Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2025 – 02:37 PM JST

PDB ID	:	8YVS
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:

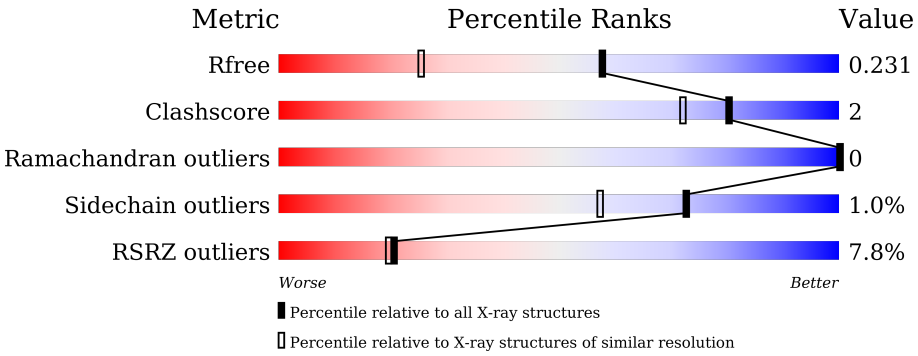
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

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 1.60 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}	164625	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (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 <=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% 92% 5%
1	B	678	20% 90% 6%
1	C	678	% 90% 6%

2 Entry composition (i)

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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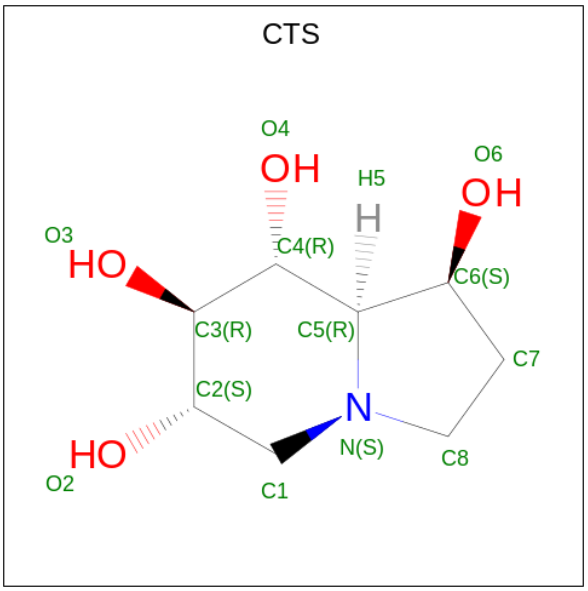
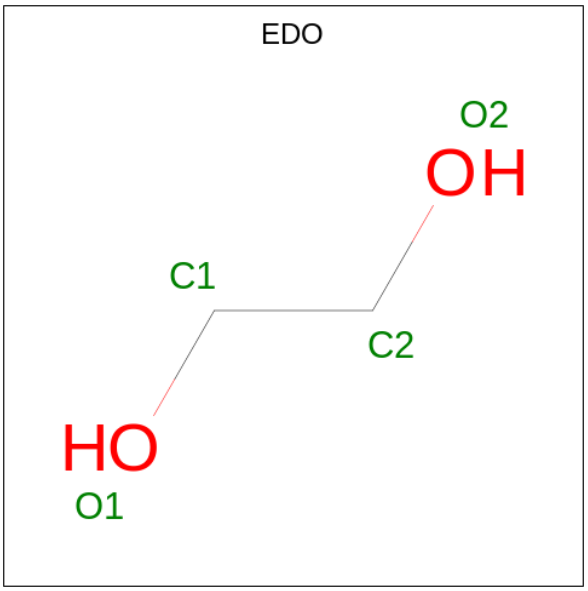
Chain	Residue	Modelled	Actual	Comment	Reference
B	6	SER	-	expression tag	UNP A5FBJ5
B	7	SER	-	expression tag	UNP A5FBJ5
B	8	HIS	-	expression tag	UNP A5FBJ5
B	9	HIS	-	expression tag	UNP A5FBJ5
B	10	HIS	-	expression tag	UNP A5FBJ5
B	11	HIS	-	expression tag	UNP A5FBJ5
B	12	HIS	-	expression tag	UNP A5FBJ5
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 (three-letter code: CTS) (formula: $C_8H_{15}NO_4$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is water.

