



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 08:29 AM UTC

PDB ID : 8YVS / pdb_00008yvs
Title : Crystal structure of GH65 alpha-1,2-glucosidase from *Flavobacterium johnsoniae* in complex with castanospermine
Authors : Nakamura, S.; Miyazaki, T.
Deposited on : 2024-03-29
Resolution : 1.60 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

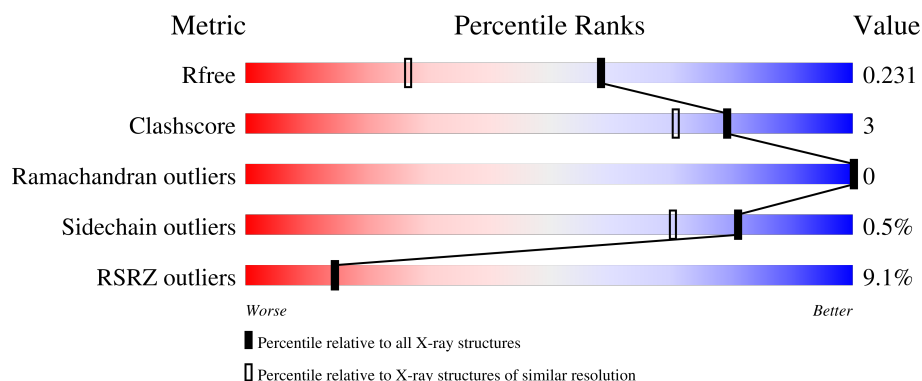
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	678	2% 91% 6% .
1	B	678	23% 89% 7% ..
1	C	678	2% 91% 6% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32723 atoms, of which 15643 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 Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	659	Total	C	H	N	O	S	155	2	0
			10425	3352	5169	883	1000	21			
1	B	659	Total	C	H	N	O	S	155	2	0
			10422	3351	5167	883	1000	21			
1	C	659	Total	C	H	N	O	S	154	1	0
			10424	3351	5169	885	998	21			

There are 60 discrepancies between the modelled and reference sequences:

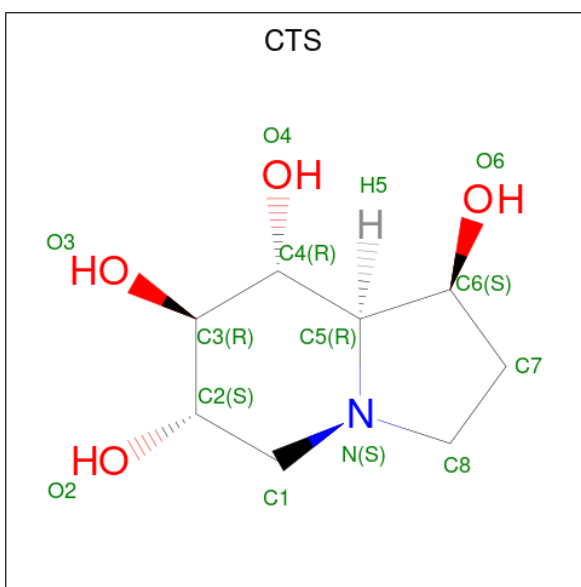
Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP A5FBJ5
A	5	GLY	-	expression tag	UNP A5FBJ5
A	6	SER	-	expression tag	UNP A5FBJ5
A	7	SER	-	expression tag	UNP A5FBJ5
A	8	HIS	-	expression tag	UNP A5FBJ5
A	9	HIS	-	expression tag	UNP A5FBJ5
A	10	HIS	-	expression tag	UNP A5FBJ5
A	11	HIS	-	expression tag	UNP A5FBJ5
A	12	HIS	-	expression tag	UNP A5FBJ5
A	13	HIS	-	expression tag	UNP A5FBJ5
A	14	SER	-	expression tag	UNP A5FBJ5
A	15	SER	-	expression tag	UNP A5FBJ5
A	16	GLY	-	expression tag	UNP A5FBJ5
A	17	LEU	-	expression tag	UNP A5FBJ5
A	18	VAL	-	expression tag	UNP A5FBJ5
A	19	PRO	-	expression tag	UNP A5FBJ5
A	20	ARG	-	expression tag	UNP A5FBJ5
A	21	GLY	-	expression tag	UNP A5FBJ5
A	22	SER	-	expression tag	UNP A5FBJ5
A	23	HIS	-	expression tag	UNP A5FBJ5
B	4	MET	-	initiating methionine	UNP A5FBJ5
B	5	GLY	-	expression tag	UNP A5FBJ5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	6	SER	-	expression tag	UNP A5FBJ5
B	7	SER	-	expression tag	UNP A5FBJ5
B	8	HIS	-	expression tag	UNP A5FBJ5
B	9	HIS	-	expression tag	UNP A5FBJ5
B	10	HIS	-	expression tag	UNP A5FBJ5
B	11	HIS	-	expression tag	UNP A5FBJ5
B	12	HIS	-	expression tag	UNP A5FBJ5
B	13	HIS	-	expression tag	UNP A5FBJ5
B	14	SER	-	expression tag	UNP A5FBJ5
B	15	SER	-	expression tag	UNP A5FBJ5
B	16	GLY	-	expression tag	UNP A5FBJ5
B	17	LEU	-	expression tag	UNP A5FBJ5
B	18	VAL	-	expression tag	UNP A5FBJ5
B	19	PRO	-	expression tag	UNP A5FBJ5
B	20	ARG	-	expression tag	UNP A5FBJ5
B	21	GLY	-	expression tag	UNP A5FBJ5
B	22	SER	-	expression tag	UNP A5FBJ5
B	23	HIS	-	expression tag	UNP A5FBJ5
C	4	MET	-	initiating methionine	UNP A5FBJ5
C	5	GLY	-	expression tag	UNP A5FBJ5
C	6	SER	-	expression tag	UNP A5FBJ5
C	7	SER	-	expression tag	UNP A5FBJ5
C	8	HIS	-	expression tag	UNP A5FBJ5
C	9	HIS	-	expression tag	UNP A5FBJ5
C	10	HIS	-	expression tag	UNP A5FBJ5
C	11	HIS	-	expression tag	UNP A5FBJ5
C	12	HIS	-	expression tag	UNP A5FBJ5
C	13	HIS	-	expression tag	UNP A5FBJ5
C	14	SER	-	expression tag	UNP A5FBJ5
C	15	SER	-	expression tag	UNP A5FBJ5
C	16	GLY	-	expression tag	UNP A5FBJ5
C	17	LEU	-	expression tag	UNP A5FBJ5
C	18	VAL	-	expression tag	UNP A5FBJ5
C	19	PRO	-	expression tag	UNP A5FBJ5
C	20	ARG	-	expression tag	UNP A5FBJ5
C	21	GLY	-	expression tag	UNP A5FBJ5
C	22	SER	-	expression tag	UNP A5FBJ5
C	23	HIS	-	expression tag	UNP A5FBJ5

- Molecule 2 is CASTANOSPERMINE (CCD ID: CTS) (formula: $C_8H_{15}NO_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 28	C 8	H 15	N 1	O 4	4	0
2	A	1	Total 28	C 8	H 15	N 1	O 4	4	0
2	B	1	Total 28	C 8	H 15	N 1	O 4	4	0
2	B	1	Total 28	C 8	H 15	N 1	O 4	4	0
2	C	1	Total 28	C 8	H 15	N 1	O 4	4	0
2	C	1	Total 28	C 8	H 15	N 1	O 4	4	0

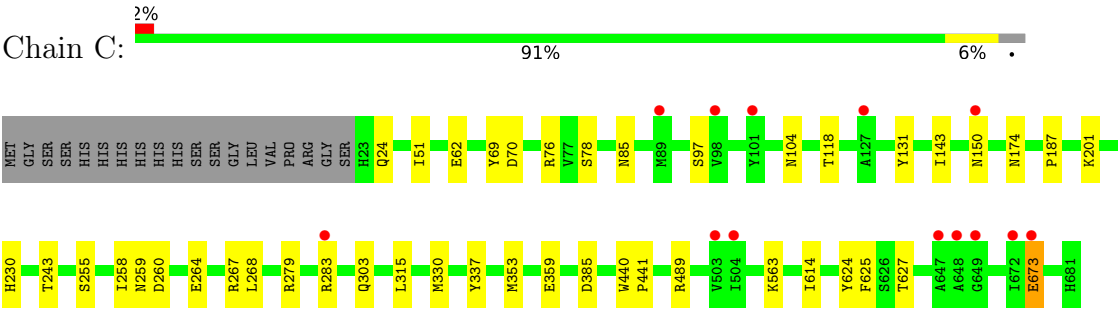
- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	2	0
			10	2	6	2		
3	A	1	Total	C	H	O	2	0
			10	2	6	2		
3	A	1	Total	C	H	O	2	0
			10	2	6	2		
3	A	1	Total	C	H	O	2	0
			10	2	6	2		
3	B	1	Total	C	H	O	2	0
			10	2	6	2		
3	C	1	Total	C	H	O	2	0
			10	2	6	2		
3	C	1	Total	C	H	O	2	0
			10	2	6	2		
3	C	1	Total	C	H	O	2	0
			10	2	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	445	Total	O	0	0
			445	445		
4	B	293	Total	O	0	0
			293	293		
4	C	466	Total	O	0	0
			466	466		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.99Å 194.51Å 112.19Å 90.00° 117.21° 90.00°	Depositor
Resolution (Å)	48.67 – 1.60 48.67 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.67-1.60) 99.9 (48.67-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.202 , 0.223 0.206 , 0.231	Depositor DCC
R_{free} test set	15471 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 33.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32723	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: CTS, EDO

