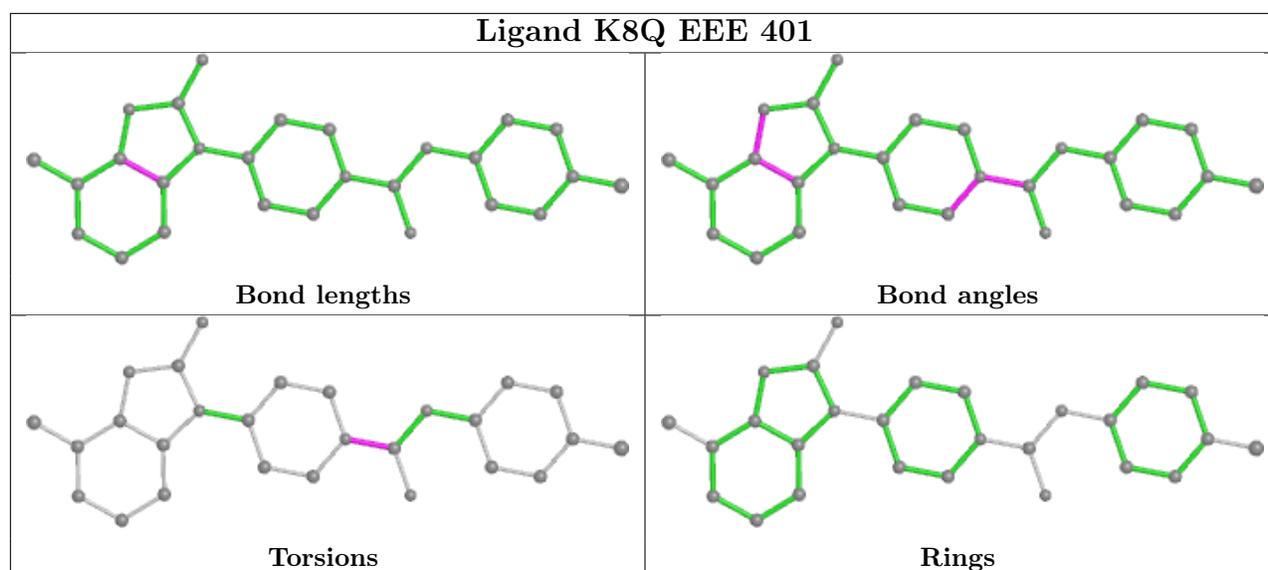
All (5) torsion outliers are listed below:

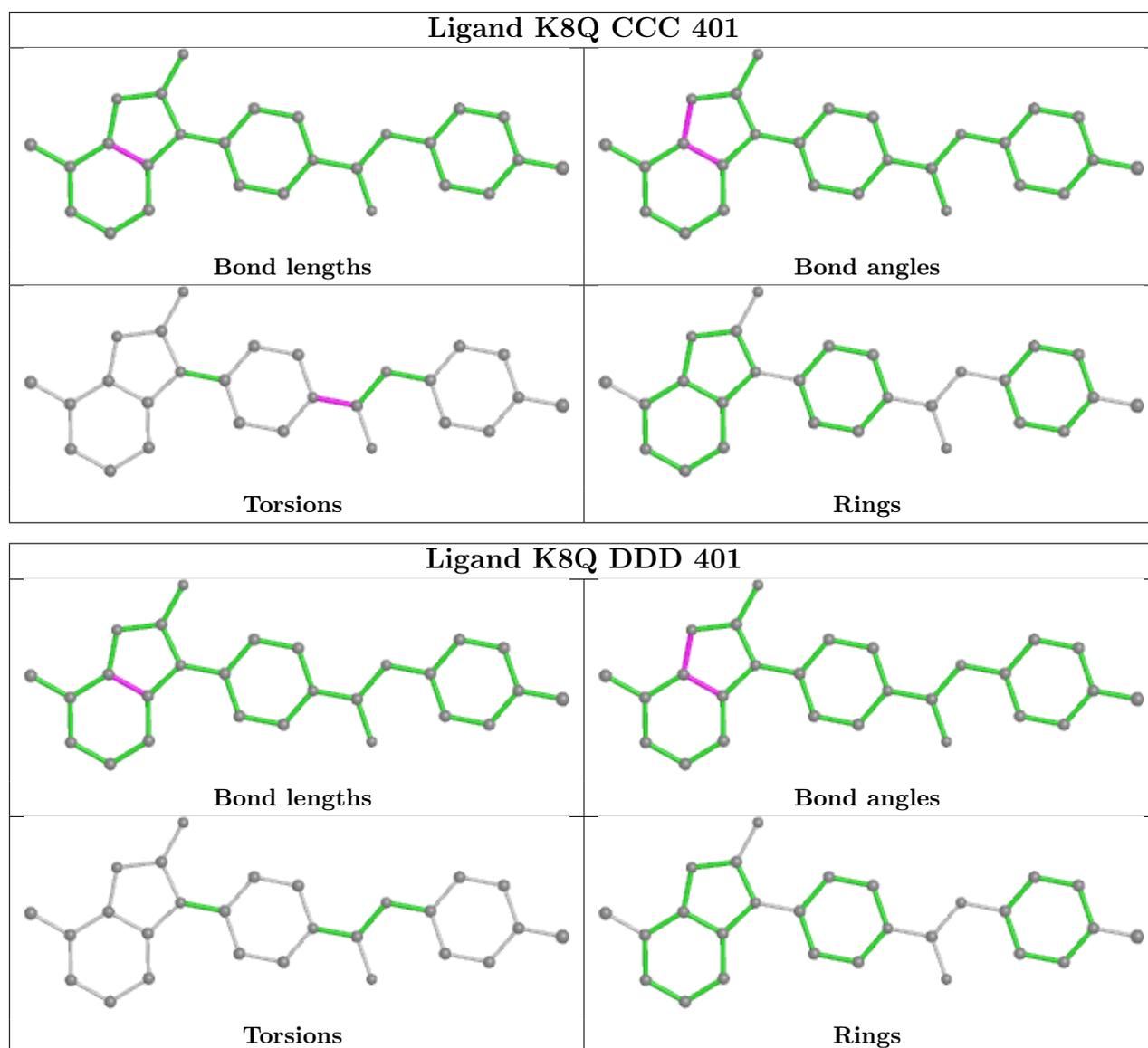
Mol	Chain	Res	Type	Atoms
2	EEE	401	K8Q	O15-C14-N11-C12
2	AAA	401	K8Q	O15-C14-N11-C12
2	EEE	401	K8Q	N16-C14-N11-C12
2	AAA	401	K8Q	N16-C14-N11-C12
2	CCC	401	K8Q	N16-C14-N11-C12

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 [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	AAA	314/337 (93%)	0.09	4 (1%) 77 76	22, 35, 58, 100	0
1	BBB	310/337 (91%)	0.15	9 (2%) 51 50	23, 35, 66, 104	0
1	CCC	303/337 (89%)	0.18	11 (3%) 42 42	25, 44, 72, 110	0
1	DDD	304/337 (90%)	0.45	24 (7%) 12 11	31, 49, 88, 111	0
1	EEE	312/337 (92%)	0.21	10 (3%) 47 46	26, 42, 71, 100	0
All	All	1543/1685 (91%)	0.22	58 (3%) 40 39	22, 41, 76, 111	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	290	GLY	7.7
1	DDD	277	ARG	7.5
1	BBB	272	TRP	6.4
1	AAA	327	ARG	5.6
1	AAA	288	ALA	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.

