



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:33 PM EDT

PDB ID : 6RLW / pdb_00006rlw
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 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

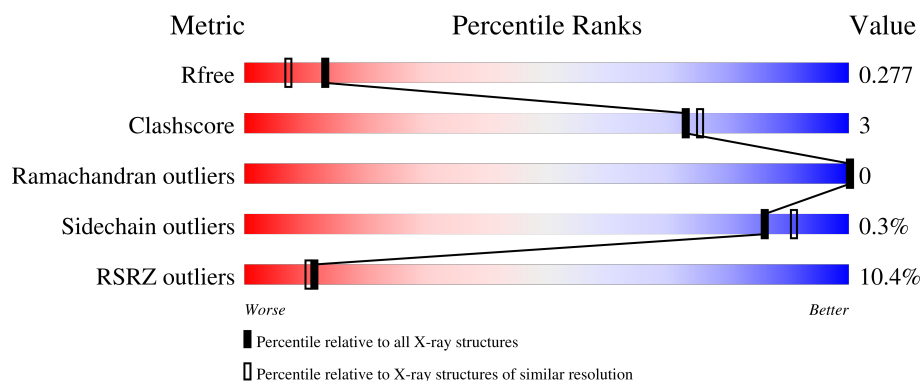
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 ≥ 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	4% 83% 10% 7%
1	BBB	337	8% 85% 7% 8%
1	CCC	337	10% 84% 6% 10%
1	DDD	337	18% 84% 7% 10%
1	EEE	337	7% 85% 7% 7%

2 Entry composition

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

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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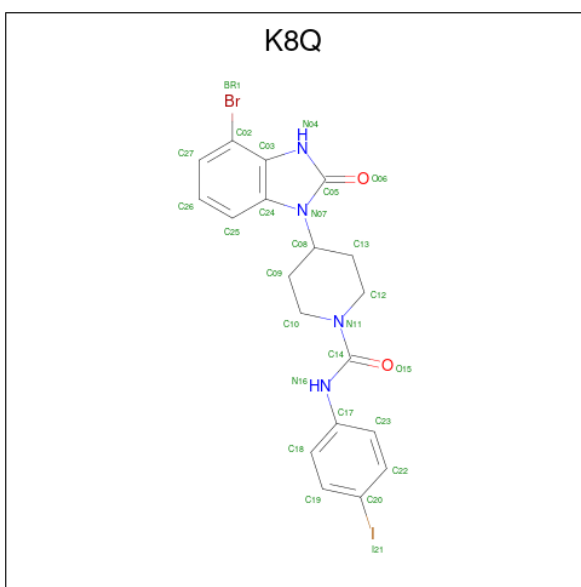
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	10	HIS	-	expression tag	UNP O15527
BBB	-9	MET	-	initiating methionine	UNP O15527
BBB	-8	GLY	-	expression tag	UNP O15527
BBB	-7	SER	-	expression tag	UNP O15527
BBB	-6	SER	-	expression tag	UNP O15527
BBB	-5	HIS	-	expression tag	UNP O15527
BBB	-4	HIS	-	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 (CCD ID: K8Q) (formula: C₁₉H₁₈BrIN₄O₂) (labeled as "Ligand of Interest" by depositor).



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

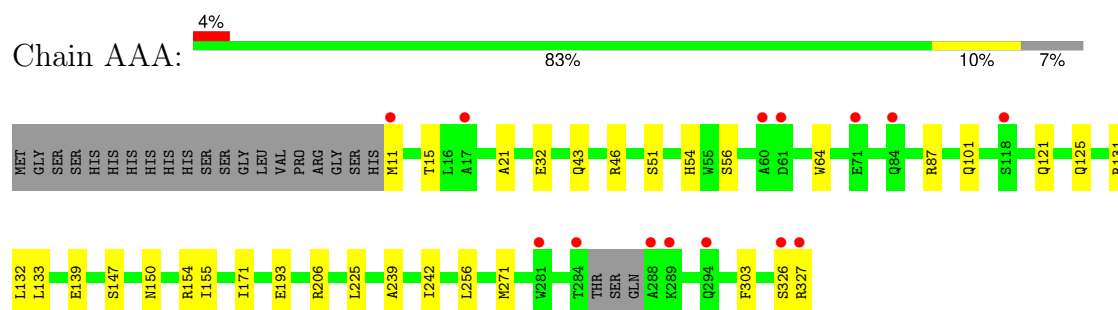
- Molecule 3 is water.

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

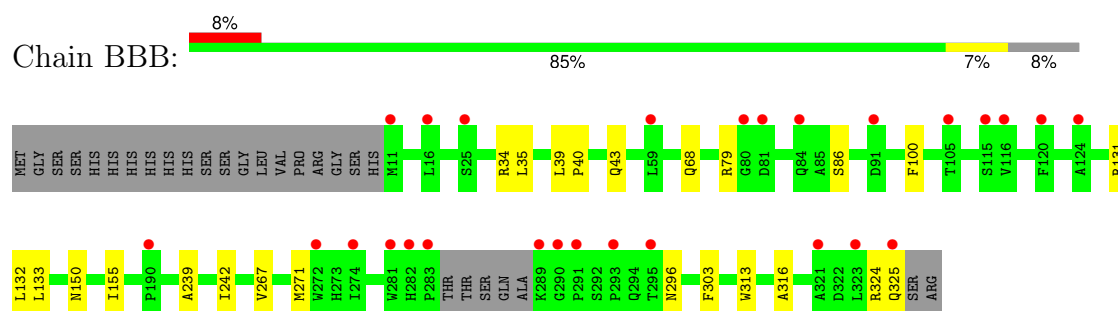
3 Residue-property plots [i](#)

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.

