



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 24, 2021 – 01:13 pm GMT

PDB ID : 7AZC
Title : DNA polymerase sliding clamp from Escherichia coli with peptide 22 bound
Authors : Monsarrat, C.; Compain, G.; Andre, C.; Martiel, I.; Engilberge, S.; Olieric, V.; Wolff, P.; Brillet, K.; Landolfo, M.; Silva da Veiga, C.; Wagner, J.; Guichard, G.; Burnouf, D.Y.
Deposited on : 2020-11-16
Resolution : 1.77 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

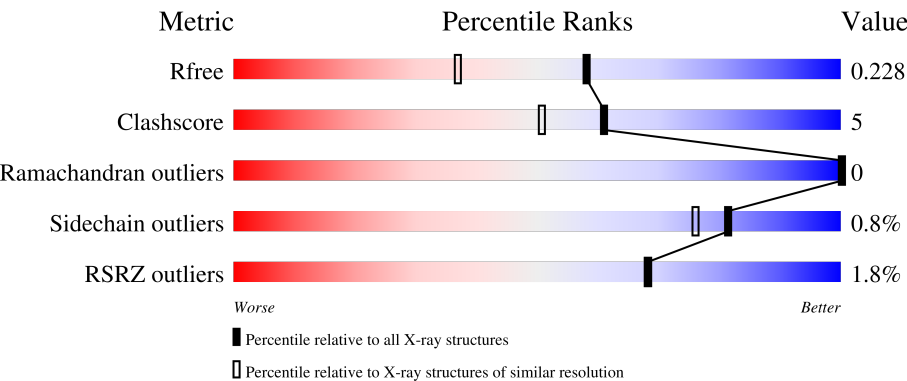
MolProbity : 4.02b-467
Mogul : 1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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.



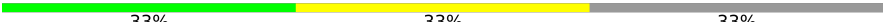


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	386	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>85%10%5%</div></div>
1	B	386	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>83%11%5%</div></div>
1	C	386	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>83%11%5%</div></div>
1	D	386	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>86%8%6%</div></div>
2	H	6	<div><div></div><div><div></div><div></div><div></div></div><div>50%17%33%</div></div>

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Mol	Chain	Length	Quality of chain
2	I	6	 33% 33% 33%
2	J	6	 50% 17% 33%
2	K	6	 50% 17% 33%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13282 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 Beta sliding clamp.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	6	0
			2899	1826	509	544	20			
1	B	365	Total	C	N	O	S	0	5	0
			2868	1806	502	541	19			
1	C	366	Total	C	N	O	S	0	7	0
			2888	1821	506	542	19			
1	D	364	Total	C	N	O	S	0	3	0
			2846	1790	502	535	19			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A073FMV0
A	-18	GLY	-	expression tag	UNP A0A073FMV0
A	-17	SER	-	expression tag	UNP A0A073FMV0
A	-16	SER	-	expression tag	UNP A0A073FMV0
A	-15	HIS	-	expression tag	UNP A0A073FMV0
A	-14	HIS	-	expression tag	UNP A0A073FMV0
A	-13	HIS	-	expression tag	UNP A0A073FMV0
A	-12	HIS	-	expression tag	UNP A0A073FMV0
A	-11	HIS	-	expression tag	UNP A0A073FMV0
A	-10	HIS	-	expression tag	UNP A0A073FMV0
A	-9	SER	-	expression tag	UNP A0A073FMV0
A	-8	SER	-	expression tag	UNP A0A073FMV0
A	-7	GLY	-	expression tag	UNP A0A073FMV0
A	-6	LEU	-	expression tag	UNP A0A073FMV0
A	-5	VAL	-	expression tag	UNP A0A073FMV0
A	-4	PRO	-	expression tag	UNP A0A073FMV0
A	-3	ARG	-	expression tag	UNP A0A073FMV0
A	-2	GLY	-	expression tag	UNP A0A073FMV0
A	-1	SER	-	expression tag	UNP A0A073FMV0
A	0	HIS	-	expression tag	UNP A0A073FMV0
B	-19	MET	-	initiating methionine	UNP A0A073FMV0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A0A073FMV0
B	-17	SER	-	expression tag	UNP A0A073FMV0
B	-16	SER	-	expression tag	UNP A0A073FMV0
B	-15	HIS	-	expression tag	UNP A0A073FMV0
B	-14	HIS	-	expression tag	UNP A0A073FMV0
B	-13	HIS	-	expression tag	UNP A0A073FMV0
B	-12	HIS	-	expression tag	UNP A0A073FMV0
B	-11	HIS	-	expression tag	UNP A0A073FMV0
B	-10	HIS	-	expression tag	UNP A0A073FMV0
B	-9	SER	-	expression tag	UNP A0A073FMV0
B	-8	SER	-	expression tag	UNP A0A073FMV0
B	-7	GLY	-	expression tag	UNP A0A073FMV0
B	-6	LEU	-	expression tag	UNP A0A073FMV0
B	-5	VAL	-	expression tag	UNP A0A073FMV0
B	-4	PRO	-	expression tag	UNP A0A073FMV0
B	-3	ARG	-	expression tag	UNP A0A073FMV0
B	-2	GLY	-	expression tag	UNP A0A073FMV0
B	-1	SER	-	expression tag	UNP A0A073FMV0
B	0	HIS	-	expression tag	UNP A0A073FMV0
C	-19	MET	-	initiating methionine	UNP A0A073FMV0
C	-18	GLY	-	expression tag	UNP A0A073FMV0
C	-17	SER	-	expression tag	UNP A0A073FMV0
C	-16	SER	-	expression tag	UNP A0A073FMV0
C	-15	HIS	-	expression tag	UNP A0A073FMV0
C	-14	HIS	-	expression tag	UNP A0A073FMV0
C	-13	HIS	-	expression tag	UNP A0A073FMV0
C	-12	HIS	-	expression tag	UNP A0A073FMV0
C	-11	HIS	-	expression tag	UNP A0A073FMV0
C	-10	HIS	-	expression tag	UNP A0A073FMV0
C	-9	SER	-	expression tag	UNP A0A073FMV0
C	-8	SER	-	expression tag	UNP A0A073FMV0
C	-7	GLY	-	expression tag	UNP A0A073FMV0
C	-6	LEU	-	expression tag	UNP A0A073FMV0
C	-5	VAL	-	expression tag	UNP A0A073FMV0
C	-4	PRO	-	expression tag	UNP A0A073FMV0
C	-3	ARG	-	expression tag	UNP A0A073FMV0
C	-2	GLY	-	expression tag	UNP A0A073FMV0
C	-1	SER	-	expression tag	UNP A0A073FMV0
C	0	HIS	-	expression tag	UNP A0A073FMV0
D	-19	MET	-	initiating methionine	UNP A0A073FMV0
D	-18	GLY	-	expression tag	UNP A0A073FMV0
D	-17	SER	-	expression tag	UNP A0A073FMV0

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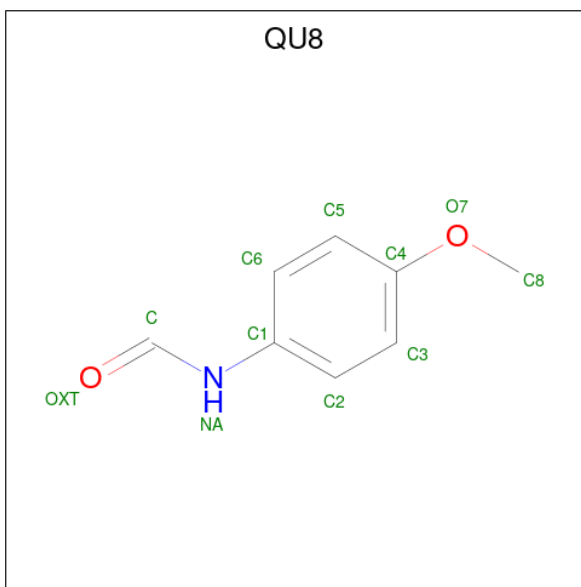
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A0A073FMV0
D	-15	HIS	-	expression tag	UNP A0A073FMV0
D	-14	HIS	-	expression tag	UNP A0A073FMV0
D	-13	HIS	-	expression tag	UNP A0A073FMV0
D	-12	HIS	-	expression tag	UNP A0A073FMV0
D	-11	HIS	-	expression tag	UNP A0A073FMV0
D	-10	HIS	-	expression tag	UNP A0A073FMV0
D	-9	SER	-	expression tag	UNP A0A073FMV0
D	-8	SER	-	expression tag	UNP A0A073FMV0
D	-7	GLY	-	expression tag	UNP A0A073FMV0
D	-6	LEU	-	expression tag	UNP A0A073FMV0
D	-5	VAL	-	expression tag	UNP A0A073FMV0
D	-4	PRO	-	expression tag	UNP A0A073FMV0
D	-3	ARG	-	expression tag	UNP A0A073FMV0
D	-2	GLY	-	expression tag	UNP A0A073FMV0
D	-1	SER	-	expression tag	UNP A0A073FMV0
D	0	HIS	-	expression tag	UNP A0A073FMV0

- Molecule 2 is a protein called Peptide 22.