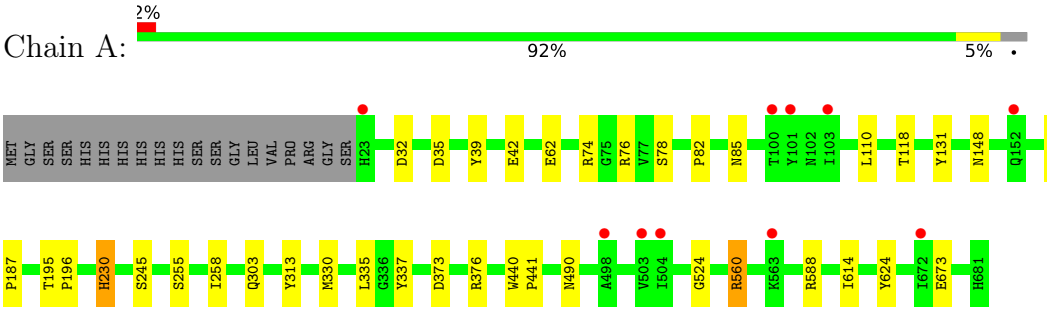
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	445	Total O 445 445	0	0
4	B	293	Total O 293 293	0	0
4	C	466	Total O 466 466	0	0

3 Residue-property plots (i)

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

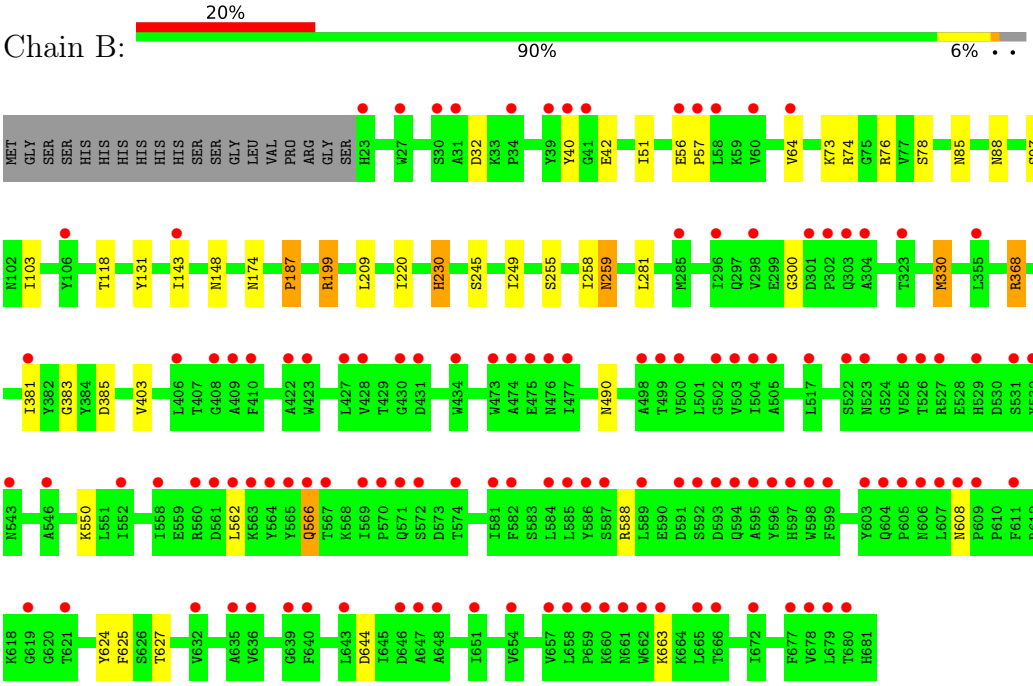
• Molecule 1: Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65

Chain A:



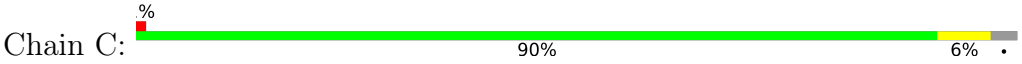
• Molecule 1: Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65