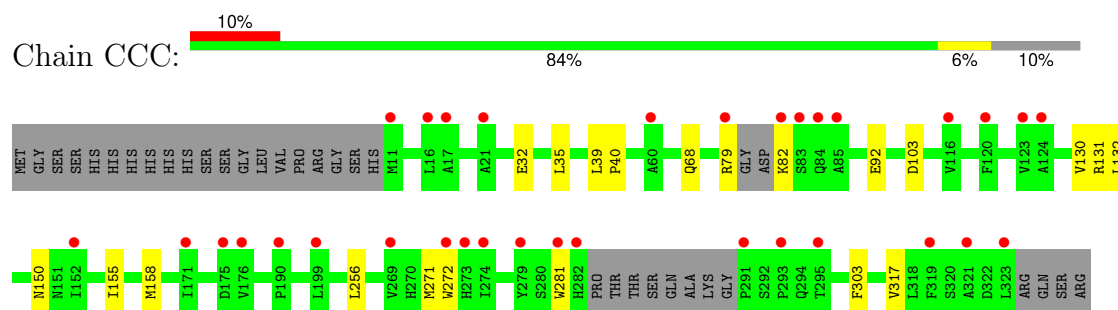
- Molecule 1: N-glycosylase/DNA lyase



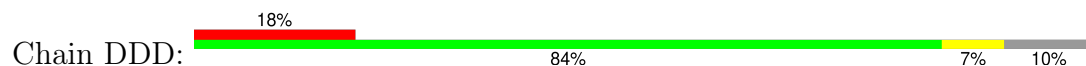
- Molecule 1: N-glycosylase/DNA lyase

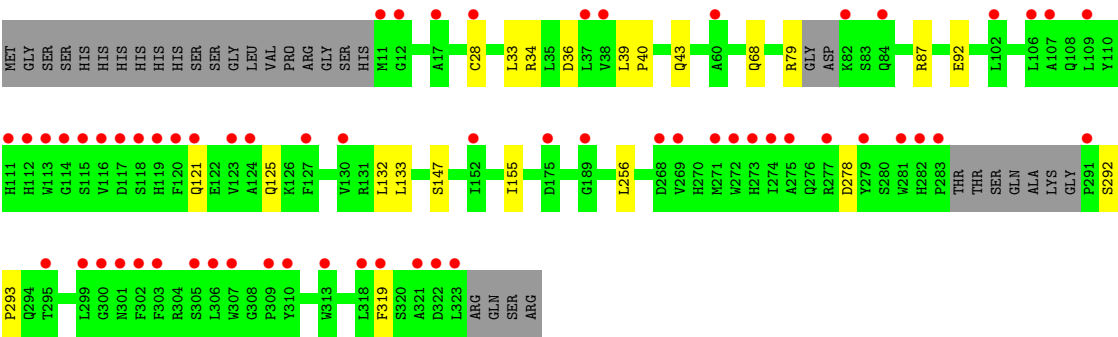


- Molecule 1: N-glycosylase/DNA lyase

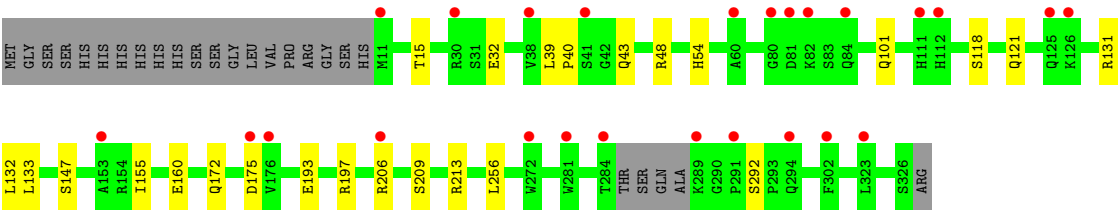
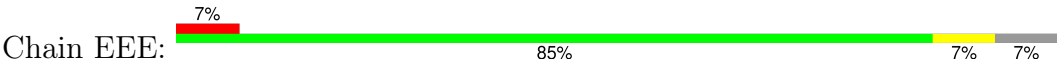


- Molecule 1: N-glycosylase/DNA lyase





● 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, α , β , γ	86.37Å 86.37Å 432.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.84 – 2.00 84.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (84.84-2.00) 99.9 (84.84-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.223 , 0.274 0.230 , 0.277	Depositor DCC
R_{free} test set	5571 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13184	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 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.*

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 [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	0.98	0/2564	1.35	0/3486
1	BBB	0.97	0/2531	1.33	0/3443
1	CCC	1.00	0/2481	1.38	0/3373
1	DDD	1.00	0/2478	1.42	0/3369
1	EEE	1.00	0/2559	1.39	0/3479
All	All	0.99	0/12613	1.37	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	20	0
1	BBB	2463	0	2396	16	0
1	CCC	2415	0	2356	13	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	77	0