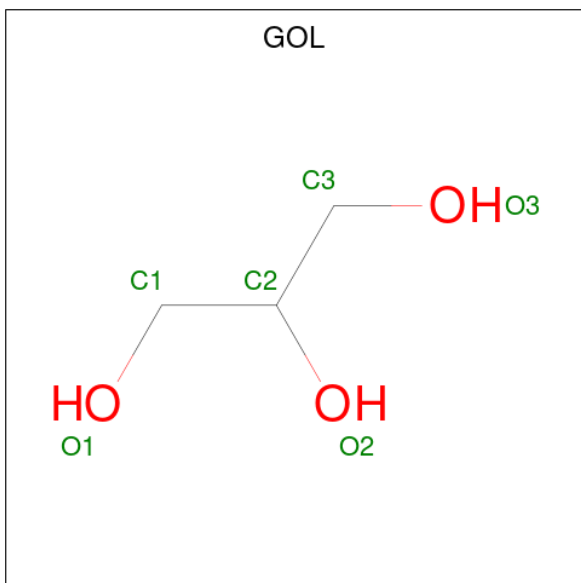
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	4	Total	C	N	O	0	0	0
			39	28	4	7			
2	I	4	Total	C	N	O	0	0	0
			39	28	4	7			
2	J	4	Total	C	N	O	0	0	0
			39	28	4	7			
2	K	4	Total	C	N	O	0	0	0
			39	28	4	7			

- Molecule 3 is {N}-(4-methoxyphenyl)methanamide (three-letter code: QU8) (formula: C₈H₉NO₂) (labeled as "Ligand of Interest" by depositor).



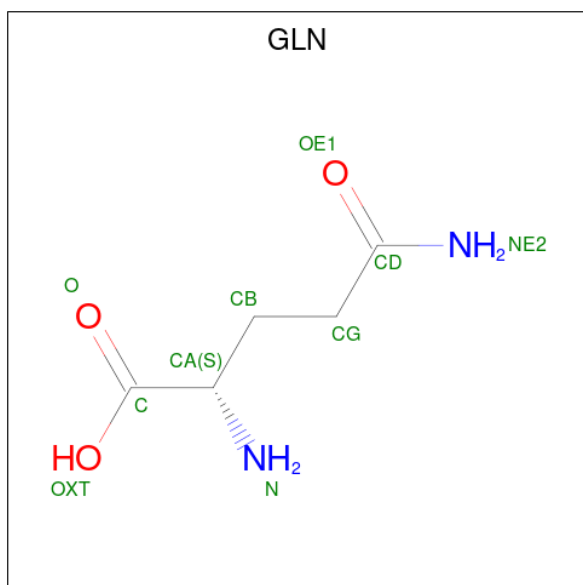
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	8	1	2		
3	B	1	Total	C	N	O	0	0
			11	8	1	2		
3	B	1	Total	C	N	O	0	0
			11	8	1	2		
3	C	1	Total	C	N	O	0	0
			11	8	1	2		

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



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

- Molecule 5 is GLUTAMINE (three-letter code: GLN) (formula: C₅H₁₀N₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	N	O	0	0
			9	5	2	2		
5	I	1	Total	C	N	O	0	0
			9	5	2	2		
5	J	1	Total	C	N	O	0	0
			9	5	2	2		
5	K	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	374	Total	O	0	8
			382	382		
6	B	367	Total	O	0	5
			372	372		
6	C	379	Total	O	0	6
			385	385		

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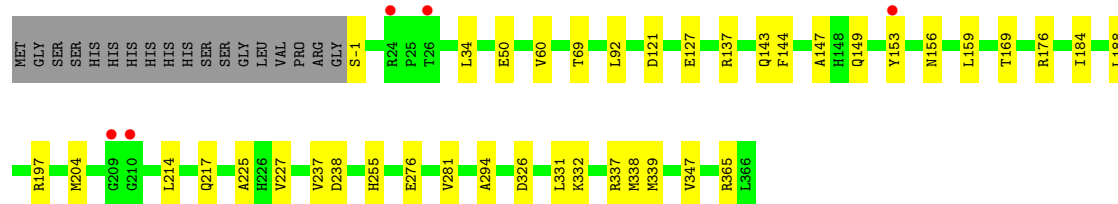
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	341	Total 343	O 343	0	2
6	H	15	Total 15	O 15	0	0
6	I	11	Total 11	O 11	0	0
6	J	14	Total 15	O 15	0	1
6	K	10	Total 10	O 10	0	0

3 Residue-property plots


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.

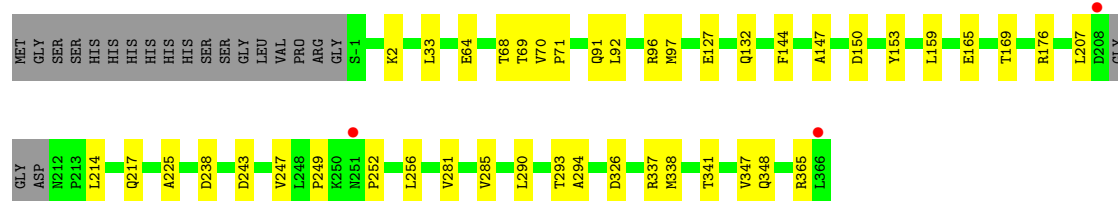
• Molecule 1: Beta sliding clamp

Chain A: 




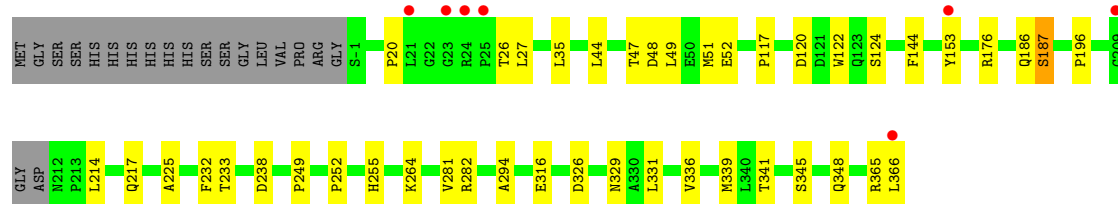
• Molecule 1: Beta sliding clamp

Chain B: 




• Molecule 1: Beta sliding clamp

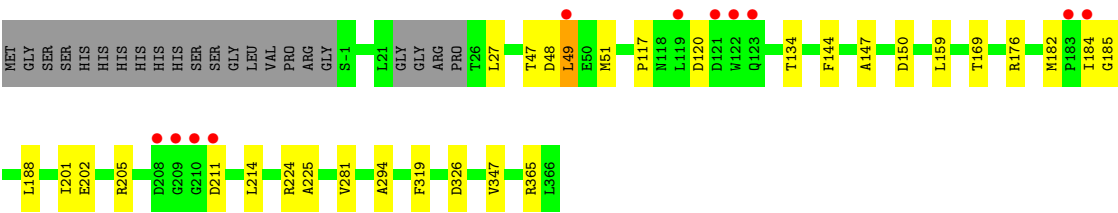
Chain C: 



• Molecule 1: Beta sliding clamp

Chain D: 

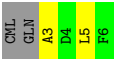




● Molecule 2: Peptide 22



● Molecule 2: Peptide 22



● Molecule 2: Peptide 22



● Molecule 2: Peptide 22



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.81Å 76.78Å 79.81Å 70.90° 68.22° 89.14°	Depositor
Resolution (Å)	25.59 – 1.77 72.02 – 1.77	Depositor EDS
% Data completeness (in resolution range)	71.8 (25.59-1.77) 71.8 (72.02-1.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 1.76Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.173 , 0.220 0.179 , 0.228	Depositor DCC
R_{free} test set	5199 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	20.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	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	0.96	EDS
Total number of atoms	13282	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, QU8, ALC