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	0.67	0/5391	1.01	4/7316 (0.1%)
1	B	0.66	1/5390 (0.0%)	1.03	7/7315 (0.1%)
1	C	0.69	0/5387	1.04	5/7310 (0.1%)
All	All	0.67	1/16168 (0.0%)	1.03	16/21941 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	3
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	78	SER	CA-CB	-5.59	1.44	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	385	ASP	CA-CB-CG	6.88	119.48	112.60
1	B	566	GLN	CB-CA-C	-6.74	99.22	110.68
1	B	85	ASN	CA-CB-CG	-6.67	105.93	112.60
1	C	260	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	560	ARG	NE-CZ-NH2	5.90	124.51	119.20
1	C	187	PRO	N-CD-CG	-5.64	94.74	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	PRO	N-CD-CG	-5.60	94.80	103.20
1	A	385	ASP	CA-CB-CG	5.49	118.09	112.60
1	B	385	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	295	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	368	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	B	490	ASN	CA-CB-CG	5.20	117.80	112.60
1	A	260	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	70	ASP	CA-CB-CG	5.14	117.74	112.60
1	C	359	GLU	CB-CG-CD	5.10	121.27	112.60
1	B	187	PRO	N-CD-CG	-5.05	95.62	103.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	588	ARG	Sidechain
1	B	368	ARG	Sidechain
1	B	76	ARG	Sidechain
1	C	279	ARG	Sidechain
1	C	489	ARG	Sidechain
1	C	76	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5256	5169	5152	20	0
1	B	5255	5167	5150	34	0
1	C	5255	5169	5152	27	0
2	A	26	30	30	4	0
2	B	26	30	30	1	0
2	C	26	30	30	4	0
3	A	16	24	23	3	0
3	B	4	6	6	0	0
3	C	12	18	18	3	0
4	A	445	0	0	4	0
4	B	293	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	466	0	0	3	0
All	All	17080	15643	15591	85	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 (85) 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)
2:A:701:CTS:H12	4:A:951:HOH:O	1.40	1.17
1:B:56:GLU:HG2	4:B:1019:HOH:O	1.57	1.04
2:C:701:CTS:H12	4:C:818:HOH:O	1.57	1.01
2:B:701:CTS:H12	4:B:999:HOH:O	1.62	0.97
1:C:614:ILE:HD11	3:C:704:EDO:H21	1.58	0.83
1:C:150:ASN:OD1	1:C:243:THR:OG1	1.98	0.81
1:B:148:ASN:OD1	1:B:245[B]:SER:OG	2.05	0.70
1:A:614:ILE:HD11	3:A:704:EDO:H12	1.73	0.69
1:B:550:LYS:NZ	1:B:644:ASP:OD1	2.25	0.69
1:C:614:ILE:CD1	3:C:704:EDO:H21	2.27	0.65
1:B:562:LEU:C	1:B:566:GLN:HE21	2.06	0.63
1:C:673:GLU:H	1:C:673:GLU:CD	2.06	0.62
1:B:403:VAL:HG12	1:C:267:ARG:HG3	1.83	0.61
1:C:201:LYS:HE3	4:C:1194:HOH:O	2.01	0.60
1:B:300:GLY:HA3	1:B:663:LYS:HE3	1.83	0.59
1:B:40:TYR:CD2	1:B:608:ASN:HB3	2.37	0.59
2:A:701:CTS:H81	2:A:702:CTS:H2	1.86	0.58
1:B:209:LEU:HD11	1:B:249:ILE:CD1	2.36	0.56
1:B:85:ASN:ND2	1:B:88[B]:ASN:OD1	2.39	0.55
1:A:303:GLN:HG2	4:A:1202:HOH:O	2.06	0.55
1:B:57:PRO:HG3	1:B:103:ILE:HD13	1.87	0.55
2:C:701:CTS:H81	2:C:702:CTS:H2	1.87	0.55
1:B:381:ILE:CG2	1:C:268:LEU:HD21	2.38	0.54
1:B:259:ASN:ND2	1:B:259:ASN:H	2.07	0.53
1:B:315:LEU:HD23	1:B:353:MET:HE3	1.91	0.53
1:B:588:ARG:NH1	1:B:644:ASP:OD2	2.40	0.51
1:C:673:GLU:CD	1:C:673:GLU:N	2.68	0.51
2:A:701:CTS:C8	2:A:702:CTS:H2	2.40	0.51
1:B:383:GLY:O	1:C:283[A]:ARG:NH2	2.44	0.51
1:B:209:LEU:HD11	1:B:249:ILE:HD11	1.94	0.50
2:C:701:CTS:C8	2:C:702:CTS:H2	2.41	0.50
1:B:51:ILE:HD11	1:B:143:ILE:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:TYR:CE2	3:A:703:EDO:H21	2.47	0.48
1:A:82:PRO:HG3	1:A:335:LEU:HD11	1.96	0.48
1:A:148:ASN:ND2	1:A:245:SER:HB2	2.29	0.48
1:C:315:LEU:HD23	1:C:353:MET:HE3	1.96	0.48
2:A:701:CTS:H82	4:A:951:HOH:O	2.14	0.47
1:B:385:ASP:HB2	4:B:1059:HOH:O	2.13	0.47
1:B:381:ILE:HG22	1:C:268:LEU:HD21	1.98	0.46
1:B:85:ASN:C	1:B:85:ASN:OD1	2.55	0.46
1:B:255:SER:HA	1:B:258:ILE:O	2.16	0.46
1:A:315:LEU:HD23	1:A:353:MET:HE3	1.97	0.45
1:C:24:GLN:NE2	1:C:303:GLN:OE1	2.49	0.45
1:C:330:MET:HA	1:C:624:TYR:O	2.17	0.45
1:C:337:TYR:HE1	2:C:702:CTS:H12	1.83	0.44
1:A:524:GLY:O	1:A:560:ARG:HD2	2.17	0.44
1:B:209:LEU:HD11	1:B:249:ILE:HD12	2.00	0.44
1:B:319:THR:HG21	1:B:364:MET:HE3	1.99	0.44
1:A:195:THR:HB	1:A:196:PRO:HD2	1.99	0.44
1:A:255:SER:HA	1:A:258:ILE:O	2.18	0.44
1:B:73:LYS:NZ	4:B:814:HOH:O	2.51	0.44
1:C:174:ASN:HB3	1:C:230:HIS:CG	2.53	0.44
1:C:104:ASN:ND2	4:C:815:HOH:O	2.49	0.44
1:A:330:MET:HA	1:A:624:TYR:O	2.18	0.43
1:B:199:ARG:HG2	4:B:892:HOH:O	2.19	0.43
1:A:477:ILE:HD12	1:A:477:ILE:C	2.44	0.43
1:A:337:TYR:CE2	3:A:703:EDO:C2	3.01	0.43
1:C:264:GLU:OE1	1:C:267:ARG:NH2	2.51	0.42
1:A:440:TRP:HB3	1:A:441:PRO:HD3	2.00	0.42
1:B:259:ASN:H	1:B:259:ASN:HD22	1.67	0.42
1:C:259:ASN:ND2	1:C:259:ASN:H	2.18	0.42
1:B:330:MET:HA	1:B:624:TYR:O	2.19	0.42
1:B:64:VAL:HA	4:B:809:HOH:O	2.20	0.42
1:A:62:GLU:HA	1:A:85:ASN:HD21	1.85	0.42
1:B:174:ASN:HB3	1:B:230:HIS:CG	2.55	0.41
1:C:62:GLU:HA	1:C:85:ASN:HD21	1.85	0.41
1:C:69:TYR:HB3	1:C:78:SER:HB2	2.01	0.41
1:A:174:ASN:HB3	1:A:230:HIS:CG	2.55	0.41
1:A:373:ASP:HB3	4:A:1043:HOH:O	2.20	0.41
1:B:281:LEU:HD23	1:B:281:LEU:HA	1.93	0.41
1:B:477:ILE:C	1:B:477:ILE:HD12	2.45	0.41
1:A:110:LEU:HD21	1:A:313:TYR:CE2	2.56	0.41
1:C:440:TRP:HB3	1:C:441:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283[B]:ARG:CZ	1:C:283[B]:ARG:HB3	2.50	0.41
1:C:255:SER:HA	1:C:258:ILE:O	2.20	0.41
1:C:614:ILE:CG1	3:C:704:EDO:H21	2.51	0.41
1:B:118:THR:HA	1:B:131:TYR:O	2.21	0.41
1:C:625:PHE:CZ	1:C:627:THR:HB	2.55	0.41
1:A:35:ASP:O	1:A:39:TYR:HB2	2.21	0.41
1:A:118:THR:HA	1:A:131:TYR:O	2.21	0.40
1:C:51:ILE:HD11	1:C:143:ILE:HD12	2.03	0.40
1:C:118:THR:HA	1:C:131:TYR:O	2.22	0.40
1:A:319:THR:HG21	1:A:364:MET:HE3	2.02	0.40
1:B:187:PRO:HG2	1:B:220:ILE:HG13	2.04	0.40
1:B:625:PHE:CZ	1:B:627:THR:HB	2.57	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	659/678 (97%)	637 (97%)	22 (3%)	0	100	100
1	B	659/678 (97%)	637 (97%)	22 (3%)	0	100	100
1	C	658/678 (97%)	638 (97%)	20 (3%)	0	100	100
All	All	1976/2034 (97%)	1912 (97%)	64 (3%)	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	567/581 (98%)	565 (100%)	2 (0%)	84	75
1	B	567/581 (98%)	563 (99%)	4 (1%)	76	63
1	C	566/581 (97%)	563 (100%)	3 (0%)	81	70
All	All	1700/1743 (98%)	1691 (100%)	9 (0%)	81	70