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

All (77) 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
1:DDD:132:LEU:HD21	1:DDD:256:LEU:HG	1.76	0.68
1:EEE:193:GLU:OE2	1:EEE:197:ARG:NH2	2.29	0.66
1:DDD:43:GLN:HE22	1:DDD:133:LEU:H	1.45	0.64
1:CCC:103:ASP:HB2	3:CCC:576:HOH:O	1.98	0.62
1:BBB:43:GLN:NE2	1:BBB:133:LEU:H	1.97	0.61
1:AAA:239:ALA:O	1:AAA:242:ILE:HG12	2.02	0.60
1:AAA:271:MET:HE3	1:AAA:303:PHE:CE2	2.40	0.57
1:EEE:43:GLN:NE2	1:EEE:133:LEU:H	2.02	0.56
1:AAA:43:GLN:NE2	1:AAA:133:LEU:H	2.01	0.56
1:DDD:292:SER:HB3	1:DDD:293:PRO:HD2	1.89	0.54
1:AAA:101:GLN:O	1:AAA:131:ARG:NH2	2.42	0.52
1:AAA:132:LEU:HD21	1:AAA:256:LEU:HG	1.92	0.51
1:CCC:79:ARG:NH1	1:CCC:92:GLU:OE2	2.43	0.51
1:DDD:34:ARG:HA	1:DDD:68:GLN:HE22	1.76	0.51
1:DDD:292:SER:HB3	1:DDD:293:PRO:CD	2.42	0.50
1:CCC:150:ASN:HB3	1:CCC:155:ILE:HG13	1.93	0.50
1:BBB:132:LEU:HD23	1:BBB:313:TRP:HA	1.94	0.50
1:DDD:79:ARG:NH1	1:DDD:92:GLU:OE2	2.44	0.49
1:BBB:79:ARG:NH2	1:BBB:86:SER:OG	2.42	0.49
1:DDD:39:LEU:N	1:DDD:40:PRO:CD	2.76	0.49
1:EEE:118:SER:O	1:EEE:121:GLN:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:DDD:43:GLN:NE2	1:DDD:133:LEU:H	2.09	0.48
1:DDD:87:ARG:NH1	3:DDD:508:HOH:O	2.45	0.48
1:CCC:82:LYS:HG2	1:CCC:82:LYS:O	2.13	0.48
1:EEE:48:ARG:NH2	1:EEE:160:GLU:OE2	2.35	0.48
1:AAA:121:GLN:O	1:AAA:125:GLN:HG2	2.14	0.47
1:CCC:150:ASN:HD21	1:CCC:158:MET:CE	2.28	0.47
1:EEE:39:LEU:N	1:EEE:40:PRO:CD	2.78	0.47
1:CCC:39:LEU:N	1:CCC:40:PRO:CD	2.78	0.47
1:AAA:46:ARG:HG3	1:AAA:139:GLU:OE2	2.14	0.46
1:CCC:35:LEU:H	1:CCC:68:GLN:HE22	1.62	0.46
1:BBB:35:LEU:H	1:BBB:68:GLN:HE22	1.64	0.46
1:BBB:39:LEU:N	1:BBB:40:PRO:CD	2.79	0.46
1:EEE:101:GLN:O	1:EEE:131:ARG:NH2	2.49	0.46
1:BBB:35:LEU:H	1:BBB:68:GLN:NE2	2.13	0.46
1:BBB:34:ARG:HA	1:BBB:68:GLN:HE22	1.82	0.45
1:BBB:150:ASN:HB3	1:BBB:155:ILE:HG13	1.98	0.45
1:AAA:132:LEU:HD21	1:AAA:256:LEU:O	2.17	0.45
1:AAA:225:LEU:HD12	1:AAA:225:LEU:N	2.31	0.45
1:BBB:324:ARG:O	1:BBB:325:GLN:HG3	2.17	0.44
1:EEE:15:THR:HA	1:EEE:54:HIS:CD2	2.52	0.44
1:DDD:121:GLN:O	1:DDD:125:GLN:HG2	2.18	0.44
1:EEE:43:GLN:HE22	1:EEE:132:LEU:HA	1.83	0.44
1:EEE:172:GLN:HE21	1:EEE:175:ASP:HA	1.83	0.44
1:AAA:21:ALA:O	1:AAA:87:ARG:HG3	2.17	0.44
1:CCC:132:LEU:CD2	1:CCC:256:LEU:HG	2.48	0.44
1:AAA:326:SER:O	1:AAA:327:ARG:CB	2.67	0.43
1:BBB:132:LEU:HD21	1:BBB:316:ALA:HB2	2.01	0.43
1:AAA:193:GLU:HG3	1:AAA:206:ARG:HA	2.01	0.43
1:DDD:34:ARG:NH2	1:DDD:36:ASP:OD2	2.52	0.42
1:BBB:267:VAL:HG11	1:BBB:296:ASN:HA	2.01	0.42
1:DDD:28:CYS:SG	1:DDD:33:LEU:HB3	2.59	0.42
1:EEE:147:SER:HA	1:EEE:155:ILE:HG12	1.99	0.42
1:EEE:209:SER:OG	1:EEE:213:ARG:NH2	2.48	0.42
1:DDD:147:SER:HA	1:DDD:155:ILE:HG12	2.00	0.42
1:AAA:11:MET:SD	1:AAA:171:ILE:HD11	2.59	0.42
1:CCC:32:GLU:O	1:CCC:131:ARG:HD2	2.19	0.42
1:AAA:147:SER:HA	1:AAA:155:ILE:HG12	2.02	0.41
1:EEE:206[B]:ARG:NH2	3:EEE:512:HOH:O	2.44	0.41
1:BBB:239:ALA:O	1:BBB:242:ILE:HG12	2.21	0.41
1:CCC:130:VAL:HG11	1:CCC:317:VAL:HA	2.02	0.41
1:BBB:271:MET:HE3	1:BBB:303:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:15:THR:HA	1:AAA:54:HIS:CD2	2.56	0.41
1:AAA:32:GLU:O	1:AAA:131:ARG:HD2	2.21	0.41
1:CCC:132:LEU:CD2	1:CCC:256:LEU:HD11	2.50	0.41
1:CCC:272:TRP:HZ3	1:CCC:281:TRP:CD1	2.39	0.41
1:EEE:32:GLU:O	1:EEE:131:ARG:HD2	2.21	0.41
1:AAA:43:GLN:HE22	1:AAA:132:LEU:HA	1.85	0.41
1:CCC:271:MET:HE3	1:CCC:303:PHE:CE2	2.56	0.41
1:AAA:150:ASN:OD1	1:AAA:154:ARG:NH1	2.54	0.40
1:BBB:324:ARG:C	1:BBB:325:GLN:HG3	2.46	0.40
1:AAA:56:SER:HA	1:AAA:64:TRP:O	2.21	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	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
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 ⓘ