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	0.47	0/2968	0.56	0/4017
1	B	0.45	0/2930	0.56	0/3965
1	C	0.47	0/2958	0.59	0/4003
1	D	0.45	0/2901	0.57	0/3923
2	H	0.74	0/28	0.61	0/35
2	I	0.67	0/28	0.56	0/35
2	J	0.88	0/28	0.66	0/35
2	K	0.57	0/28	0.57	0/35
All	All	0.47	0/11869	0.57	0/16048

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	A	2899	0	2918	26	0
1	B	2868	0	2895	29	0
1	C	2888	0	2916	35	0
1	D	2846	0	2863	17	0
2	H	39	0	38	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	39	0	38	3	0
2	J	39	0	38	1	0
2	K	39	0	38	1	0
3	A	11	0	0	0	0
3	B	22	0	0	0	0
3	C	11	0	0	0	0
4	B	6	0	8	1	0
4	C	6	0	8	0	0
5	H	9	0	7	0	0
5	I	9	0	7	0	0
5	J	9	0	7	0	0
5	K	9	0	7	0	0
6	A	382	0	0	4	0
6	B	372	0	0	5	0
6	C	385	0	0	6	0
6	D	343	0	0	1	0
6	H	15	0	0	0	0
6	I	11	0	0	0	0
6	J	15	0	0	0	0
6	K	10	0	0	0	0
All	All	13282	0	11788	107	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 5.

All (107) 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:255[A]:HIS:CE1	1:A:337:ARG:HH11	1.98	0.82
1:A:255[A]:HIS:CE1	1:A:337:ARG:NH1	2.50	0.80
1:C:252:PRO:HA	1:C:341:THR:HG22	1.64	0.79
1:C:233:THR:HG22	6:C:575:HOH:O	1.83	0.78
1:B:214:LEU:HD11	1:B:225:ALA:HB1	1.68	0.74
1:C:282:ARG:HG2	1:C:366:LEU:HD22	1.71	0.72
1:C:35:LEU:HD22	1:C:44[A]:LEU:HD23	1.72	0.72
1:D:214:LEU:HD11	1:D:225:ALA:HB1	1.71	0.72
1:D:201:ILE:O	1:D:205[A]:ARG:HG2	1.89	0.71
1:A:255[A]:HIS:HE1	1:A:337:ARG:NH1	1.89	0.69
1:A:214:LEU:HD11	1:A:225:ALA:HB1	1.75	0.68
1:C:47:THR:HG21	1:C:117:PRO:HG2	1.75	0.67
1:B:96:ARG:HG3	6:B:816:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:LEU:HD22	1:C:44[A]:LEU:CD2	2.26	0.66
1:B:252:PRO:HA	1:B:341:THR:HG22	1.78	0.64
1:C:196:PRO:HG2	6:C:628:HOH:O	1.97	0.64
1:A:184:ILE:HD11	1:A:188:LEU:HD11	1.79	0.63
1:D:51:MET:HE3	1:D:202:GLU:HG2	1.80	0.63
1:C:214:LEU:HD11	1:C:225:ALA:HB1	1.83	0.60
1:C:48:ASP:O	1:C:49:LEU:HB2	2.02	0.57
1:A:147:ALA:O	1:A:197:ARG:HD2	2.04	0.57
1:C:20:PRO:HG3	1:C:51:MET:HE1	1.85	0.57
1:D:134:THR:HG23	1:D:182:MET:HE2	1.87	0.57
1:D:47:THR:HG21	1:D:117:PRO:HG2	1.87	0.57
1:B:338:MET:HE3	1:B:347:VAL:HG11	1.86	0.57
1:A:255[B]:HIS:CE1	1:A:339:MET:HG2	2.40	0.56
1:A:153[A]:TYR:CE2	1:A:238:ASP:O	2.60	0.55
1:A:-1:SER:HB3	1:A:92:LEU:CD1	2.36	0.55
1:B:243:ASP:H	4:B:401:GOL:C3	2.20	0.55
1:C:153[A]:TYR:CE2	1:C:238:ASP:O	2.60	0.55
1:B:64:GLU:HG3	6:B:681:HOH:O	2.07	0.54
1:C:264:LYS:HD2	1:C:329:ASN:OD1	2.09	0.53
1:D:120:ASP:CB	1:D:224:ARG:HH22	2.22	0.52
1:B:256:LEU:HD12	1:B:285[B]:VAL:HG11	1.92	0.52
1:C:365:ARG:HB2	2:J:3:ALC:HZ3	1.91	0.52
1:B:256:LEU:HD12	1:B:285[A]:VAL:HG21	1.92	0.51
1:C:52:GLU:OE2	1:C:120:ASP:HB2	2.10	0.51
1:B:70:VAL:HG11	1:B:97:MET:SD	2.51	0.51
1:D:48:ASP:O	1:D:49:LEU:HD22	2.11	0.51
1:C:281:VAL:HG12	1:C:294:ALA:HB2	1.93	0.51
1:A:156:ASN:C	1:A:197:ARG:HG3	2.31	0.51
1:D:144:PHE:CD1	1:D:326:ASP:HB3	2.46	0.50
1:C:282:ARG:HG2	1:C:366:LEU:CD2	2.40	0.50
1:D:185:GLY:HA2	6:D:508:HOH:O	2.10	0.50
1:B:132:GLN:HB2	1:B:207:LEU:HD22	1.92	0.50
1:A:144:PHE:CD1	1:A:326:ASP:HB3	2.47	0.49
1:C:26:THR:HA	6:C:801:HOH:O	2.11	0.49
1:C:144:PHE:CD1	1:C:326:ASP:HB3	2.47	0.49
1:A:60:VAL:HG22	6:A:671:HOH:O	2.13	0.49
1:A:365:ARG:HB2	2:H:3:ALC:HZ3	1.95	0.49
1:B:247:VAL:HG13	2:I:5:LEU:HD22	1.93	0.49
1:B:285[B]:VAL:HG22	1:B:290:LEU:HD13	1.95	0.49
1:C:153[B]:TYR:HE1	6:C:648:HOH:O	1.95	0.48
1:A:153[B]:TYR:CD2	1:A:237:VAL:HG13	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:861:HOH:O	1:D:27:LEU:HD21	2.13	0.47
1:C:316:GLU:HG2	1:C:366:LEU:HD13	1.96	0.47
1:D:49:LEU:C	1:D:49:LEU:HD23	2.35	0.47
1:B:337:ARG:NH1	6:B:503:HOH:O	2.48	0.46
1:A:159:LEU:O	1:A:169:THR:HA	2.16	0.46
1:A:127:GLU:HG2	1:A:217:GLN:HG2	1.98	0.45
1:C:341:THR:HG21	6:C:788:HOH:O	2.15	0.45
6:A:542:HOH:O	1:B:71:PRO:HG3	2.16	0.45
1:B:365:ARG:HG2	2:I:3:ALC:HZ3	1.99	0.45
1:D:184:ILE:HD11	1:D:188:LEU:HD11	1.98	0.45
1:A:153[B]:TYR:HD2	1:A:237:VAL:HG13	1.82	0.45
1:A:50:GLU:HB2	6:A:784:HOH:O	2.17	0.45
1:C:20:PRO:HG3	1:C:51:MET:CE	2.46	0.45
1:B:68:THR:HG21	1:B:92:LEU:HD21	1.99	0.44
1:C:35:LEU:CD2	1:C:44[A]:LEU:HD23	2.46	0.44
1:A:338:MET:HE3	1:A:347[B]:VAL:HG21	1.99	0.44
1:B:293:THR:HG23	6:B:715:HOH:O	2.16	0.44
1:B:2:LYS:HG2	1:B:91:GLN:CB	2.48	0.44
1:C:51:MET:HE3	1:C:232:PHE:CE1	2.53	0.44
6:B:720:HOH:O	1:C:27:LEU:HD12	2.17	0.43
1:D:159:LEU:O	1:D:169:THR:HA	2.18	0.43
1:A:281:VAL:HG12	1:A:294:ALA:HB2	2.01	0.43
1:C:51:MET:HE3	1:C:232:PHE:HE1	1.83	0.43
1:D:319:PHE:HZ	1:D:347:VAL:HG13	1.84	0.43
1:D:365:ARG:HB2	2:K:3:ALC:HZ3	1.99	0.43
1:B:159:LEU:O	1:B:169:THR:HA	2.18	0.43
1:B:365:ARG:CG	2:I:3:ALC:HZ3	2.49	0.43
1:C:124:SER:HB2	1:C:217:GLN:HB3	2.00	0.43
1:B:144:PHE:CD1	1:B:326:ASP:HB3	2.54	0.43
1:C:316:GLU:HG2	1:C:366:LEU:CD1	2.49	0.42
1:A:-1:SER:HB3	1:A:92:LEU:HD13	2.00	0.42
1:B:153:TYR:HE2	1:B:238:ASP:O	2.01	0.42
1:C:35:LEU:CD2	1:C:44[A]:LEU:CD2	2.97	0.42
1:A:214:LEU:HD13	1:A:227:VAL:CG2	2.50	0.42
1:C:331:LEU:HD13	1:C:336[A]:VAL:HG12	2.01	0.42
1:A:331:LEU:O	1:A:332:LYS:C	2.59	0.41
1:A:276:GLU:CD	1:A:276:GLU:H	2.24	0.41
1:B:147:ALA:HB1	1:B:150:ASP:HB2	2.02	0.41
1:B:249:PRO:HD2	1:B:348:GLN:OE1	2.20	0.41
1:C:186:GLN:O	1:C:187:SER:C	2.59	0.41
1:C:341:THR:OG1	1:C:345:SER:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LEU:HA	1:A:69:THR:HG22	2.03	0.41
1:A:143:GLN:OE1	1:A:204[A]:MET:SD	2.79	0.41
1:B:281:VAL:HG12	1:B:294:ALA:HB2	2.02	0.41
1:B:127:GLU:HG2	1:B:217:GLN:HG2	2.02	0.41
1:D:281:VAL:HG12	1:D:294:ALA:HB2	2.03	0.41
1:B:33:LEU:O	1:B:69:THR:HA	2.21	0.40
1:C:255:HIS:CD2	1:C:339:MET:HG2	2.55	0.40
1:C:249:PRO:HD2	1:C:348:GLN:OE1	2.22	0.40
1:C:122:TRP:HB3	6:C:580:HOH:O	2.22	0.40
1:D:147:ALA:HB1	1:D:150:ASP:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	372/386 (96%)	360 (97%)	12 (3%)	0	100	100
1	B	366/386 (95%)	359 (98%)	7 (2%)	0	100	100
1	C	369/386 (96%)	362 (98%)	7 (2%)	0	100	100
1	D	363/386 (94%)	353 (97%)	10 (3%)	0	100	100
2	H	2/6 (33%)	2 (100%)	0	0	100	100
2	I	2/6 (33%)	2 (100%)	0	0	100	100
2	J	2/6 (33%)	2 (100%)	0	0	100	100
2	K	2/6 (33%)	2 (100%)	0	0	100	100
All	All	1478/1568 (94%)	1442 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	320/330 (97%)	316 (99%)	4 (1%)	69	59
1	B	318/330 (96%)	317 (100%)	1 (0%)	92	90
1	C	320/330 (97%)	318 (99%)	2 (1%)	86	82
1	D	312/330 (94%)	309 (99%)	3 (1%)	76	68
2	H	3/4 (75%)	3 (100%)	0	100	100
2	I	3/4 (75%)	3 (100%)	0	100	100
2	J	3/4 (75%)	3 (100%)	0	100	100
2	K	3/4 (75%)	3 (100%)	0	100	100
All	All	1282/1336 (96%)	1272 (99%)	10 (1%)	81	76