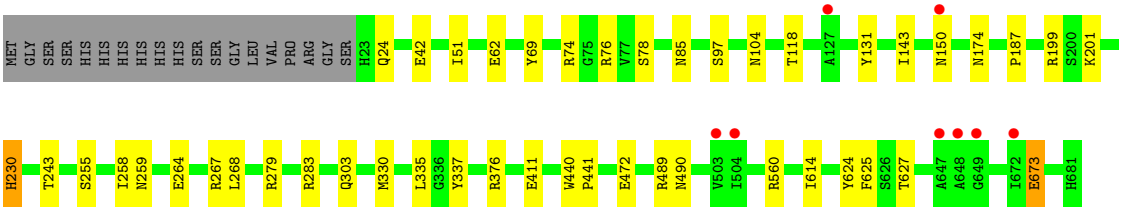
Chain B:



• Molecule 1: Candidate alpha glycoside phosphorylase Glycoside hydrolase family 65

Chain C:




MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER H23 Q24 E42 I51 E62 Y69 R74 G75 R76 V77 S78 N85 S97 N104 T118 A127 Y131 I143 N150 N174 P187 R199 S200 K201
H230 T243 S255 I258 N259 E264 R267 L268 R279 R283 Q303 M330 L335 G336 Y337 R376 E411 W440 P441 E472 R489 N490 V503 I504 R560 I614 Y624 F625 S626 T627 A647 A648 G649 I672 E673 H681

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	15491 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]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, CTS

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	0.52	1/5391 (0.0%)	0.86	7/7316 (0.1%)
1	B	0.50	1/5390 (0.0%)	0.85	6/7315 (0.1%)
1	C	0.54	2/5387 (0.0%)	0.88	7/7310 (0.1%)
All	All	0.52	4/16168 (0.0%)	0.86	20/21941 (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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	78	SER	CA-CB	-6.01	1.44	1.52
1	C	411	GLU	CD-OE1	5.50	1.31	1.25
1	A	78	SER	CA-CB	-5.22	1.45	1.52
1	C	472	GLU	CD-OE1	5.16	1.31	1.25

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	560	ARG	NE-CZ-NH2	8.42	124.51	120.30
1	B	368	ARG	NE-CZ-NH1	-8.04	116.28	120.30
1	A	376	ARG	NE-CZ-NH2	-7.90	116.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	74	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	A	74	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	A	74	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	C	199	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	C	74	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	76	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	199	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	C	335	LEU	CB-CG-CD2	5.86	120.96	111.00
1	B	376	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	74	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	C	187	PRO	N-CD-CG	-5.64	94.74	103.20
1	A	187	PRO	N-CD-CG	-5.60	94.80	103.20
1	B	566	GLN	CB-CA-C	-5.59	99.22	110.40
1	A	560	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	C	560	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	376	ARG	NE-CZ-NH2	-5.06	117.77	120.30
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 (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	5256	5169	5152	17	0
1	B	5255	5167	5150	31	0
1	C	5255	5169	5152	26	0
2	A	26	30	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
4	C	466	0	0	3	0
All	All	17080	15643	15591	78	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 2.

All (78) 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: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
1:B:562:LEU:C	1:B:566:GLN:HE21	2.06	0.58
2:A:701:CTS:H81	2:A:702:CTS:H2	1.86	0.58
1:C:673:GLU:H	1:C:673:GLU:CD	2.06	0.57
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:588:ARG:NH1	1:B:644:ASP:OD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:255:SER:HA	1:B:258:ILE:O	2.16	0.46
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:673:GLU:CD	1:C:673:GLU:N	2.68	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: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: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: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:B:85:ASN:OD1	1:B:85:ASN:C	2.55	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: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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	567/581 (98%)	562 (99%)	5 (1%)	75	62
1	B	567/581 (98%)	560 (99%)	7 (1%)	67	50
1	C	566/581 (97%)	561 (99%)	5 (1%)	75	62
All	All	1700/1743 (98%)	1683 (99%)	17 (1%)	73	57

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ASP
1	A	42	GLU
1	A	230	HIS
1	A	490	ASN
1	A	673	GLU
1	B	32	ASP
1	B	42	GLU
1	B	97	SER
1	B	230	HIS
1	B	259	ASN
1	B	330	MET
1	B	490	ASN
1	C	42	GLU
1	C	97	SER
1	C	230	HIS
1	C	490	ASN
1	C	673	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	85	ASN
1	A	105	ASN
1	A	148	ASN
1	A	158	ASN
1	B	259	ASN
1	B	282	ASN
1	B	566	GLN
1	C	85	ASN