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%)	84	89
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%)	73	80
1	EEE	264/284 (93%)	263 (100%)	1 (0%)	84	89
All	All	1300/1420 (92%)	1296 (100%)	4 (0%)	86	91

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 ⓘ

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 ⓘ

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	0.63	1 (3%)	43,43,43	0.67	3 (6%)
2	K8Q	CCC	401	-	30,30,30	0.60	1 (3%)	43,43,43	0.63	2 (4%)
2	K8Q	AAA	401	-	30,30,30	0.63	1 (3%)	43,43,43	0.67	1 (2%)
2	K8Q	BBB	401	-	30,30,30	0.68	1 (3%)	43,43,43	0.68	2 (4%)
2	K8Q	DDD	401	-	30,30,30	0.62	1 (3%)	43,43,43	0.64	2 (4%)

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	CCC	401	-	-	0/12/22/22	0/4/4/4
2	K8Q	AAA	401	-	-	1/12/22/22	0/4/4/4
2	K8Q	BBB	401	-	-	0/12/22/22	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	-2.89	1.36	1.45
2	BBB	401	K8Q	C03-C24	-2.89	1.36	1.45
2	EEE	401	K8Q	C03-C24	-2.79	1.36	1.45
2	CCC	401	K8Q	C03-C24	-2.76	1.36	1.45
2	AAA	401	K8Q	C03-C24	-2.59	1.37	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	401	K8Q	C24-C03-N04	2.38	109.30	106.53
2	BBB	401	K8Q	C24-N07-C05	-2.34	107.66	109.24
2	BBB	401	K8Q	C24-C03-N04	2.25	109.14	106.53
2	EEE	401	K8Q	C10-N11-C14	-2.19	113.88	121.83
2	DDD	401	K8Q	C24-C03-N04	2.18	109.06	106.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	EEE	401	K8Q	C24-C03-N04	2.11	108.99	106.53
2	CCC	401	K8Q	C24-N07-C05	-2.11	107.82	109.24
2	DDD	401	K8Q	C24-N07-C05	-2.08	107.84	109.24
2	CCC	401	K8Q	C24-C03-N04	2.05	108.92	106.53
2	EEE	401	K8Q	C24-N07-C05	-2.02	107.88	109.24

There are no chirality outliers.

All (3) torsion outliers are listed below:

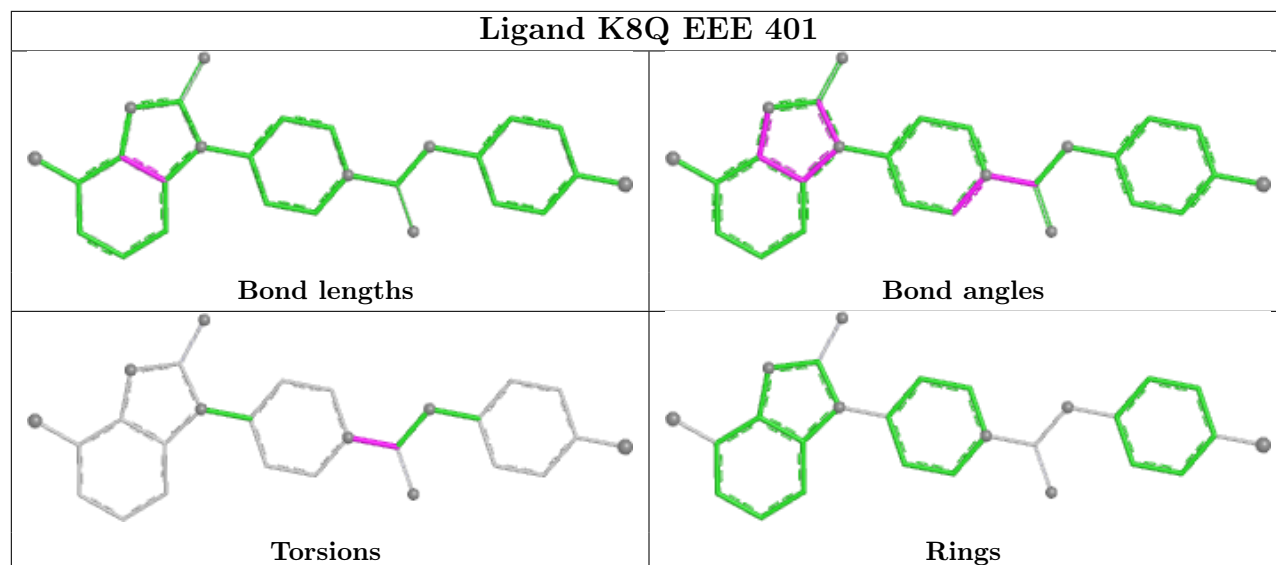
Mol	Chain	Res	Type	Atoms
2	EEE	401	K8Q	O15-C14-N11-C12
2	AAA	401	K8Q	O15-C14-N11-C12
2	EEE	401	K8Q	N16-C14-N11-C12

There are no ring outliers.