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ASP
1	A	137	ARG
1	A	149	GLN
1	A	176	ARG
1	B	176	ARG
1	C	176	ARG
1	C	187	SER
1	D	49	LEU
1	D	176	ARG
1	D	211	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	221	ASN
1	B	226	HIS
1	C	221	ASN
1	C	265	GLN

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Mol	Chain	Res	Type
1	D	191	HIS
1	D	289	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 ligands are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

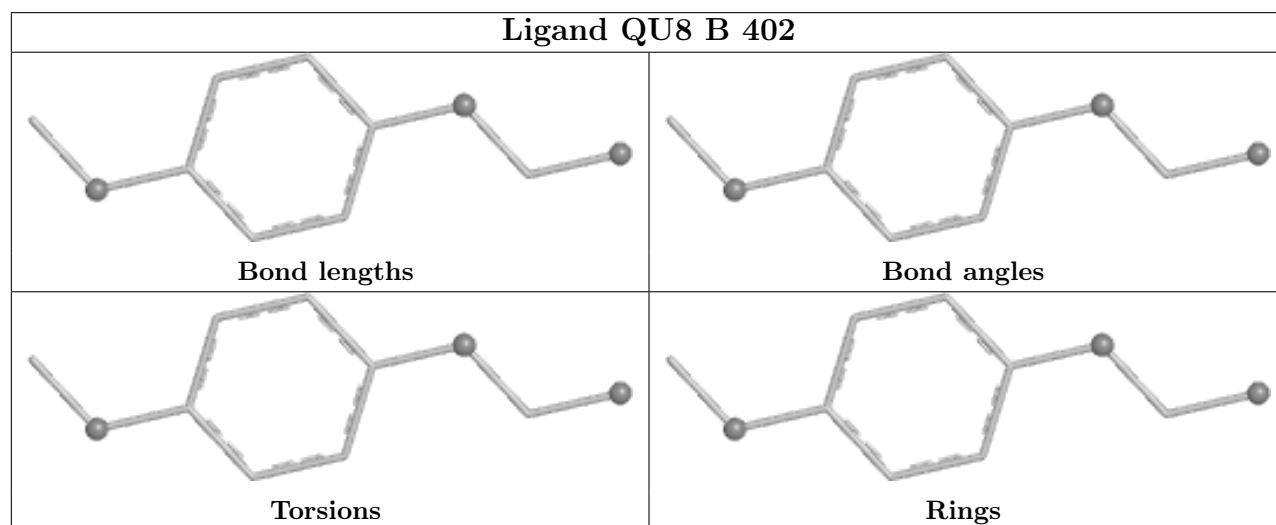
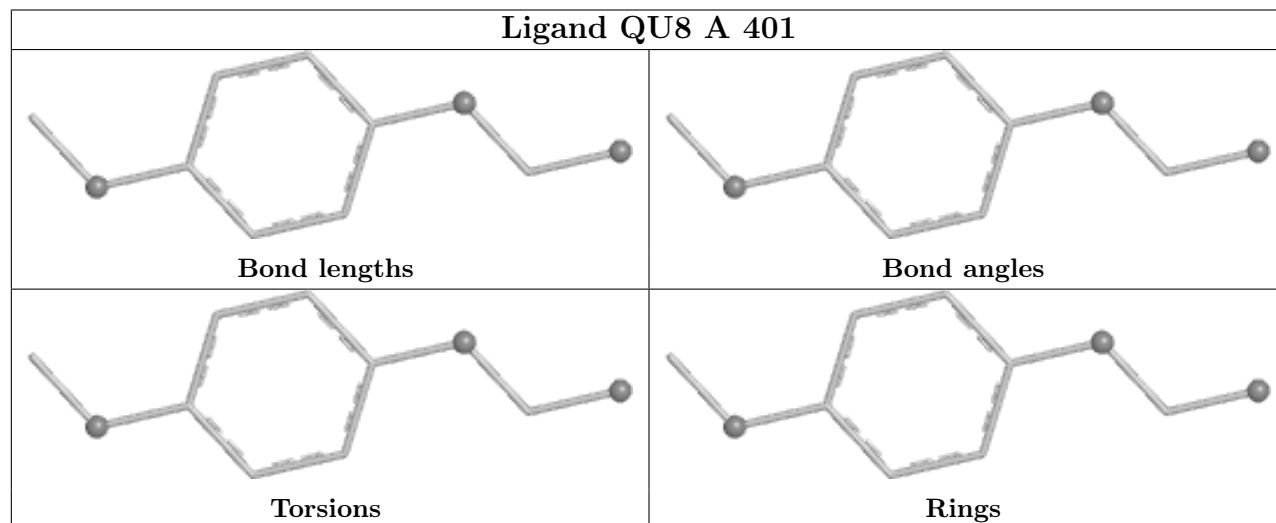
There are no torsion outliers.

There are no ring outliers.