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Mol	Chain	Res	Type
1	C	158	ASN
1	C	259	ASN
1	C	293	GLN
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	A	702	-	14,14,14	0.87	0	16,21,21	1.51	3 (18%)
2	CTS	B	701	-	14,14,14	0.96	1 (7%)	16,21,21	1.28	2 (12%)
3	EDO	C	704	-	3,3,3	0.53	0	2,2,2	0.27	0
2	CTS	C	701	-	14,14,14	1.16	1 (7%)	16,21,21	1.84	4 (25%)
3	EDO	C	705	-	3,3,3	0.35	0	2,2,2	0.22	0
2	CTS	C	702	-	14,14,14	0.81	0	16,21,21	1.65	5 (31%)
3	EDO	A	703	-	3,3,3	0.73	0	2,2,2	0.27	0
2	CTS	B	702	-	14,14,14	0.56	0	16,21,21	1.46	2 (12%)
3	EDO	B	703	-	3,3,3	0.60	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	EDO	C	703	-	3,3,3	0.37	0	2,2,2	0.62	0
2	CTS	A	701	-	14,14,14	0.95	1 (7%)	16,21,21	1.62	3 (18%)
3	EDO	A	704	-	3,3,3	0.40	0	2,2,2	0.32	0
3	EDO	A	706	-	3,3,3	0.35	0	2,2,2	0.45	0
3	EDO	A	705	-	3,3,3	0.06	0	2,2,2	0.12	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
3	EDO	C	704	-	-	0/1/1/1	-
2	CTS	A	702	-	-	-	0/2/2/2
2	CTS	B	701	-	-	-	0/2/2/2
2	CTS	C	701	-	-	-	0/2/2/2
3	EDO	C	705	-	-	0/1/1/1	-
2	CTS	C	702	-	-	-	0/2/2/2
3	EDO	B	703	-	-	0/1/1/1	-
3	EDO	A	703	-	-	1/1/1/1	-
2	CTS	B	702	-	-	-	0/2/2/2
3	EDO	C	703	-	-	0/1/1/1	-
2	CTS	A	701	-	-	-	0/2/2/2
3	EDO	A	704	-	-	0/1/1/1	-
3	EDO	A	706	-	-	0/1/1/1	-
3	EDO	A	705	-	-	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	-2.38	1.43	1.47
2	B	701	CTS	C2-C3	-2.10	1.49	1.52
2	A	701	CTS	C2-C3	-2.10	1.49	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	702	CTS	C2-C1-N	4.20	118.01	110.54
2	A	701	CTS	C2-C1-N	3.79	117.28	110.54
2	C	701	CTS	C2-C1-N	3.64	117.02	110.54
2	B	701	CTS	C2-C1-N	3.57	116.88	110.54
2	C	702	CTS	C2-C1-N	3.20	116.24	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	CTS	C7-C6-C5	-3.11	98.90	102.80
2	C	702	CTS	O6-C6-C7	2.96	118.58	111.54
2	A	702	CTS	O4-C4-C5	-2.90	101.59	109.16
2	C	701	CTS	O2-C2-C1	2.89	115.18	109.62
2	A	702	CTS	C2-C1-N	2.72	115.38	110.54
2	C	701	CTS	O4-C4-C5	-2.61	102.35	109.16
2	C	701	CTS	C7-C6-C5	-2.60	99.55	102.80
2	A	702	CTS	O6-C6-C7	2.51	117.51	111.54
2	B	701	CTS	O2-C2-C1	2.37	114.19	109.62
2	C	702	CTS	C1-C2-C3	2.30	112.87	110.24
2	C	702	CTS	O4-C4-C5	-2.15	103.55	109.16
2	C	702	CTS	O3-C3-C2	-2.07	106.03	109.99
2	A	701	CTS	O3-C3-C2	-2.06	106.05	109.99
2	B	702	CTS	C2-C3-C4	-2.02	107.40	110.89

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.