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASP
1	A	673	GLU
1	B	32	ASP
1	B	97	SER
1	B	149	ILE
1	B	259	ASN
1	C	97	SER
1	C	563	LYS
1	C	673	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	85	ASN
1	A	94	ASN
1	A	104	ASN
1	A	105	ASN
1	A	108	GLN
1	A	122	GLN
1	A	148	ASN
1	A	171	ASN
1	A	178	ASN
1	A	183	HIS
1	A	185	ASN
1	A	206	ASN
1	A	476	ASN
1	A	539	GLN
1	A	594	GLN
1	A	608	ASN

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Mol	Chain	Res	Type
1	B	94	ASN
1	B	108	GLN
1	B	150	ASN
1	B	178	ASN
1	B	183	HIS
1	B	185	ASN
1	B	206	ASN
1	B	259	ASN
1	B	282	ASN
1	B	476	ASN
1	B	539	GLN
1	B	566	GLN
1	B	571	GLN
1	B	594	GLN
1	B	608	ASN
1	C	85	ASN
1	C	94	ASN
1	C	108	GLN
1	C	171	ASN
1	C	178	ASN
1	C	183	HIS
1	C	185	ASN
1	C	206	ASN
1	C	259	ASN
1	C	293	GLN
1	C	594	GLN
1	C	608	ASN
1	C	681	HIS

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

14 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	CTS	B	702	-	14,14,14	0.56	0	17,21,21	1.64	2 (11%)
2	CTS	C	701	-	14,14,14	1.17	1 (7%)	17,21,21	2.09	5 (29%)
3	EDO	C	704	-	3,3,3	0.52	0	2,2,2	0.20	0
2	CTS	A	701	-	14,14,14	0.94	1 (7%)	17,21,21	1.90	3 (17%)
2	CTS	B	701	-	14,14,14	0.96	1 (7%)	17,21,21	1.46	3 (17%)
2	CTS	C	702	-	14,14,14	0.80	0	17,21,21	2.07	5 (29%)
3	EDO	C	705	-	3,3,3	0.32	0	2,2,2	0.18	0
3	EDO	A	704	-	3,3,3	0.40	0	2,2,2	0.28	0
3	EDO	A	703	-	3,3,3	0.74	0	2,2,2	0.30	0
3	EDO	A	705	-	3,3,3	0.06	0	2,2,2	0.13	0
3	EDO	C	703	-	3,3,3	0.37	0	2,2,2	0.52	0
3	EDO	A	706	-	3,3,3	0.34	0	2,2,2	0.36	0
2	CTS	A	702	-	14,14,14	0.87	0	17,21,21	1.77	4 (23%)
3	EDO	B	703	-	3,3,3	0.57	0	2,2,2	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CTS	B	702	-	-	-	0/2/2/2
2	CTS	C	701	-	-	-	0/2/2/2
3	EDO	C	704	-	-	0/1/1/1	-
2	CTS	A	701	-	-	-	0/2/2/2
2	CTS	B	701	-	-	-	0/2/2/2
2	CTS	C	702	-	-	-	0/2/2/2
3	EDO	C	705	-	-	0/1/1/1	-
3	EDO	A	704	-	-	0/1/1/1	-
3	EDO	A	703	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	705	-	-	0/1/1/1	-
3	EDO	C	703	-	-	0/1/1/1	-
3	EDO	A	706	-	-	0/1/1/1	-
2	CTS	A	702	-	-	-	0/2/2/2
3	EDO	B	703	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	CTS	C1-N	-2.39	1.43	1.47
2	B	701	CTS	C2-C3	-2.01	1.49	1.52
2	A	701	CTS	C2-C3	-2.00	1.49	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	702	CTS	C1-N-C5	5.57	120.45	110.62
2	C	701	CTS	C1-N-C5	4.72	118.95	110.62
2	A	701	CTS	C1-N-C5	4.59	118.72	110.62
2	A	702	CTS	C1-N-C5	4.26	118.13	110.62
2	B	702	CTS	C2-C1-N	3.93	118.01	110.72
2	B	702	CTS	C1-N-C5	3.65	117.07	110.62
2	A	701	CTS	C2-C1-N	3.53	117.28	110.72
2	C	701	CTS	C2-C1-N	3.39	117.02	110.72
2	B	701	CTS	C1-N-C5	3.39	116.59	110.62
2	B	701	CTS	C2-C1-N	3.32	116.88	110.72
2	A	701	CTS	C7-C6-C5	-3.11	98.90	102.80
2	C	702	CTS	O6-C6-C7	3.05	118.58	111.43
2	C	702	CTS	C2-C1-N	2.97	116.24	110.72
2	A	702	CTS	O4-C4-C5	-2.92	101.59	109.14
2	C	701	CTS	O2-C2-C1	2.89	115.18	109.66
2	C	701	CTS	O4-C4-C5	-2.62	102.35	109.14
2	C	701	CTS	C7-C6-C5	-2.60	99.55	102.80
2	A	702	CTS	O6-C6-C7	2.59	117.51	111.43
2	A	702	CTS	C2-C1-N	2.51	115.38	110.72
2	B	701	CTS	O2-C2-C1	2.37	114.19	109.66
2	C	702	CTS	C1-C2-C3	2.27	112.87	110.17
2	C	702	CTS	O4-C4-C5	-2.16	103.55	109.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	703	EDO	O1-C1-C2-O2