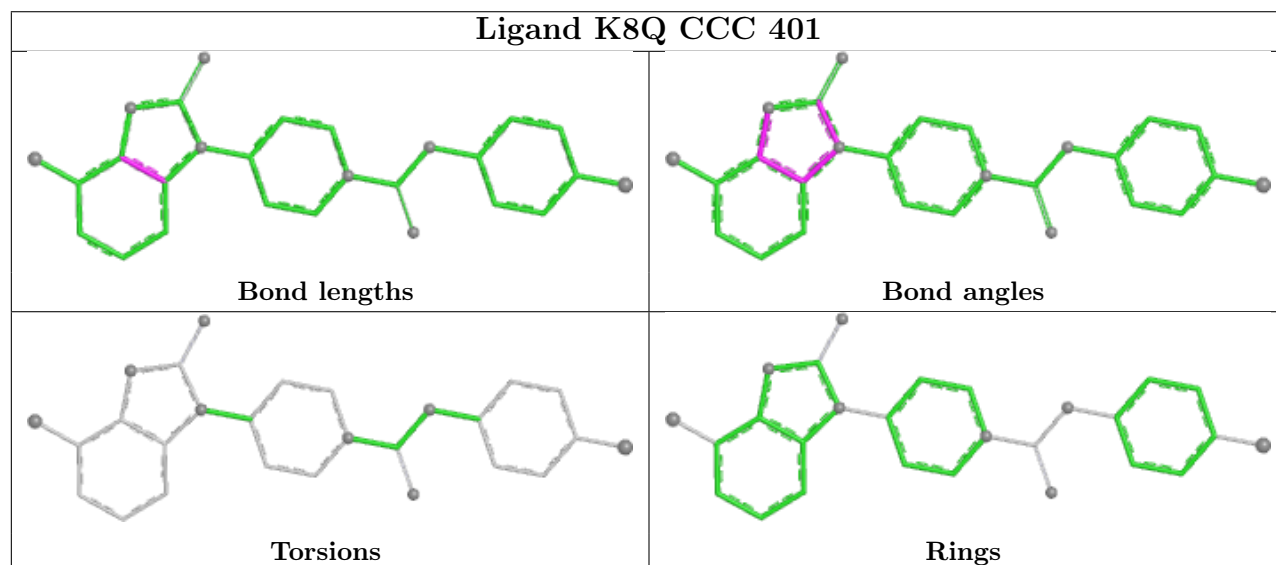
No monomer is involved in short contacts.

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.