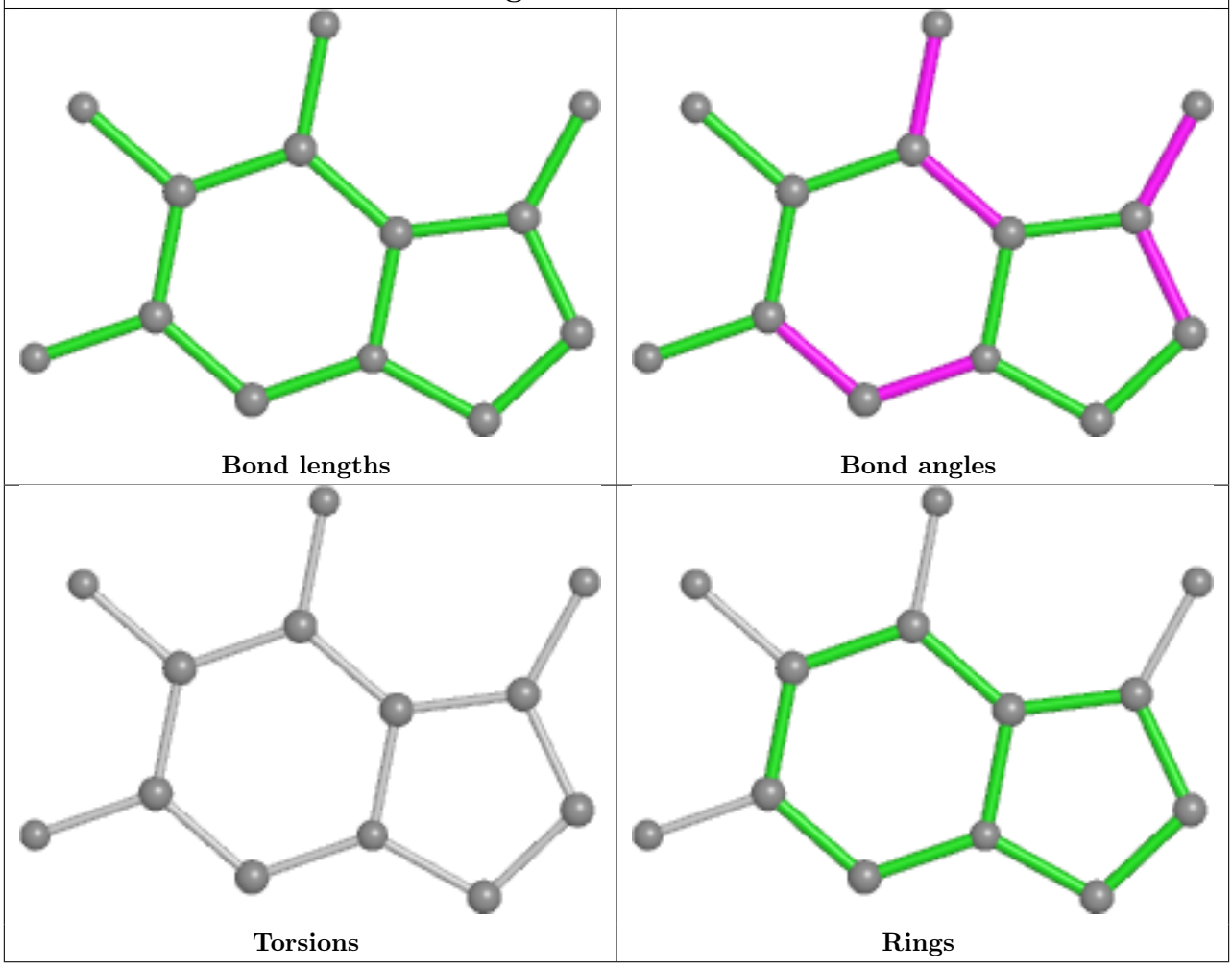
8 monomers are involved in 15 short contacts:

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

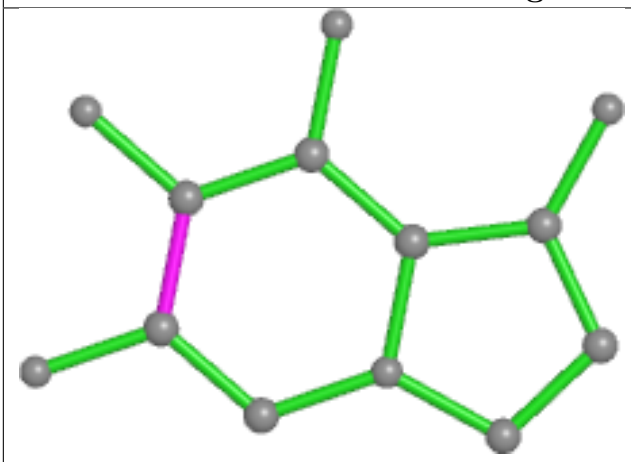
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