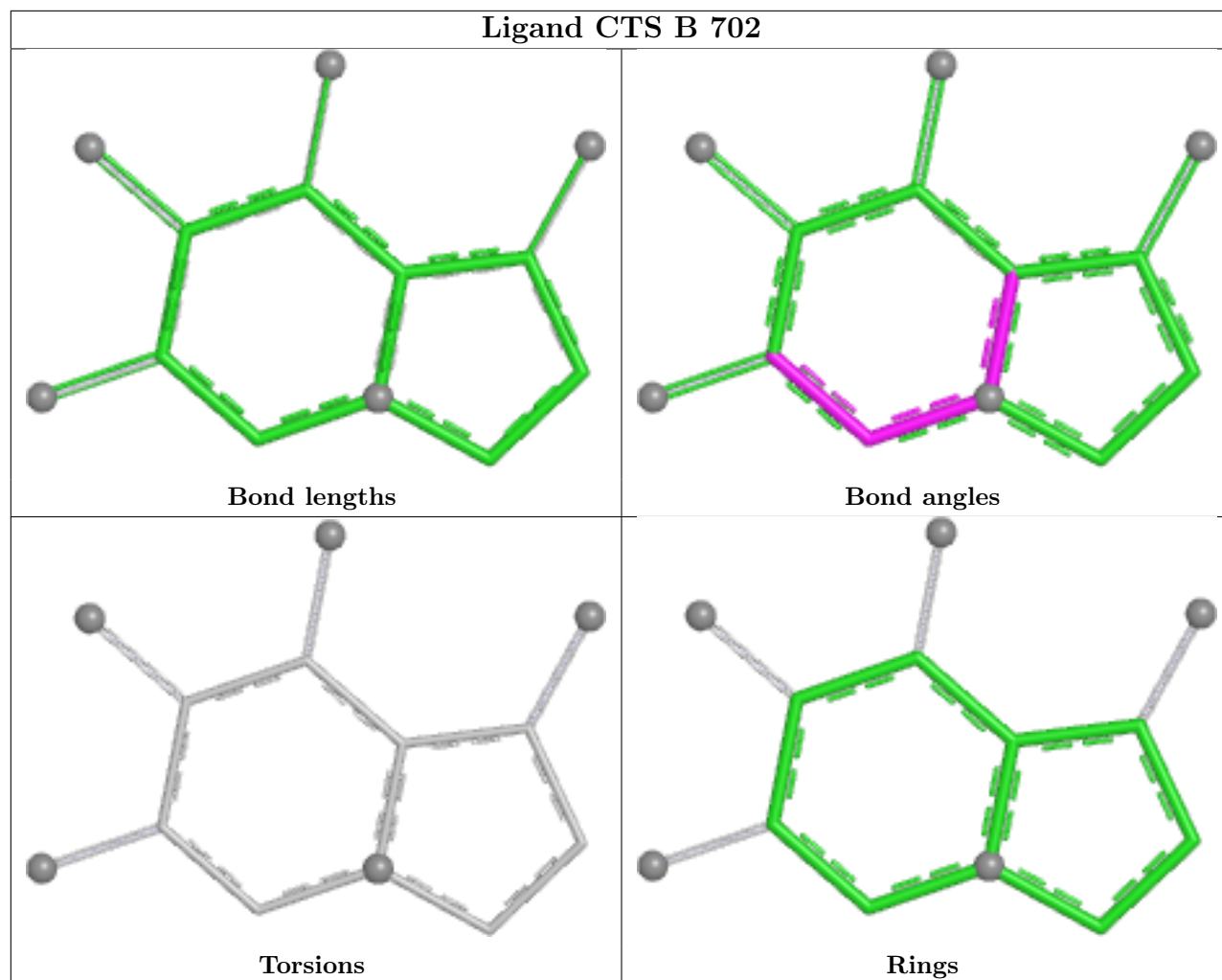
There are no ring outliers.

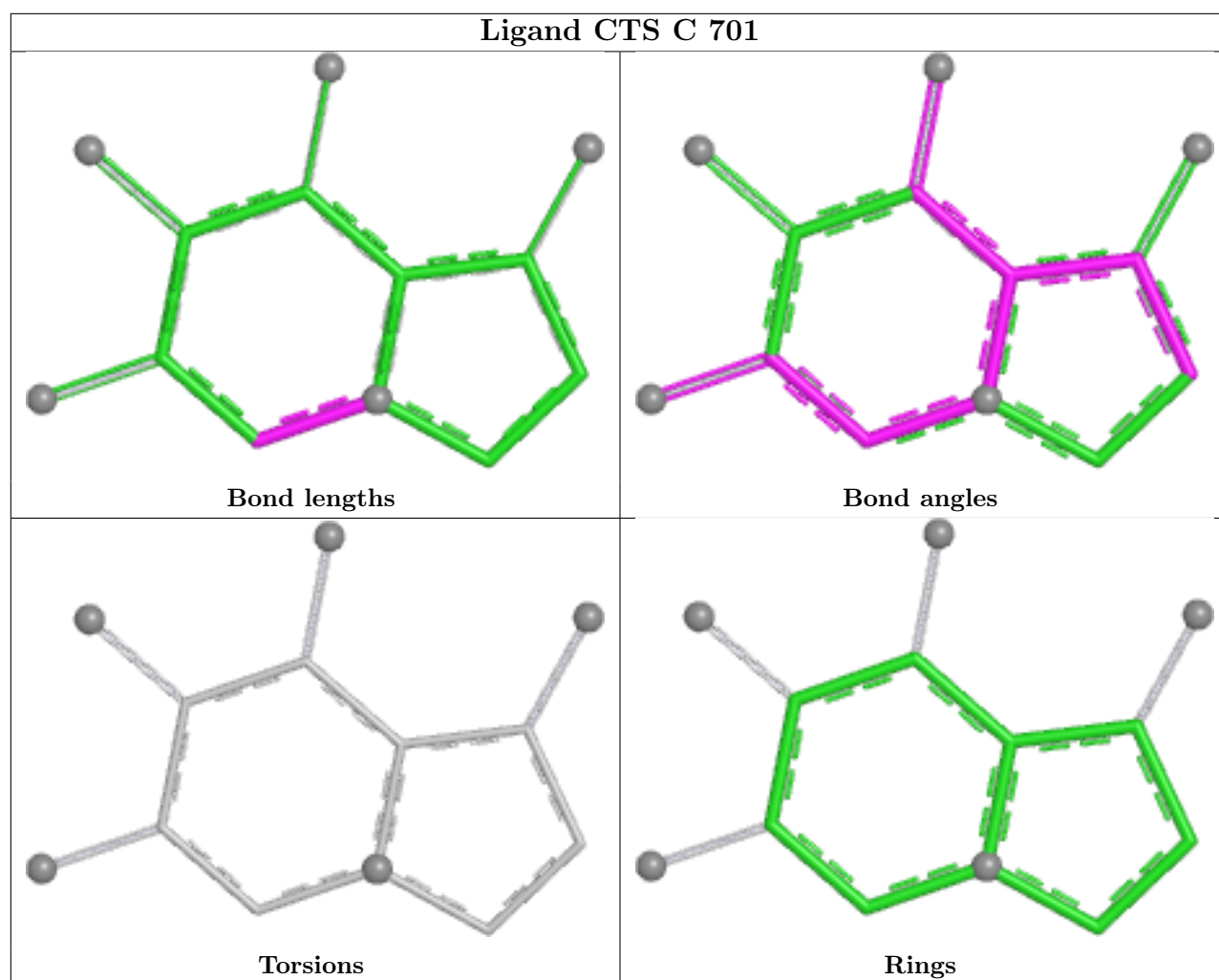
8 monomers are involved in 15 short contacts:

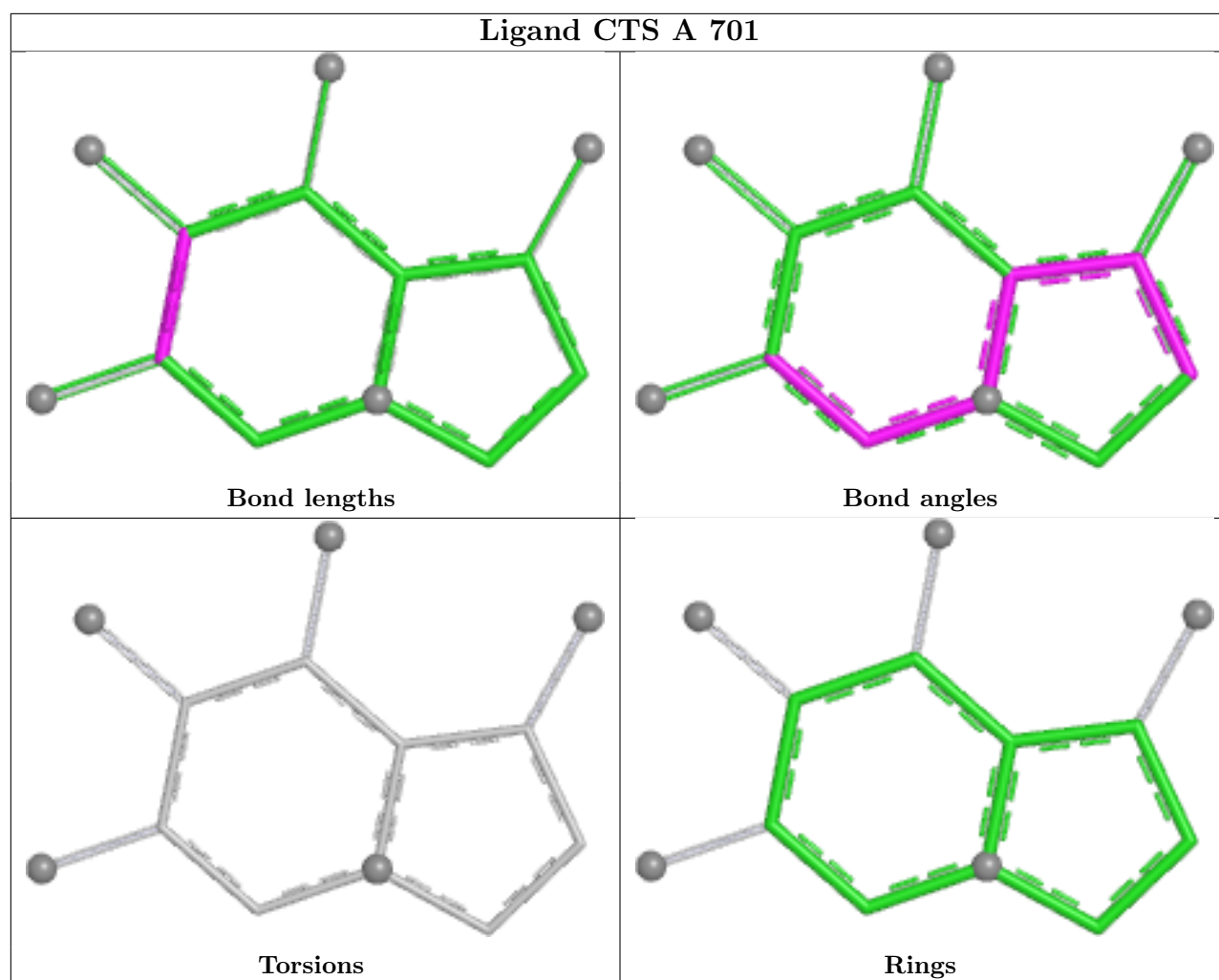
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	701	CTS	3	0
3	C	704	EDO	3	0
2	A	701	CTS	4	0
2	B	701	CTS	1	0
2	C	702	CTS	3	0
3	A	704	EDO	1	0
3	A	703	EDO	2	0
2	A	702	CTS	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