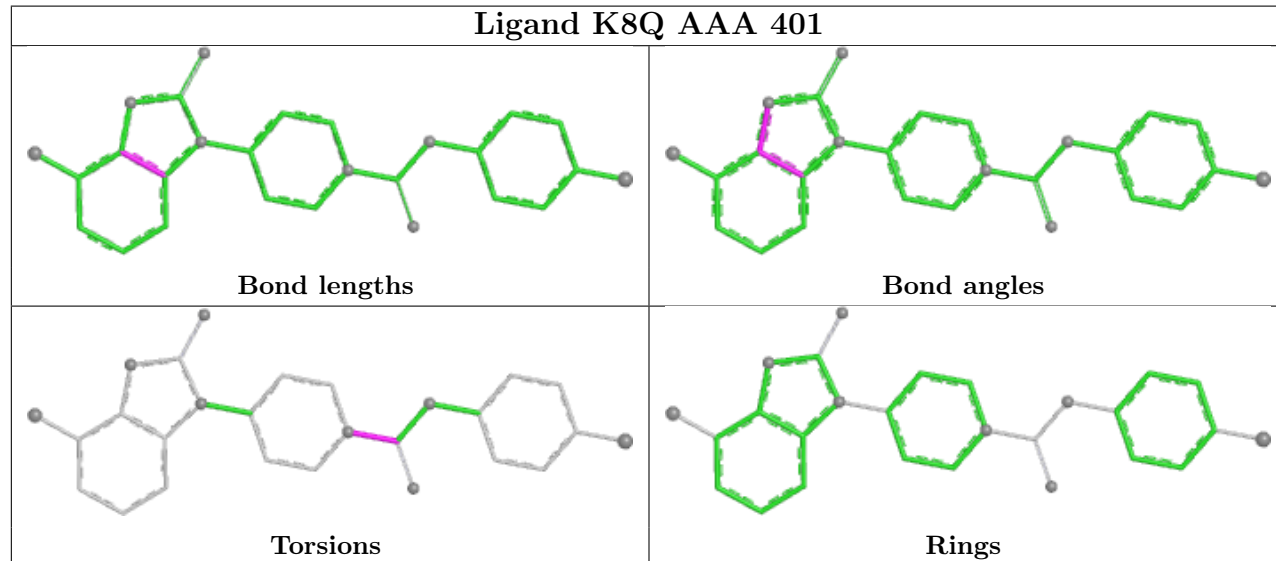
Ligand K8Q EEE 401

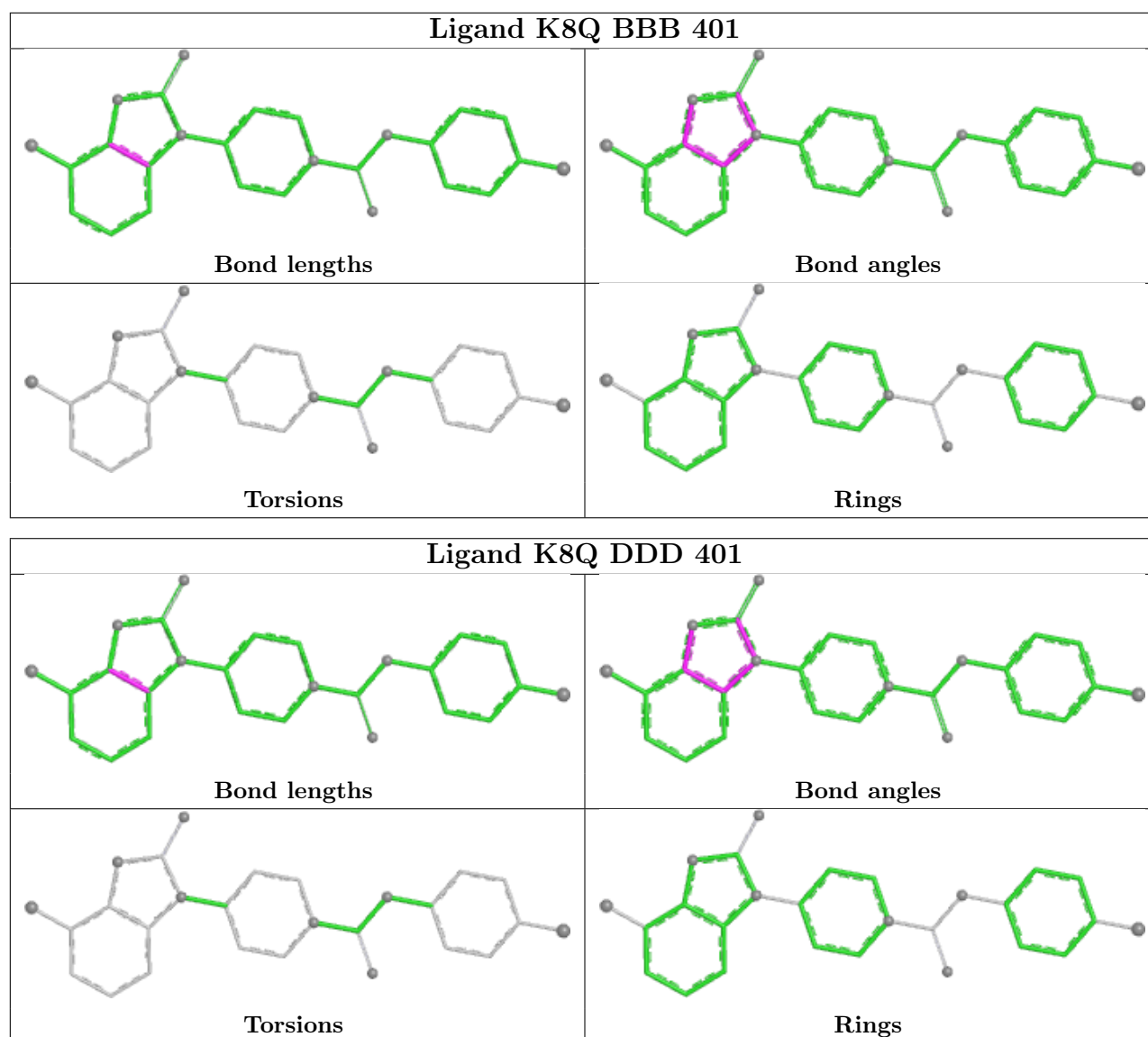


Ligand K8Q CCC 401



Ligand K8Q AAA 401





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	AAA	314/337 (93%)	0.43	14 (4%) 38 37	22, 35, 58, 100	0
1	BBB	310/337 (91%)	0.54	27 (8%) 16 15	23, 35, 66, 104	0
1	CCC	303/337 (89%)	0.76	33 (10%) 10 9	25, 44, 72, 110	0
1	DDD	304/337 (90%)	1.21	61 (20%) 3 2	31, 49, 88, 111	0
1	EEE	312/337 (92%)	0.78	25 (8%) 18 17	18, 42, 71, 100	1 (0%)
All	All	1543/1685 (91%)	0.74	160 (10%) 11 10	18, 41, 76, 111	1 (0%)