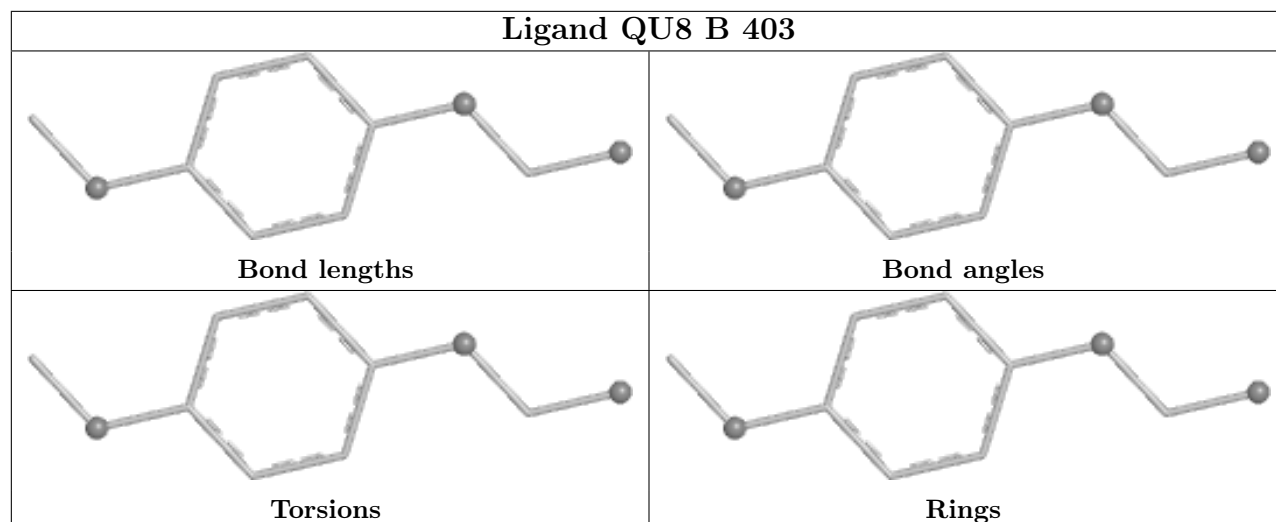
No monomer is involved in short contacts.

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

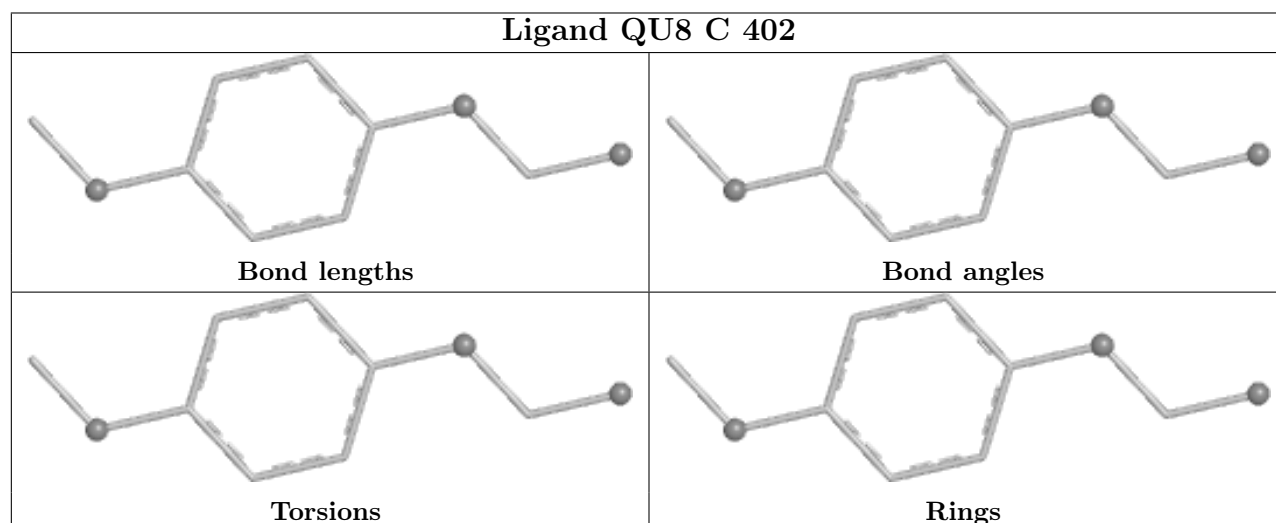
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