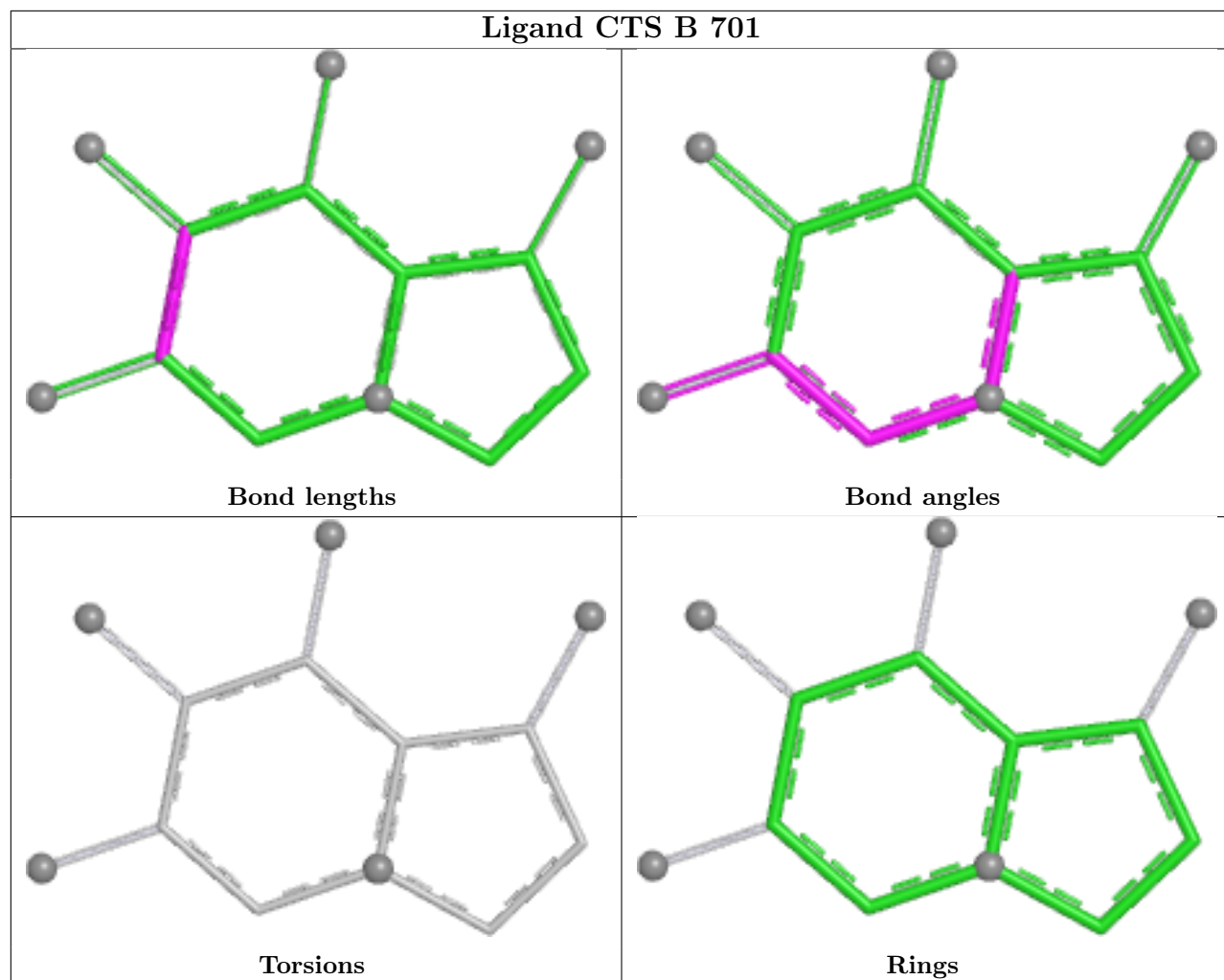
Ligand CTS B 702

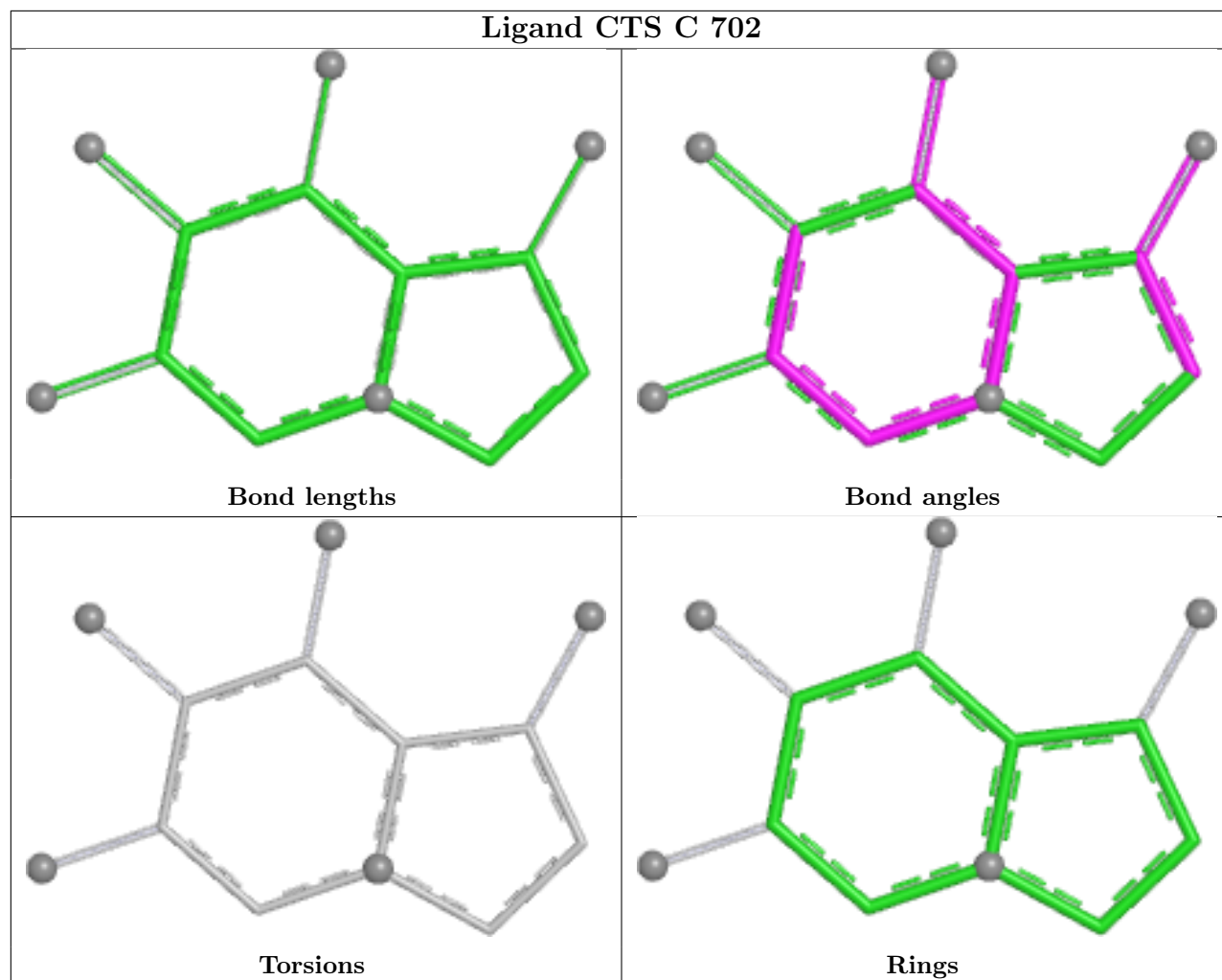


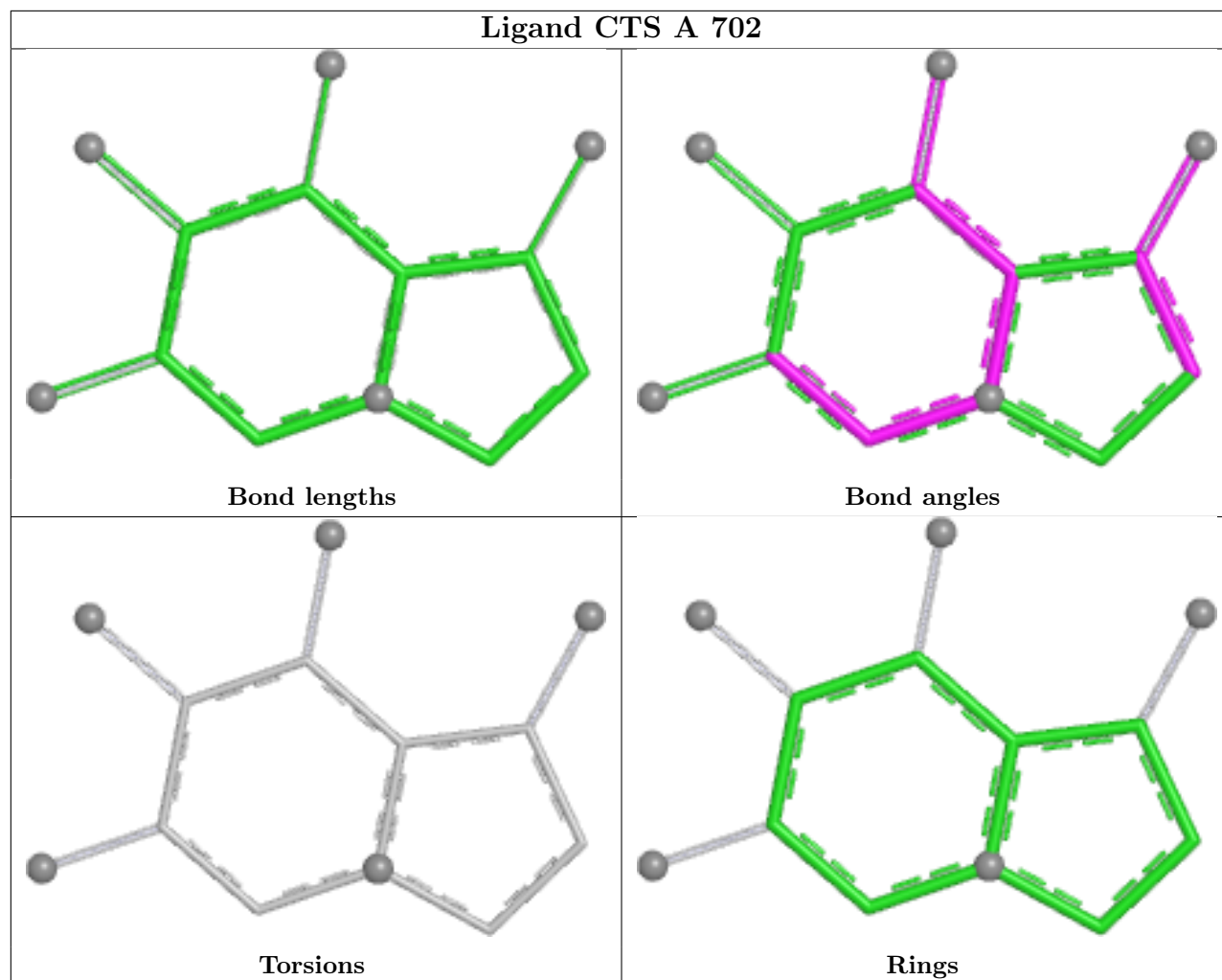




Ligand CTS B 701







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	659/678 (97%)	0.41	13 (1%) 65 69	11, 27, 49, 70	2 (0%)
1	B	659/678 (97%)	1.16	153 (23%) 2 2	14, 35, 64, 88	2 (0%)
1	C	659/678 (97%)	0.37	13 (1%) 65 69	17, 27, 44, 60	1 (0%)
All	All	1977/2034 (97%)	0.65	179 (9%) 15 15	11, 29, 55, 88	5 (0%)

All (179) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	101	TYR	5.5
1	B	298	VAL	4.9
1	B	406	LEU	4.9
1	B	409	ALA	4.8
1	B	672	ILE	4.4
1	B	564	TYR	4.2
1	B	533	THR	4.2
1	B	504	ILE	4.2
1	B	562	LEU	4.1
1	B	678	VAL	4.0
1	B	532	TYR	3.9
1	B	662	TRP	3.9
1	C	504	ILE	3.9
1	B	657	VAL	3.8
1	C	672	ILE	3.8
1	B	596	TYR	3.8
1	B	569	ILE	3.7
1	B	428	VAL	3.7
1	B	40	TYR	3.7
1	B	522	SER	3.6
1	B	477	ILE	3.6
1	B	567	THR	3.6
1	B	525	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	58	LEU	3.6
1	B	408	GLY	3.5
1	B	639	GLY	3.5
1	A	672	ILE	3.4
1	B	614	ILE	3.4
1	B	661	ASN	3.4
1	B	517	LEU	3.4
1	B	635	ALA	3.4
1	B	473	TRP	3.4
1	B	427	LEU	3.3
1	B	23	HIS	3.3
1	B	589	LEU	3.3
1	B	474	ALA	3.3
1	B	592	SER	3.2
1	B	570	PRO	3.2
1	B	523	ASN	3.2
1	B	302	PRO	3.2
1	A	504	ILE	3.2
1	B	531	SER	3.2
1	B	304	ALA	3.1
1	B	563	LYS	3.1
1	B	677	PHE	3.1
1	B	599	PHE	3.1
1	A	152	GLN	3.0
1	B	680	THR	3.0
1	B	566	GLN	3.0
1	B	660	LYS	3.0
1	B	598	TRP	3.0
1	B	101	TYR	3.0
1	B	502	GLY	3.0
1	B	143	ILE	3.0
1	C	150	ASN	3.0
1	B	611	PHE	3.0
1	C	648	ALA	2.9
1	B	582	PHE	2.9
1	B	586	TYR	2.9
1	B	34	PRO	2.9
1	B	381	ILE	2.9
1	A	23	HIS	2.9
1	B	574	THR	2.8
1	B	613	VAL	2.8
1	B	39	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	103	ILE	2.8
1	B	434	TRP	2.8
1	C	647	ALA	2.8
1	B	665	LEU	2.8
1	B	558	ILE	2.8
1	B	647	ALA	2.8
1	B	503	VAL	2.8
1	B	603	TYR	2.8
1	B	658	LEU	2.8