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	272	TRP	5.7
1	DDD	323	LEU	5.5
1	DDD	283	PRO	5.1
1	DDD	115	SER	5.1
1	BBB	272	TRP	4.9
1	BBB	283	PRO	4.8
1	BBB	290	GLY	4.7
1	DDD	291	PRO	4.7
1	DDD	120	PHE	4.6
1	DDD	116	VAL	4.5
1	AAA	288	ALA	4.3
1	CCC	323	LEU	4.3
1	CCC	282	HIS	4.1
1	DDD	113	TRP	4.1
1	DDD	302	PHE	4.0
1	EEE	284	THR	3.9
1	DDD	123	VAL	3.9
1	DDD	281	TRP	3.9
1	BBB	11	MET	3.8
1	DDD	130	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	DDD	274	ILE	3.7
1	BBB	80	GLY	3.6
1	DDD	124	ALA	3.6
1	DDD	279	TYR	3.6
1	BBB	120	PHE	3.6
1	CCC	11	MET	3.5
1	DDD	306	LEU	3.5
1	DDD	127	PHE	3.5
1	BBB	116	VAL	3.5
1	CCC	272	TRP	3.5
1	BBB	291	PRO	3.4
1	DDD	319	PHE	3.4
1	DDD	277	ARG	3.4
1	DDD	275	ALA	3.3
1	CCC	16	LEU	3.3
1	BBB	59	LEU	3.2
1	EEE	82	LYS	3.2
1	CCC	85	ALA	3.1
1	DDD	109	LEU	3.1
1	CCC	281	TRP	3.1
1	DDD	118	SER	3.1
1	DDD	175	ASP	3.1
1	BBB	282	HIS	3.1
1	EEE	11	MET	3.0
1	CCC	83	SER	3.0
1	AAA	327	ARG	3.0
1	BBB	289	LYS	3.0
1	DDD	299	LEU	3.0
1	DDD	114	GLY	3.0
1	DDD	313	TRP	3.0
1	EEE	125	GLN	2.9
1	DDD	28	CYS	2.9
1	DDD	82	LYS	2.9
1	CCC	279	TYR	2.9
1	AAA	60	ALA	2.9
1	DDD	111	HIS	2.8
1	EEE	206[A]	ARG	2.8
1	DDD	318	LEU	2.8
1	BBB	293	PRO	2.8
1	CCC	175	ASP	2.8
1	EEE	126	LYS	2.8
1	BBB	81	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	CCC	60	ALA	2.8
1	DDD	152	ILE	2.8
1	BBB	115	SER	2.7
1	CCC	321	ALA	2.7
1	DDD	321	ALA	2.7
1	DDD	106	LEU	2.7
1	BBB	84	GLN	2.7
1	AAA	284	THR	2.7
1	CCC	291	PRO	2.7
1	CCC	274	ILE	2.7
1	DDD	307	TRP	2.7
1	EEE	289	LYS	2.7
1	CCC	84	GLN	2.6
1	DDD	300	GLY	2.6
1	EEE	112	HIS	2.6
1	AAA	281	TRP	2.6
1	EEE	323	LEU	2.6
1	DDD	121	GLN	2.5
1	DDD	112	HIS	2.5
1	DDD	282	HIS	2.5
1	EEE	111	HIS	2.5
1	DDD	295	THR	2.5
1	CCC	120	PHE	2.5
1	DDD	107	ALA	2.5
1	DDD	309	PRO	2.5
1	EEE	60	ALA	2.5
1	EEE	291	PRO	2.5
1	CCC	116	VAL	2.5
1	CCC	123	VAL	2.5
1	CCC	152	ILE	2.5
1	CCC	269	VAL	2.5
1	EEE	175	ASP	2.5
1	BBB	124	ALA	2.5
1	CCC	21	ALA	2.5
1	DDD	119	HIS	2.5
1	BBB	281	TRP	2.5
1	EEE	176	VAL	2.4
1	DDD	310	TYR	2.4
1	DDD	11	MET	2.4
1	AAA	118	SER	2.4
1	EEE	302	PHE	2.4
1	DDD	269	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	CCC	79	ARG	2.4
1	DDD	322	ASP	2.3
1	EEE	81	ASP	2.3
1	AAA	11	MET	2.3
1	DDD	271	MET	2.3
1	EEE	38	VAL	2.3
1	DDD	60	ALA	2.3
1	DDD	301	ASN	2.3
1	CCC	82	LYS	2.3
1	CCC	293	PRO	2.3
1	EEE	294	GLN	2.3
1	CCC	17	ALA	2.3
1	CCC	124	ALA	2.3
1	EEE	272	TRP	2.3
1	EEE	281	TRP	2.3
1	AAA	289	LYS	2.3
1	BBB	325	GLN	2.3
1	DDD	84	GLN	2.3
1	BBB	321	ALA	2.3
1	AAA	294	GLN	2.2
1	BBB	274	ILE	2.2
1	CCC	190	PRO	2.2
1	DDD	38	VAL	2.2
1	BBB	16	LEU	2.2
1	AAA	71	GLU	2.2
1	DDD	17	ALA	2.2
1	DDD	102	LEU	2.2
1	BBB	295	THR	2.2
1	CCC	171	ILE	2.2
1	CCC	176	VAL	2.2
1	EEE	30	ARG	2.2
1	DDD	273	HIS	2.1
1	DDD	305	SER	2.1
1	DDD	268	ASP	2.1
1	BBB	105	THR	2.1
1	BBB	190	PRO	2.1
1	DDD	303	PHE	2.1
1	CCC	273	HIS	2.1
1	EEE	153	ALA	2.1
1	AAA	326	SER	2.1
1	EEE	41	SER	2.1
1	EEE	84	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	CCC	319	PHE	2.1
1	BBB	25	SER	2.1
1	BBB	323	LEU	2.1
1	CCC	199	LEU	2.1
1	AAA	61	ASP	2.1
1	DDD	12	GLY	2.1
1	DDD	189	GLY	2.1
1	EEE	80	GLY	2.1
1	AAA	17	ALA	2.1
1	DDD	37	LEU	2.0
1	BBB	91	ASP	2.0
1	DDD	117	ASP	2.0
1	CCC	295	THR	2.0
1	AAA	84	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](#)

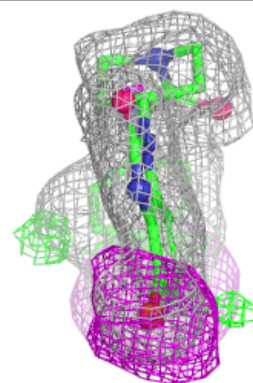
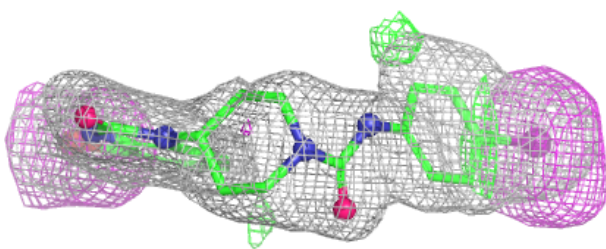
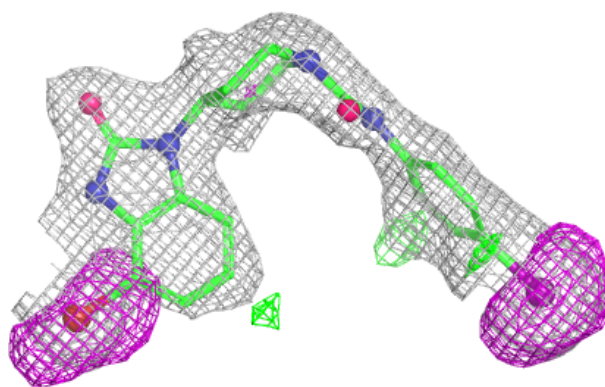
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	K8Q	BBB	401	27/27	0.93	0.15	38,50,61,78	0
2	K8Q	DDD	401	27/27	0.93	0.14	45,61,93,117	0
2	K8Q	CCC	401	27/27	0.94	0.14	55,68,77,96	0
2	K8Q	EEE	401	27/27	0.97	0.10	34,43,55,75	0
2	K8Q	AAA	401	27/27	0.99	0.08	27,31,33,49	0