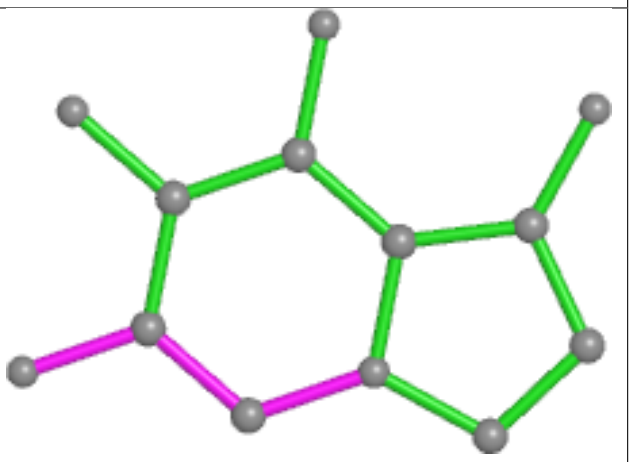
Ligand CTS A 702



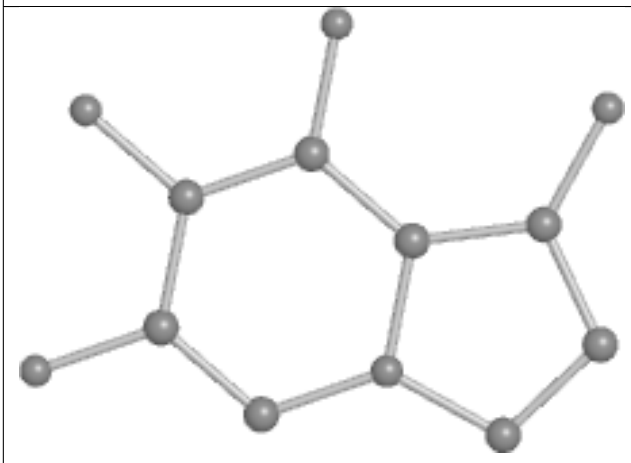
Ligand CTS B 701



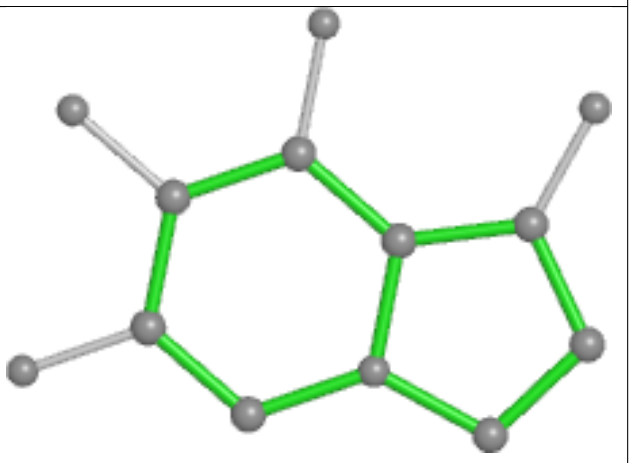
Bond lengths



Bond angles

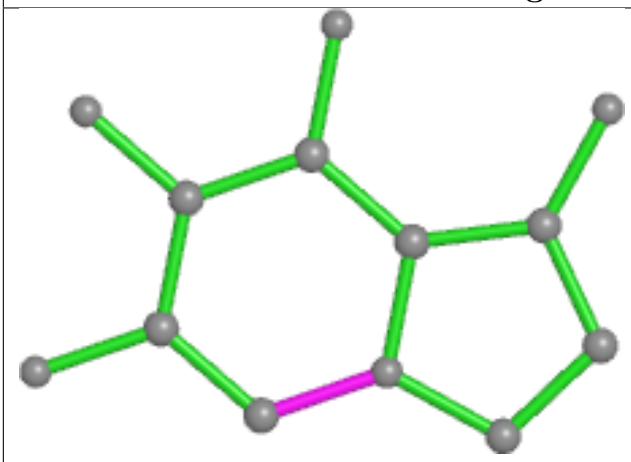


Torsions

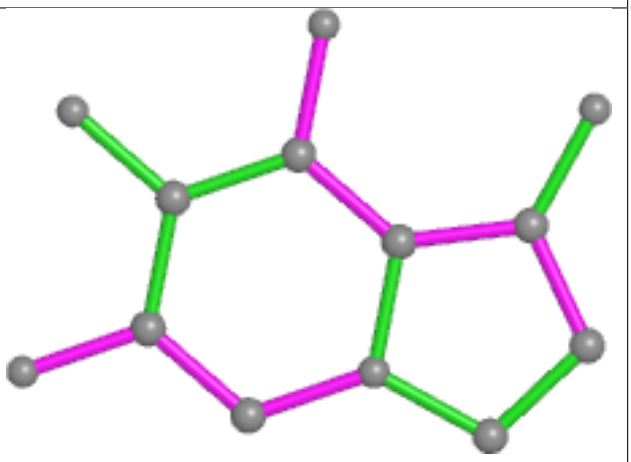


Rings