1	B	476	ASN	2.7
1	B	565	TYR	2.7
1	B	552	ILE	2.7
1	B	604	GLN	2.7
1	C	649	GLY	2.7
1	B	373	ASP	2.7
1	C	127	ALA	2.7
1	B	608	ASN	2.6
1	B	617	CYS	2.6
1	B	619	GLY	2.6
1	B	654	VAL	2.6
1	B	285	MET	2.6
1	B	585	LEU	2.6
1	B	537	ILE	2.6
1	B	303	GLN	2.6
1	B	372	LEU	2.6
1	B	584	LEU	2.6
1	B	605	PRO	2.6
1	B	431	ASP	2.5
1	B	621	THR	2.5
1	B	30	SER	2.5
1	B	106	TYR	2.5
1	B	56	GLU	2.5
1	B	500	VAL	2.5
1	B	607	LEU	2.5
1	B	679	LEU	2.5
1	B	594	GLN	2.5
1	B	659	PRO	2.5
1	B	355	LEU	2.5
1	B	505	ALA	2.5
1	B	609	PRO	2.5
1	B	323	THR	2.5
1	B	593	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	643	LEU	2.4
1	B	57	PRO	2.4
1	B	648	ALA	2.4
1	A	503	VAL	2.4
1	B	499	THR	2.4
1	B	632	VAL	2.4
1	B	301	ASP	2.4
1	B	572	SER	2.4
1	B	571	GLN	2.4
1	B	651	ILE	2.4
1	B	60	VAL	2.4
1	B	430	GLY	2.3
1	B	606	ASN	2.3
1	B	561	ASP	2.3
1	B	27	TRP	2.3
1	B	296	ILE	2.3
1	B	595	ALA	2.3
1	B	597	HIS	2.3
1	B	98	VAL	2.3
1	C	503	VAL	2.3
1	A	563	LYS	2.3
1	B	646	ASP	2.3
1	B	100	THR	2.3
1	B	526	THR	2.3
1	B	31	ALA	2.3
1	B	529	HIS	2.3
1	B	636	VAL	2.3
1	A	498	ALA	2.2
1	B	41	GLY	2.2
1	B	475	GLU	2.2
1	A	100	THR	2.2
1	B	527	ARG	2.2
1	B	543	ASN	2.2
1	B	546	ALA	2.2
1	B	410	PHE	2.2
1	B	640	PHE	2.2
1	B	498	ALA	2.2
1	B	581	ILE	2.2
1	A	182	THR	2.2
1	B	587	SER	2.2
1	B	591	ASP	2.1
1	B	64	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	422	ALA	2.1
1	B	423	TRP	2.1
1	B	666	THR	2.1
1	B	663	LYS	2.1
1	B	435	LEU	2.1
1	B	358	PRO	2.1
1	B	560	ARG	2.1
1	B	670	ILE	2.1
1	B	405	ALA	2.1
1	B	642	GLY	2.1
1	C	89	MET	2.1
1	C	673	GLU	2.1
1	B	534	ASP	2.1
1	C	283[A]	ARG	2.1
1	B	33	LYS	2.1
1	B	436	LYS	2.1
1	B	37	ASN	2.0
1	B	36	SER	2.0
1	B	467	VAL	2.0
1	B	501	LEU	2.0
1	B	429	THR	2.0
1	B	553	THR	2.0
1	A	57	PRO	2.0
1	C	101	TYR	2.0
1	B	542	ALA	2.0
1	B	580	ALA	2.0
1	A	98	VAL	2.0
1	B	63	VAL	2.0
1	C	98	VAL	2.0
1	B	652	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