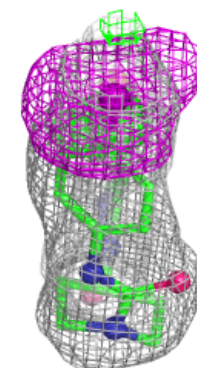
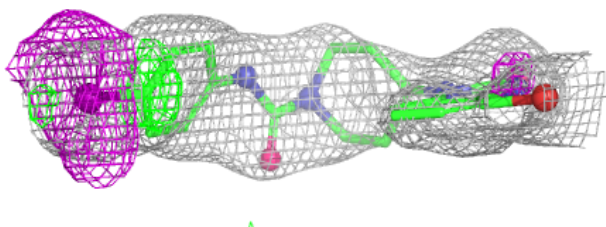
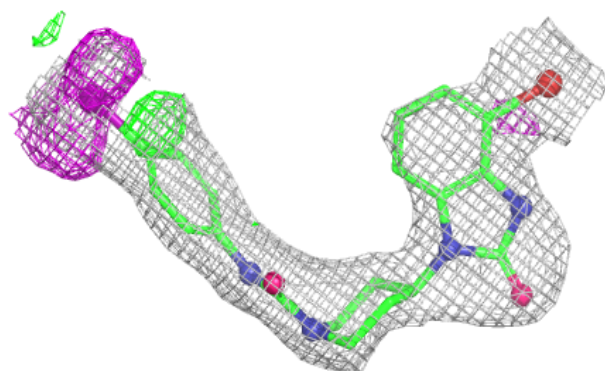
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around K8Q BBB 401:

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

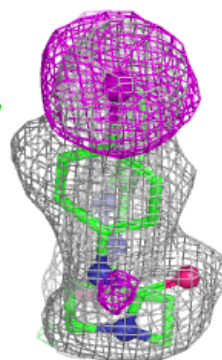
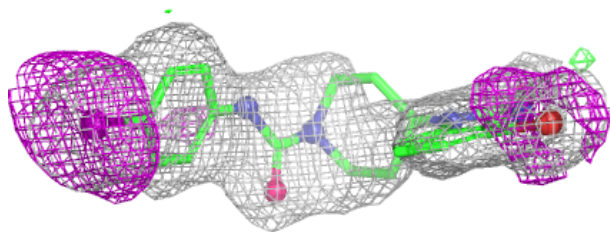
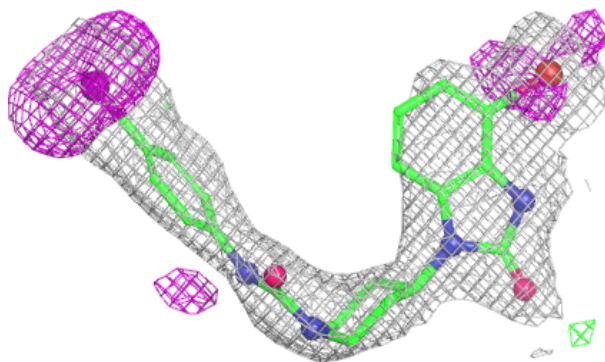
**Electron density around K8Q DDD 401:**

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

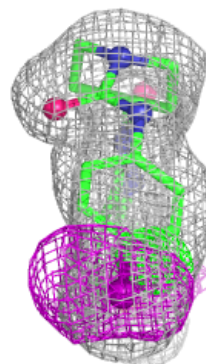
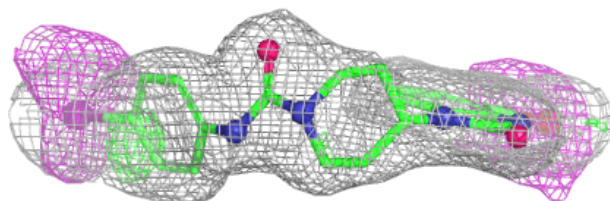
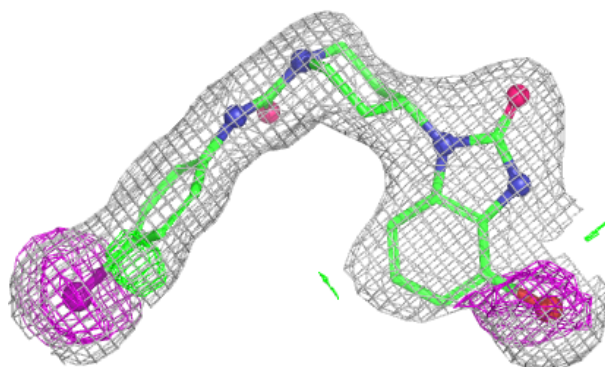


Electron density around K8Q CCC 401:

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

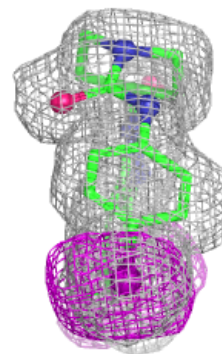
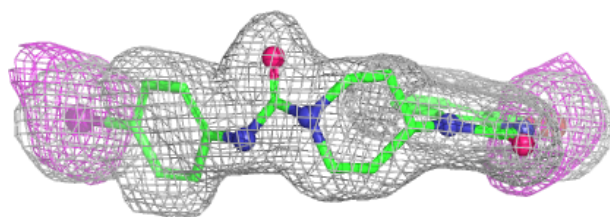
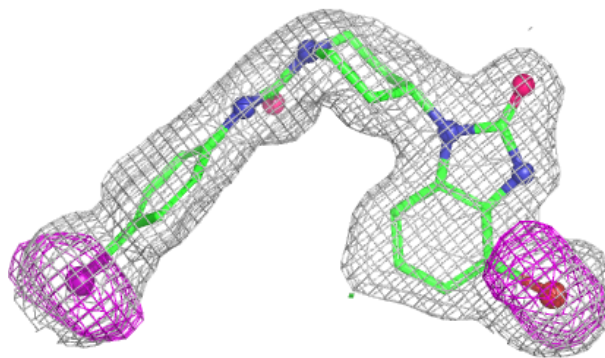
**Electron density around K8Q EEE 401:**

$2mF_o-DF_c$ (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.