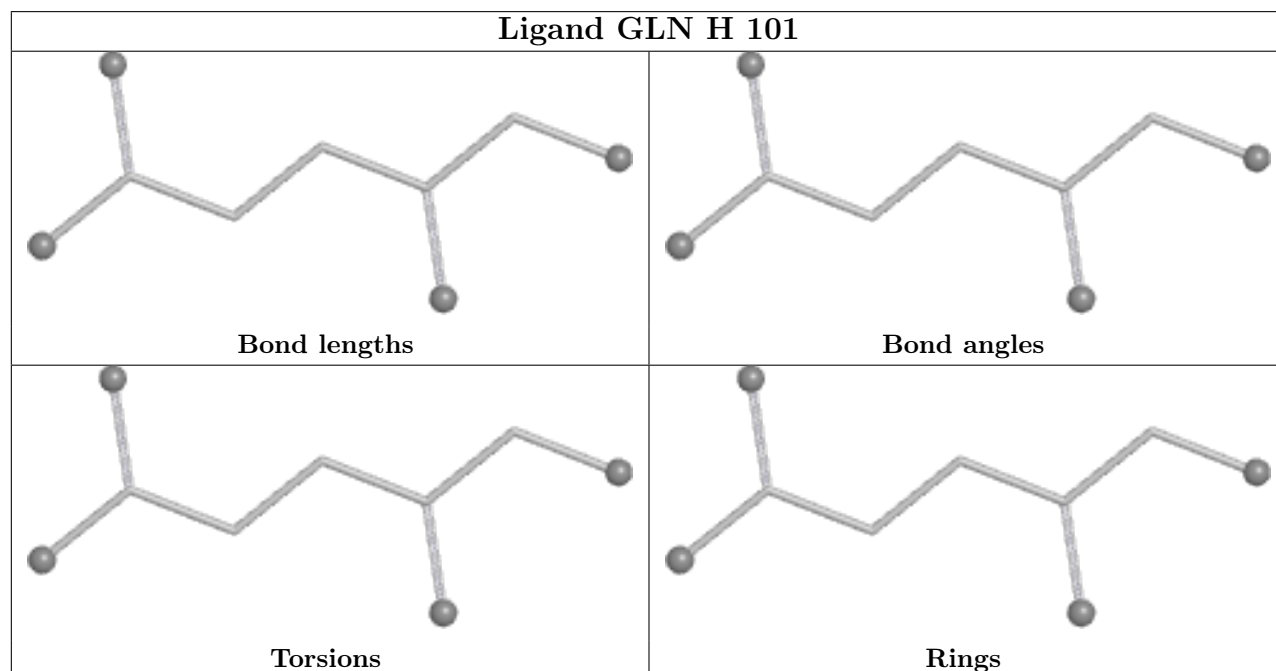
Ligand QU8 B 403



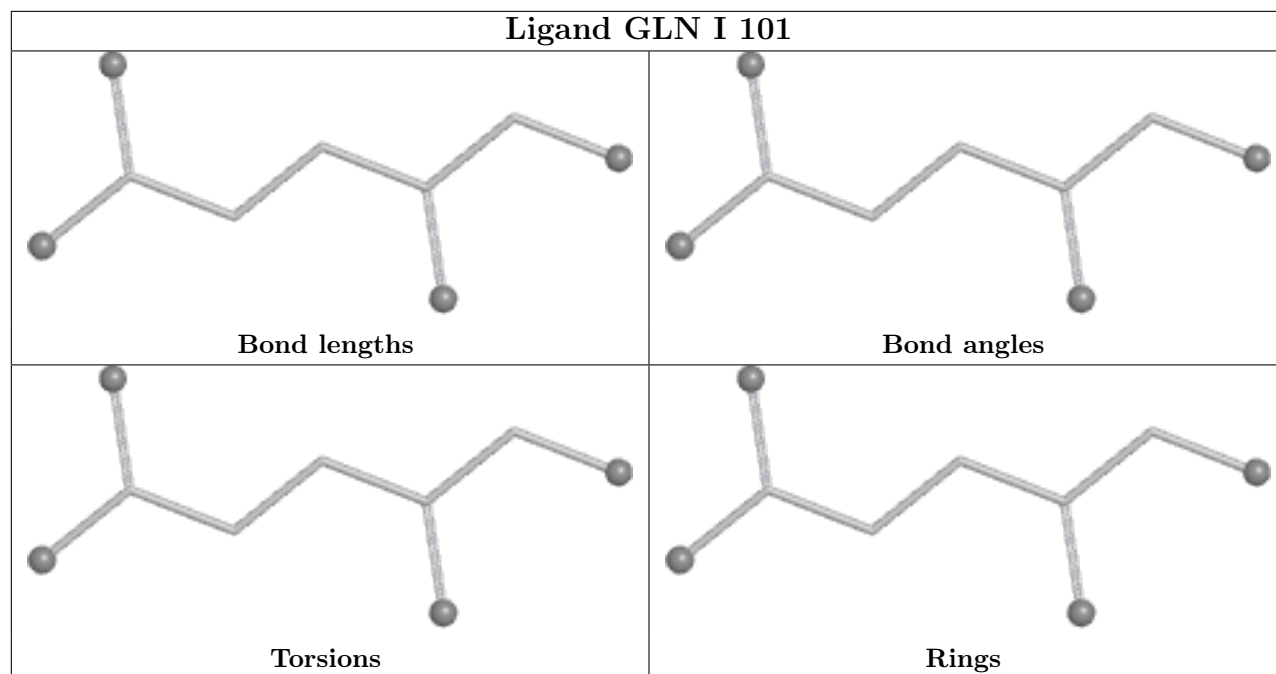
Ligand QU8 C 402



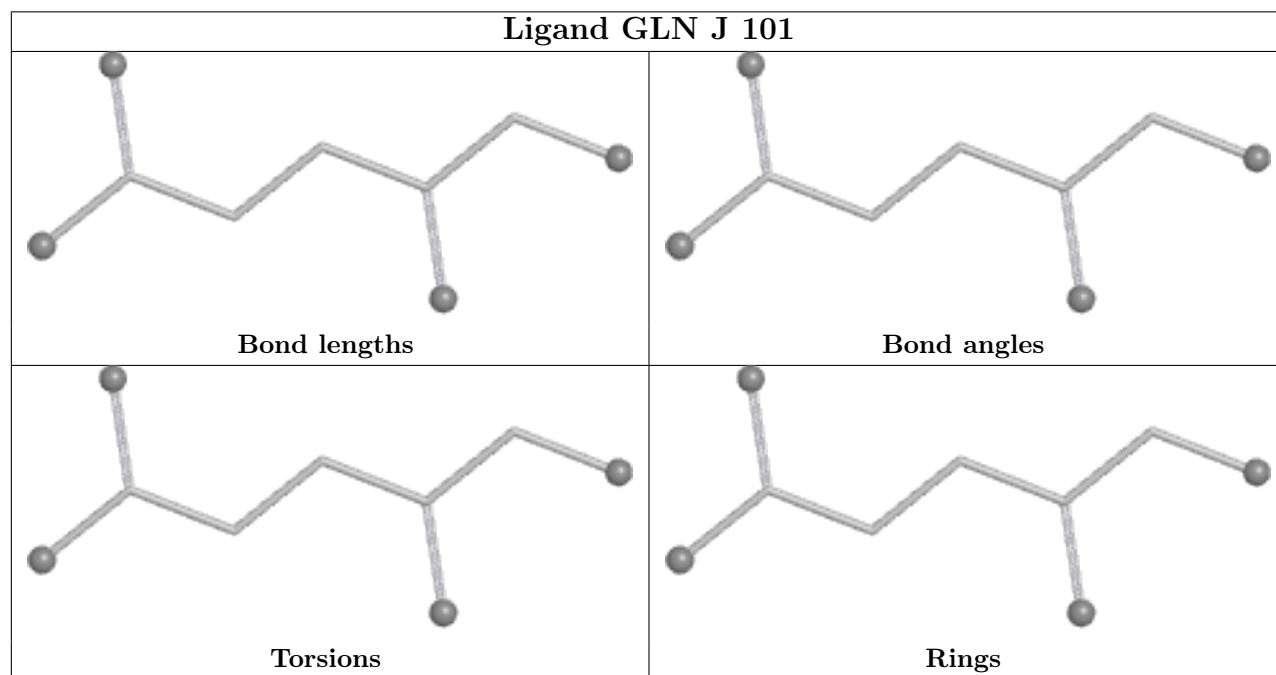
Ligand GLN H 101

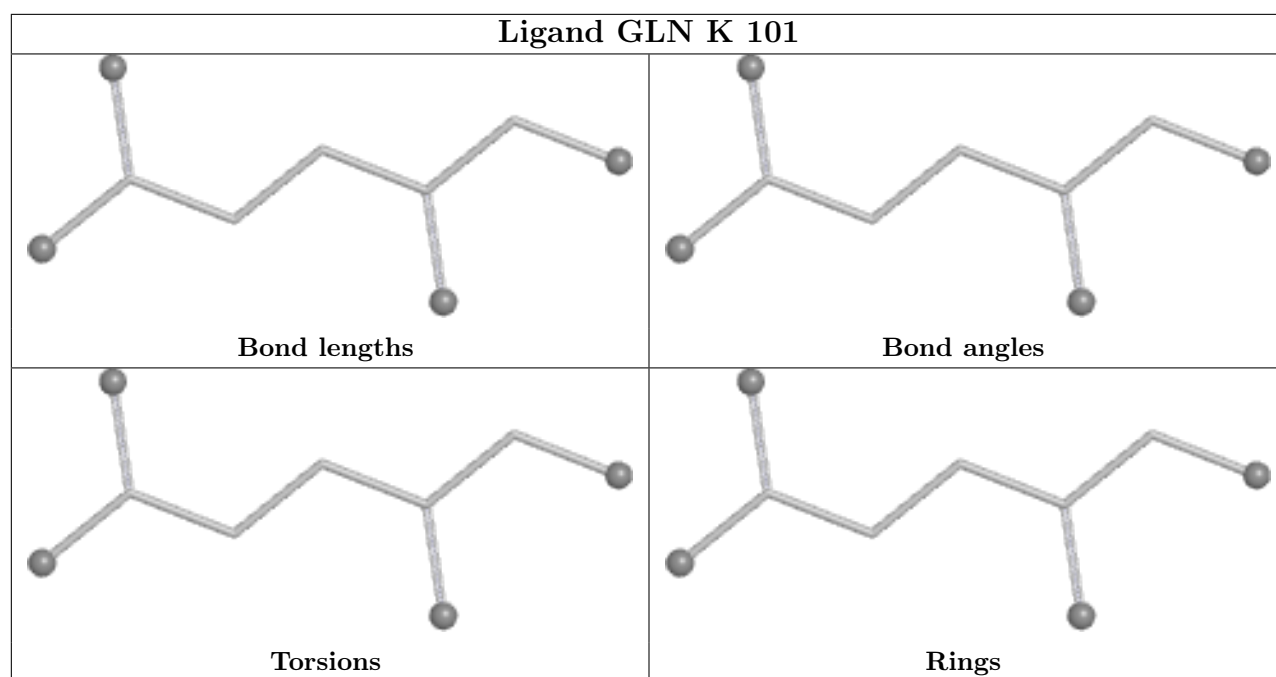


Ligand GLN I 101



Ligand GLN J 101





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	368/386 (95%)	-0.32	5 (1%) 75 75	10, 23, 51, 105	0
1	B	365/386 (94%)	-0.31	3 (0%) 86 86	14, 25, 50, 87	0
1	C	366/386 (94%)	-0.34	7 (1%) 66 67	12, 22, 49, 103	0
1	D	364/386 (94%)	-0.15	11 (3%) 50 48	14, 27, 57, 83	0
2	H	3/6 (50%)	-0.73	0 100 100	16, 16, 16, 20	0
2	I	3/6 (50%)	0.01	0 100 100	23, 23, 34, 36	0
2	J	3/6 (50%)	-0.78	0 100 100	17, 17, 20, 20	0
2	K	3/6 (50%)	-0.22	0 100 100	26, 26, 28, 31	0
All	All	1475/1568 (94%)	-0.28	26 (1%) 68 68	10, 24, 53, 105	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	24	ARG	6.3
1	D	123	GLN	5.7
1	D	122	TRP	5.1
1	A	26	THR	4.8
1	D	184	ILE	4.3
1	C	23	GLY	4.3
1	D	211	ASP	4.0
1	D	210	GLY	3.8
1	D	209	GLY	3.7
1	D	49	LEU	3.7
1	A	209	GLY	3.3
1	B	366	LEU	3.3
1	A	24	ARG	3.1
1	D	208	ASP	3.1
1	C	25	PRO	3.0
1	A	210	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	366	LEU	2.9
1	C	209	GLY	2.8
1	B	251	ASN	2.7
1	D	119	LEU	2.6
1	D	183	PRO	2.5
1	B	208	ASP	2.3
1	C	153[A]	TYR	2.2
1	D	121	ASP	2.2
1	A	153[A]	TYR	2.0
1	C	21	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ALC	I	3	11/12	0.94	0.08	18,22,26,28	0
2	ALC	K	3	11/12	0.96	0.07	18,21,31,31	0
2	ALC	J	3	11/12	0.97	0.07	13,17,25,27	0
2	ALC	H	3	11/12	0.97	0.08	10,19,28,29	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	GOL	B	401	6/6	0.75	0.16	40,42,45,46	6
4	GOL	C	401	6/6	0.86	0.21	55,55,59,60	0
3	QU8	B	402	11/11	0.94	0.10	18,41,44,44	0
3	QU8	B	403	11/11	0.94	0.09	23,28,41,45	0