Ligand CTS C 701



Bond lengths



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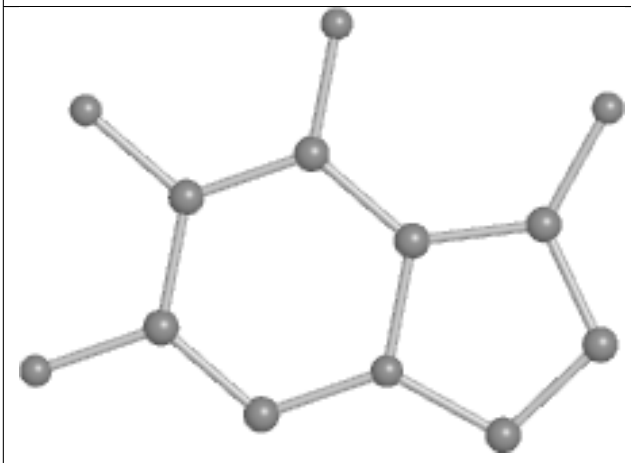

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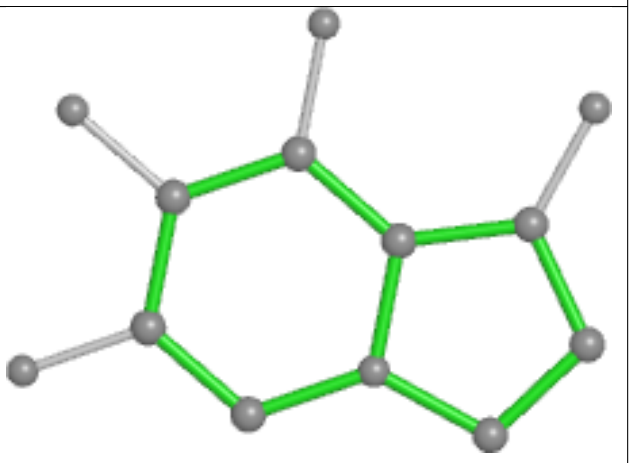
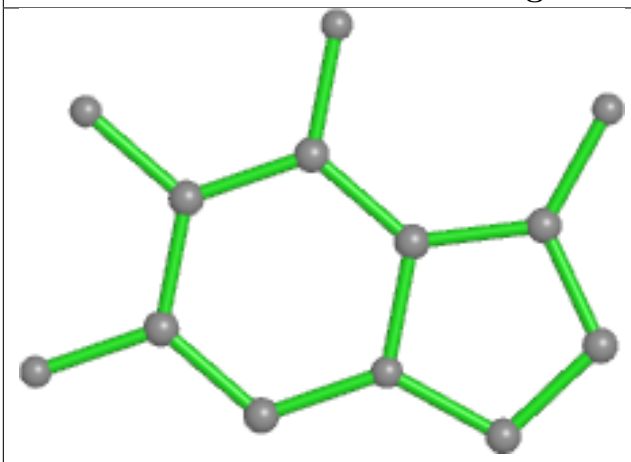
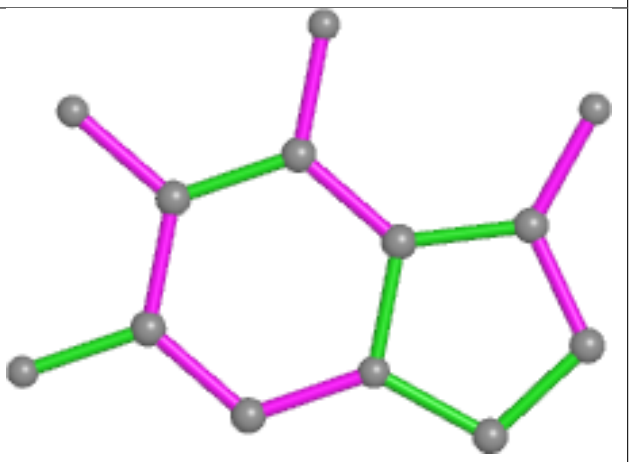