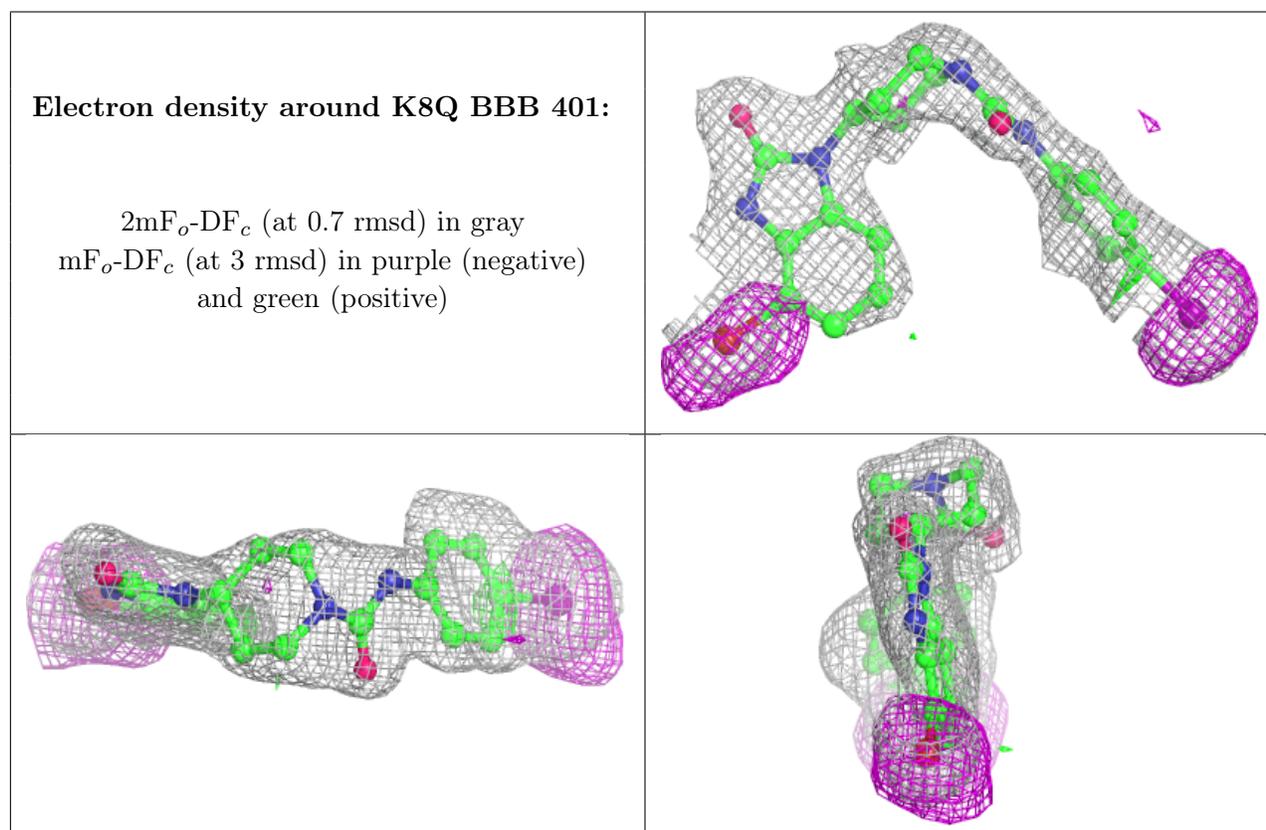
### 6.4 Ligands [i](#)

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, 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.

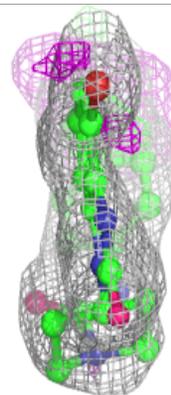
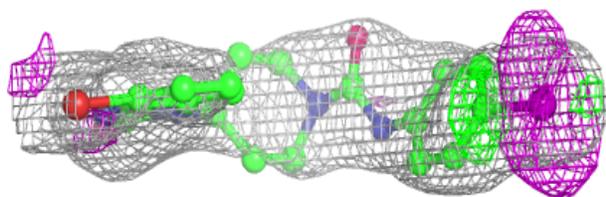
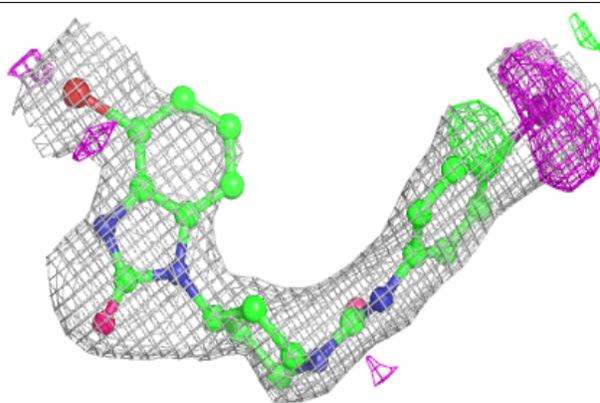
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	K8Q	BBB	401	27/27	0.94	0.17	38,50,61,78	0
2	K8Q	DDD	401	27/27	0.95	0.18	45,61,93,117	0
2	K8Q	CCC	401	27/27	0.96	0.16	55,68,77,96	0
2	K8Q	EEE	401	27/27	0.97	0.12	34,43,55,75	0
2	K8Q	AAA	401	27/27	0.99	0.09	27,31,33,49	0

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.