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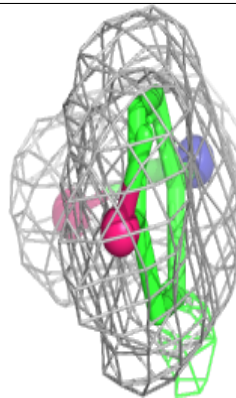
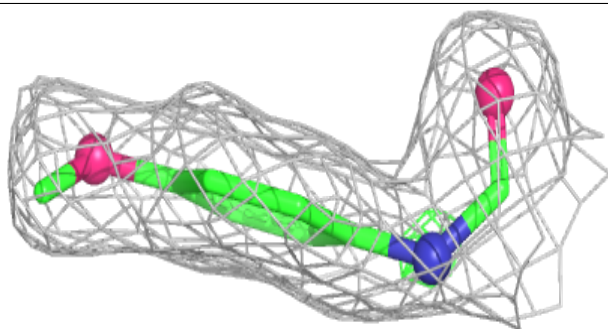
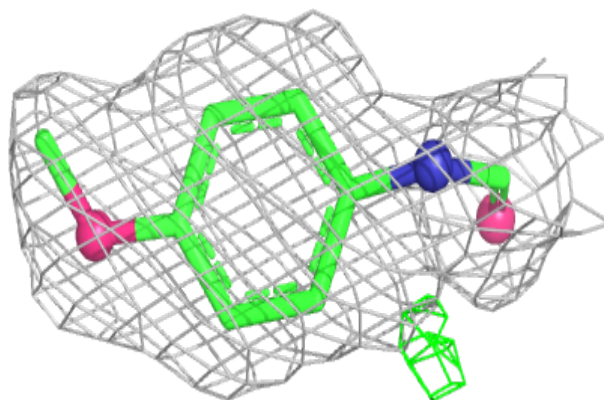
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	QU8	A	401	11/11	0.97	0.09	17,21,36,37	0
3	QU8	C	402	11/11	0.97	0.06	12,16,20,21	0
5	GLN	I	101	9/10	0.97	0.07	16,22,26,27	0
5	GLN	J	101	9/10	0.97	0.06	8,13,18,18	0
5	GLN	K	101	9/10	0.97	0.06	15,22,26,28	0
5	GLN	H	101	9/10	0.98	0.07	11,12,15,15	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.

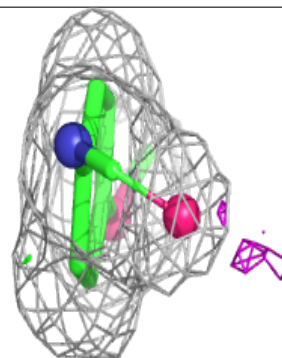
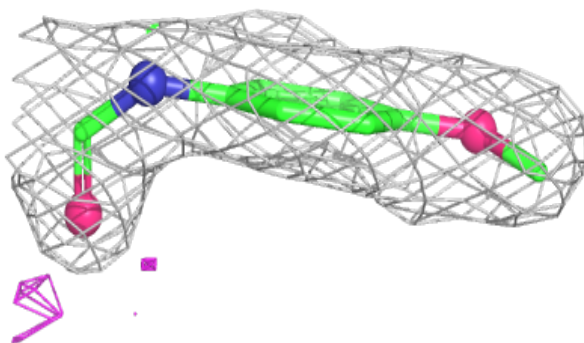
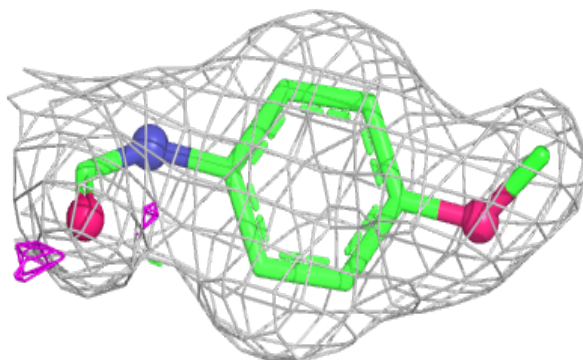
Electron density around QU8 B 402:

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

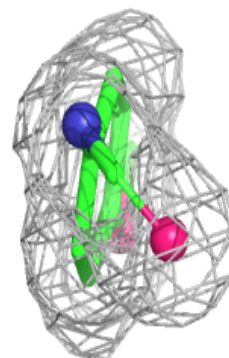
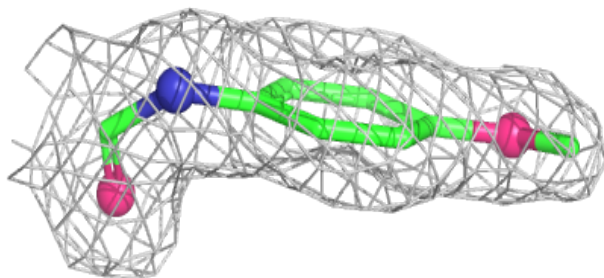
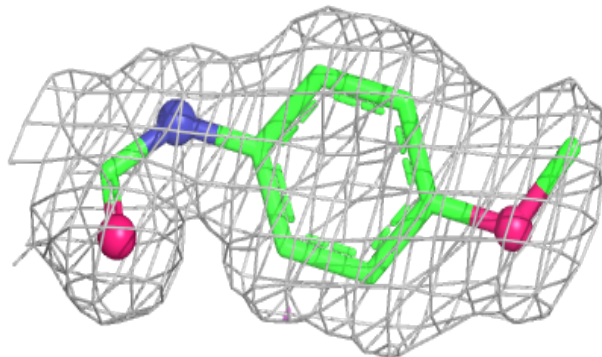


Electron density around QU8 B 403:

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

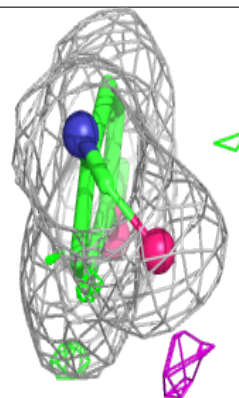
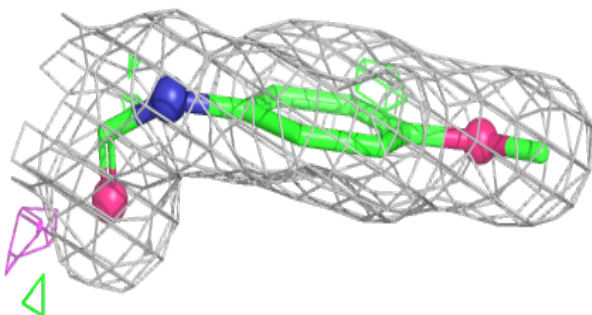
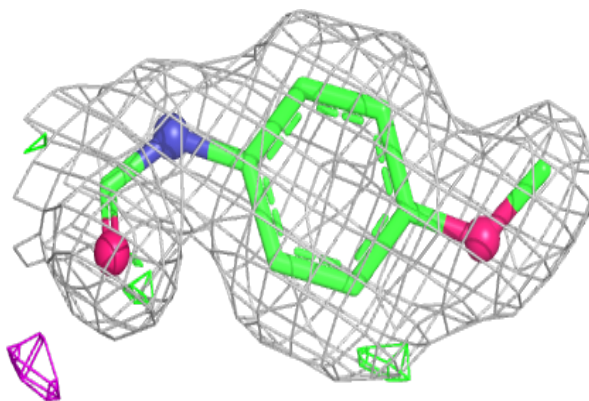
**Electron density around QU8 A 401:**