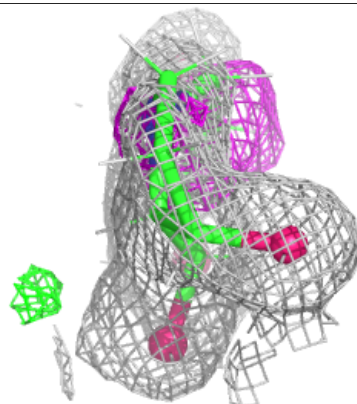
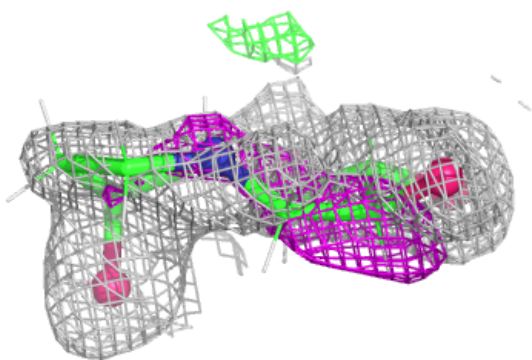
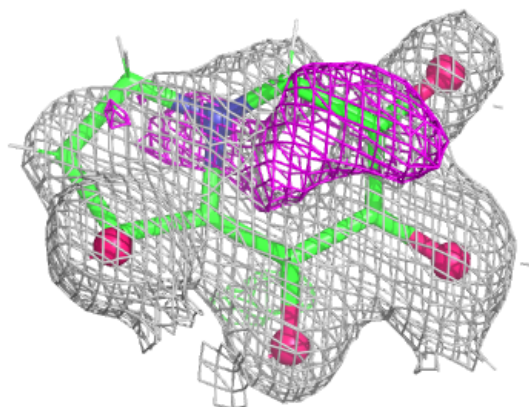
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	CTS	B	702	13/13	0.84	0.14	30,39,44,45	4
2	CTS	A	702	13/13	0.87	0.15	21,30,36,37	4
2	CTS	C	702	13/13	0.87	0.14	21,30,36,37	4
3	EDO	C	704	4/4	0.88	0.13	28,31,33,33	2
3	EDO	A	704	4/4	0.89	0.12	30,36,36,39	2
3	EDO	C	705	4/4	0.89	0.12	30,36,37,39	2
3	EDO	A	705	4/4	0.91	0.09	30,38,40,42	2
3	EDO	A	706	4/4	0.92	0.13	30,32,35,35	2
3	EDO	B	703	4/4	0.93	0.09	30,32,33,35	2
3	EDO	C	703	4/4	0.93	0.11	24,30,33,37	2
2	CTS	B	701	13/13	0.93	0.09	26,29,31,32	4
2	CTS	C	701	13/13	0.93	0.09	19,21,30,30	4
2	CTS	A	701	13/13	0.95	0.07	20,22,30,30	4
3	EDO	A	703	4/4	0.96	0.07	24,27,30,30	2

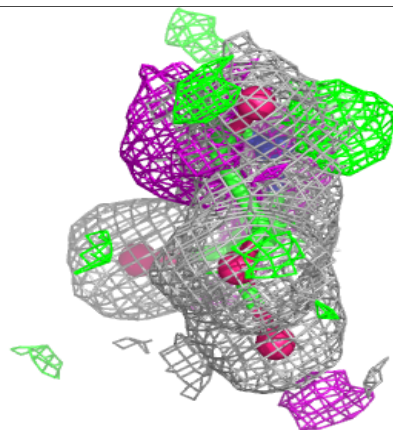
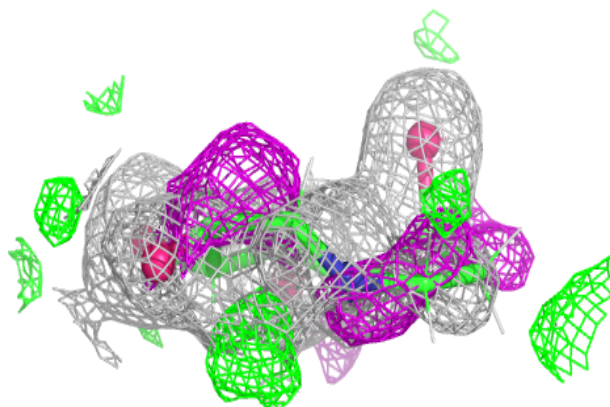
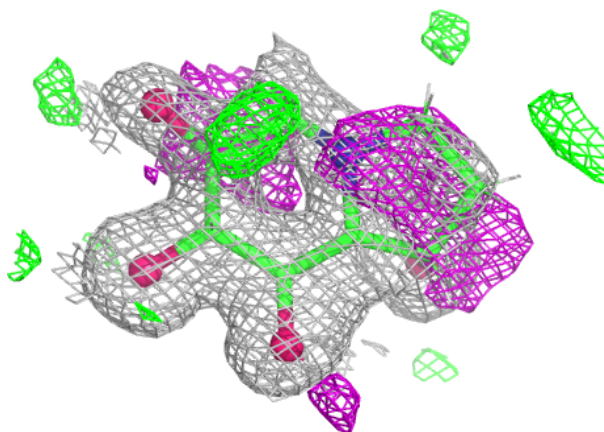
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CTS B 702:

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

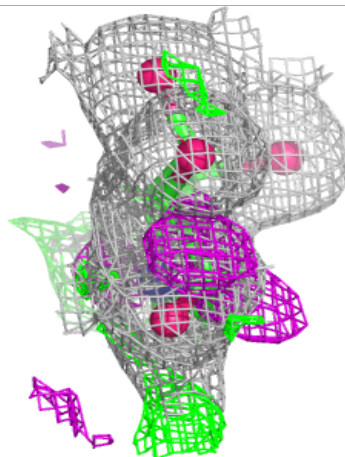
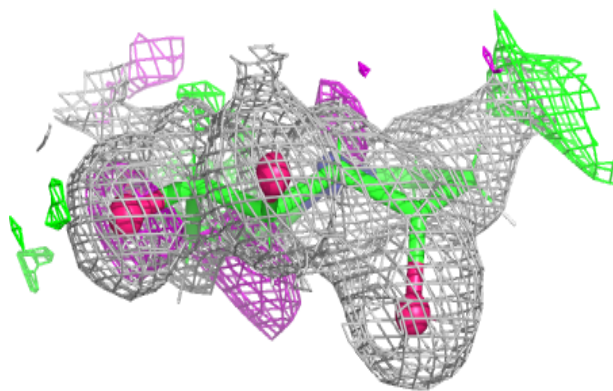
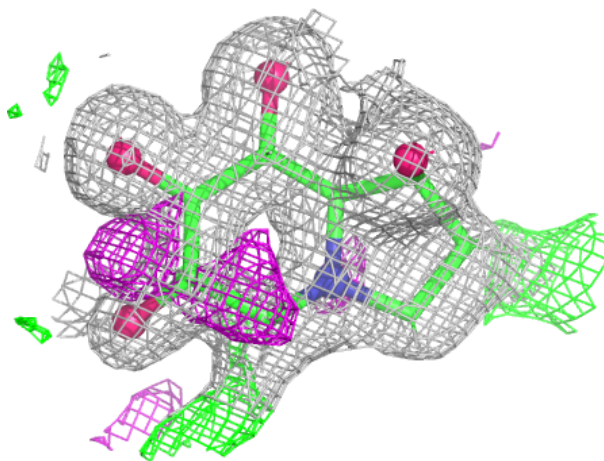
**Electron density around CTS A 702:**

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



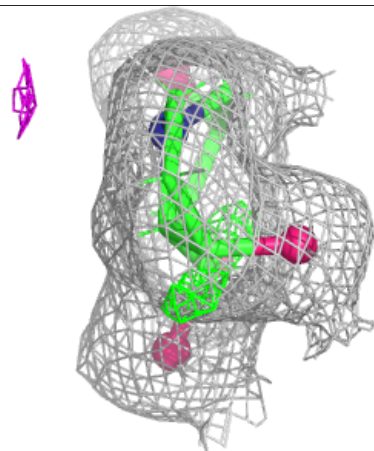
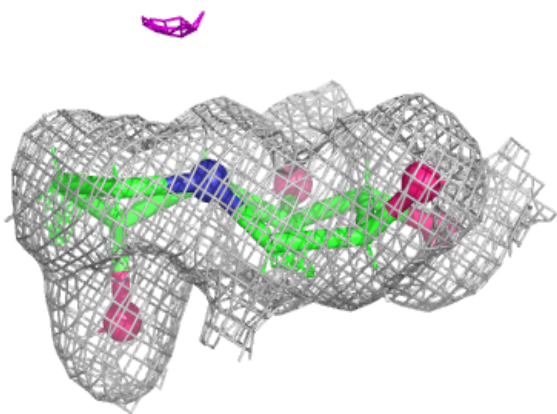
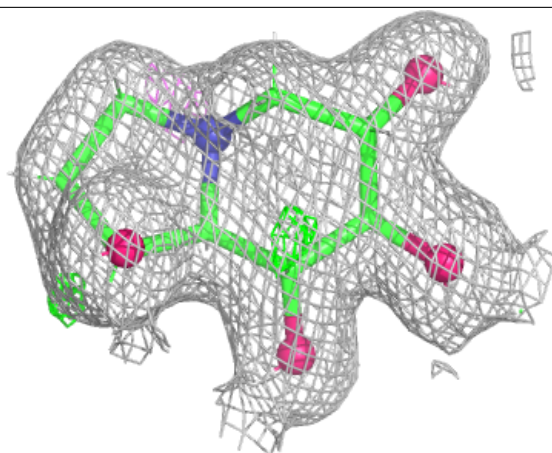
Electron density around CTS C 702:

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



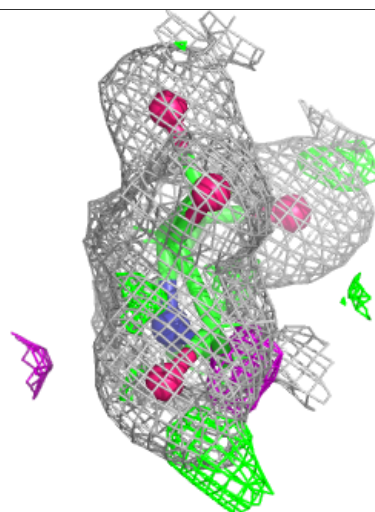
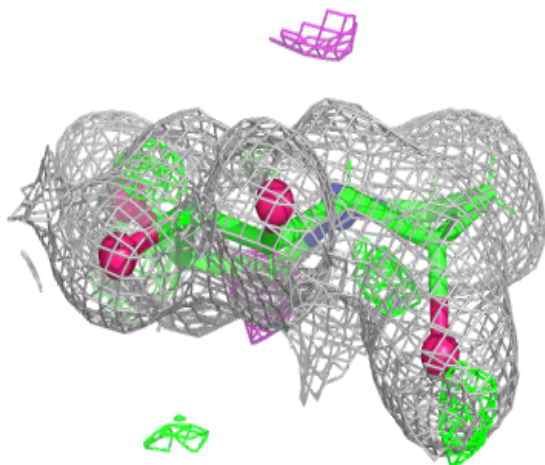
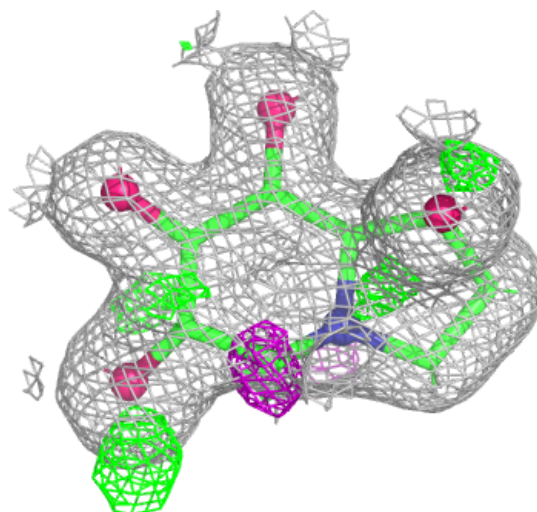
Electron density around CTS B 701:

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



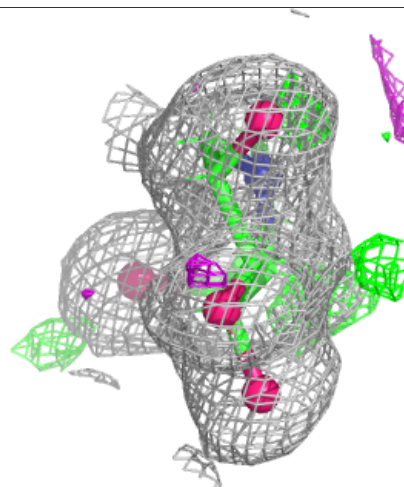
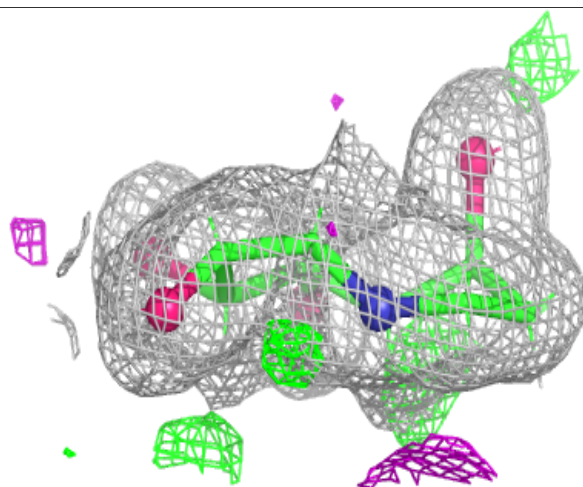
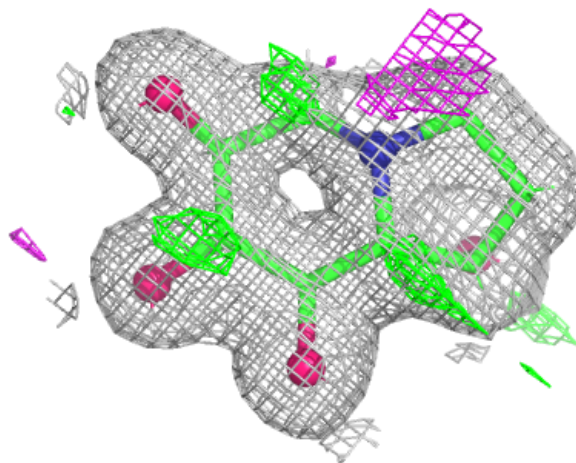
Electron density around CTS C 701:

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



Electron density around CTS A 701:

$2mF_o-DF_c$ (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.