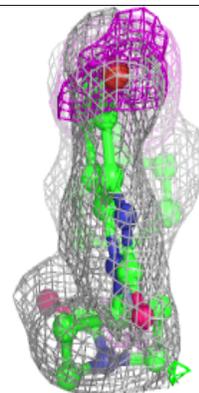
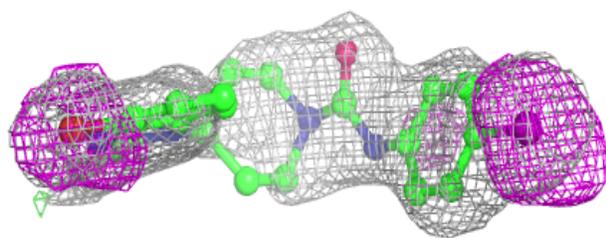
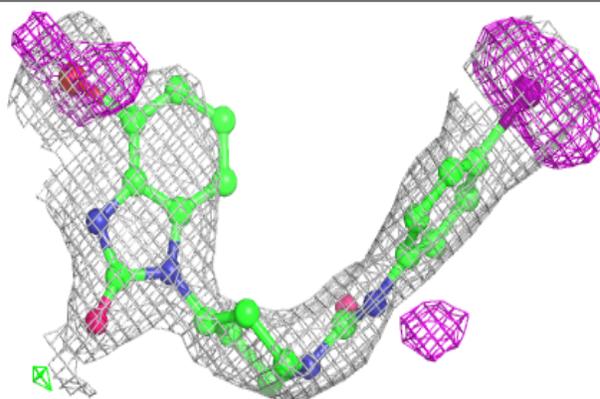


**Electron density around K8Q DDD 401:**

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

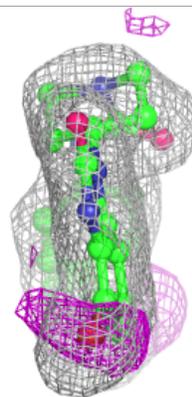
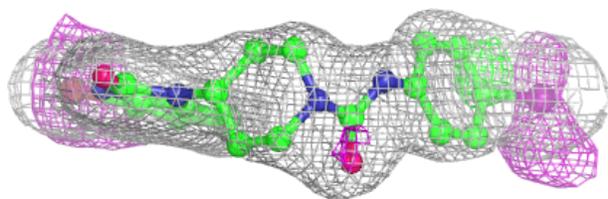
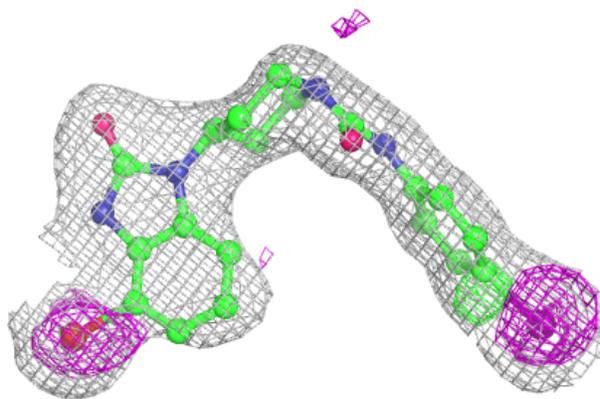
**Electron density around K8Q CCC 401:**

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

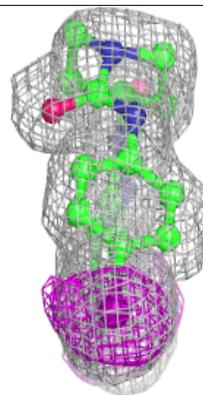
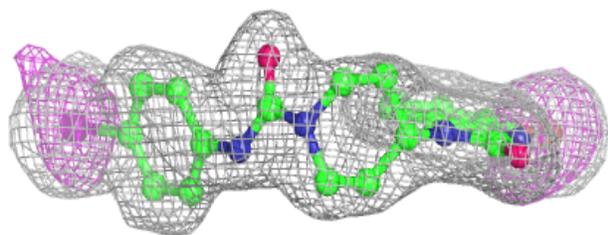
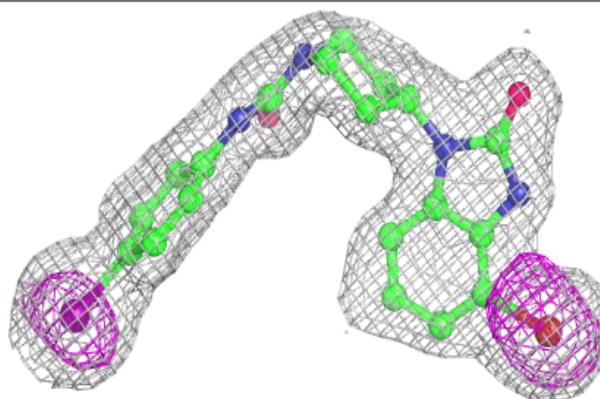


**Electron density around K8Q EEE 401:**

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

**Electron density around K8Q AAA 401:**

$2mF_o-DF_c$  (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.