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

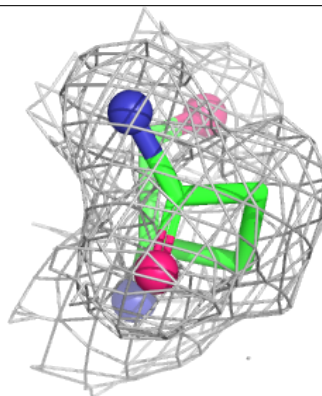
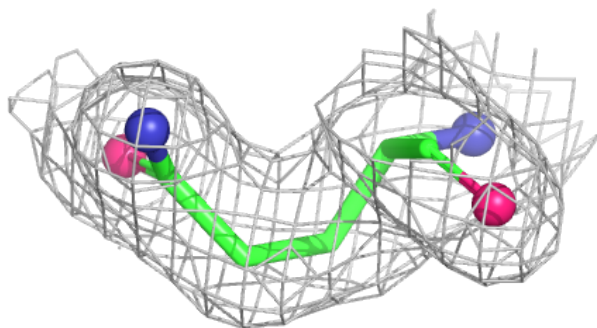
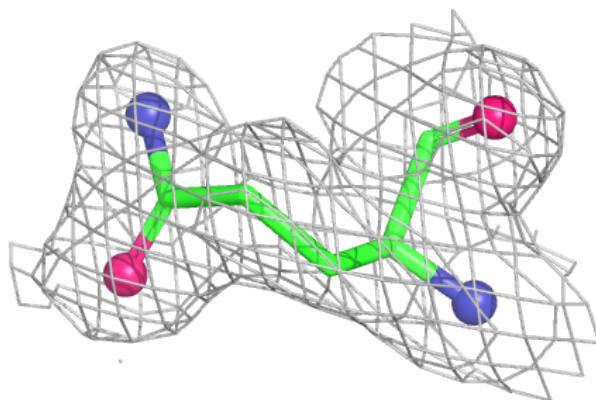


Electron density around QU8 C 402:

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

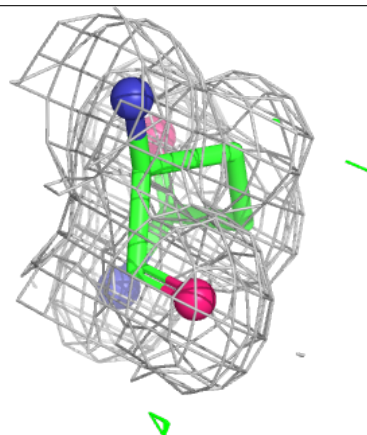
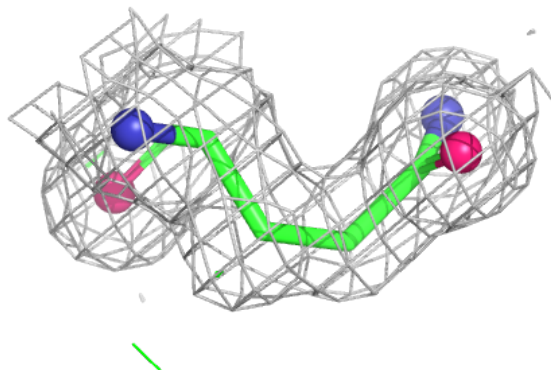
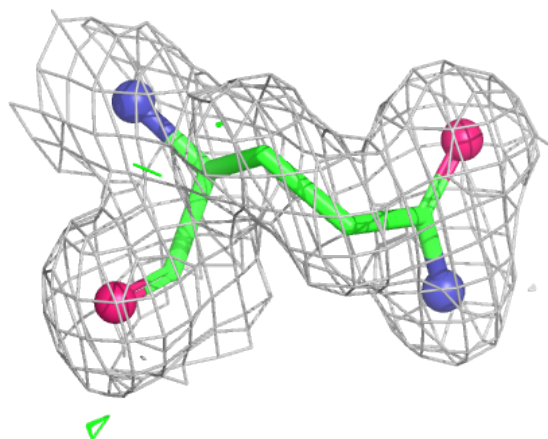
**Electron density around GLN I 101:**

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



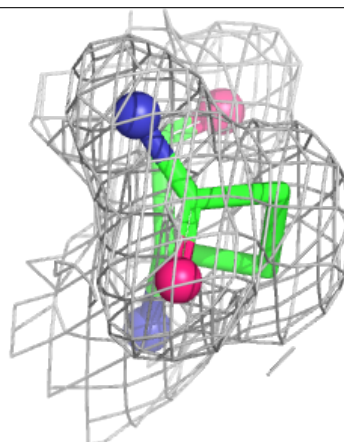
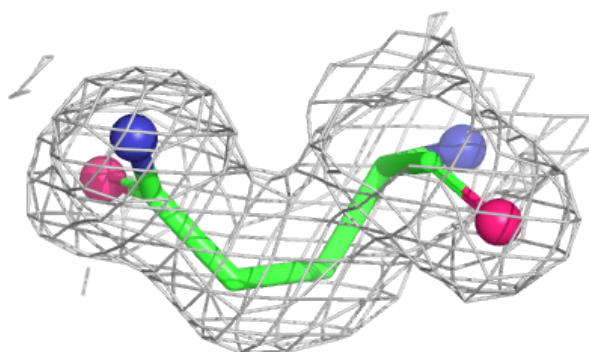
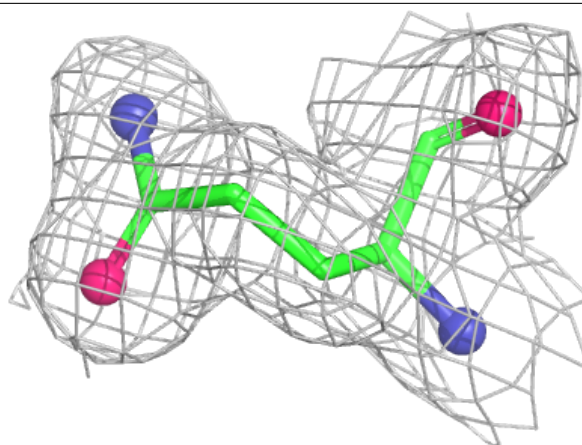
Electron density around GLN J 101:

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

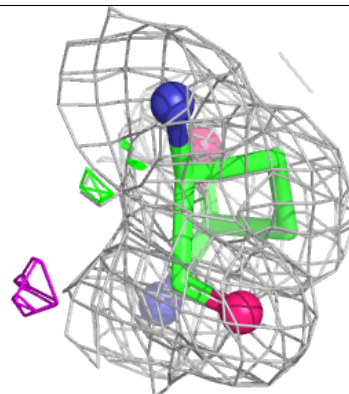
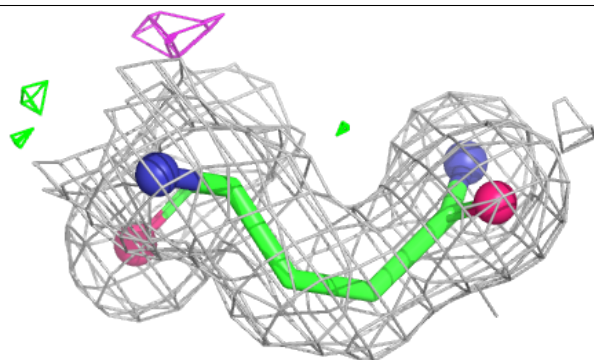
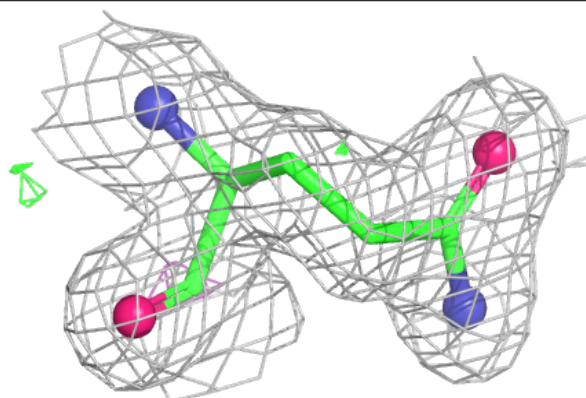


Electron density around GLN K 101:

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

**Electron density around GLN H 101:**

$2mF_o-DF_c$ (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.