Rings

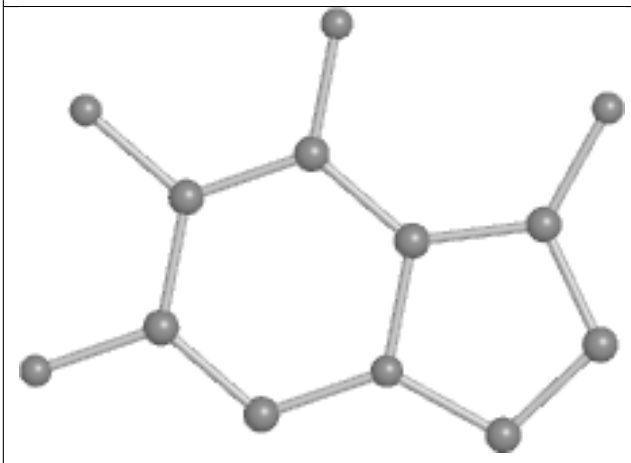
Ligand CTS C 702



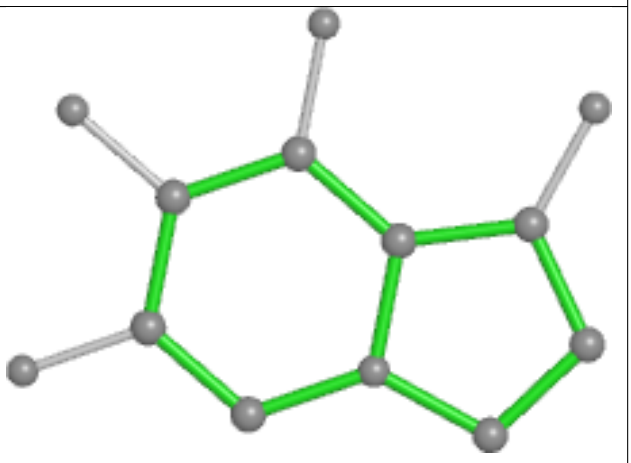
Bond lengths



Bond angles

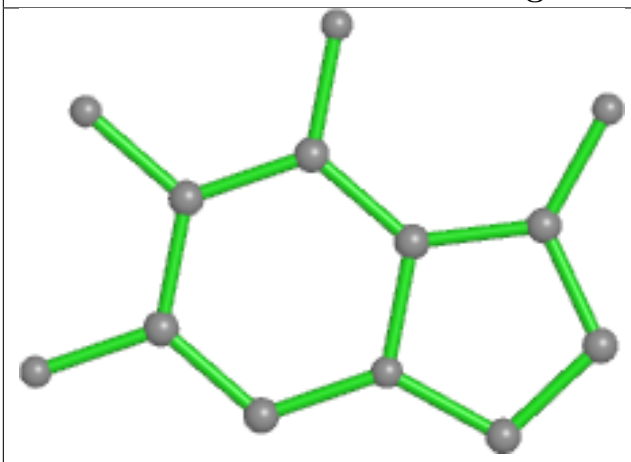


Torsions

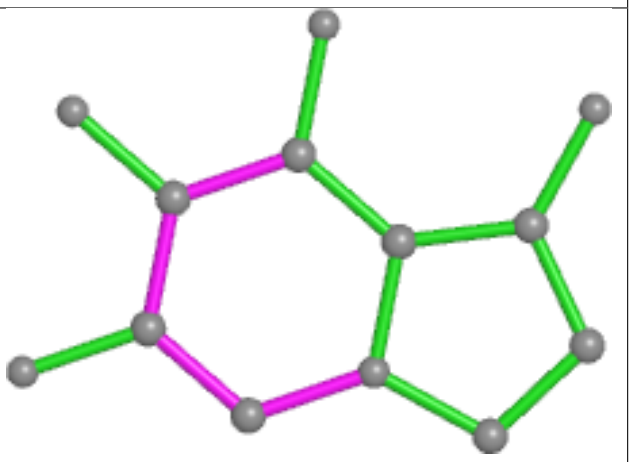


Rings

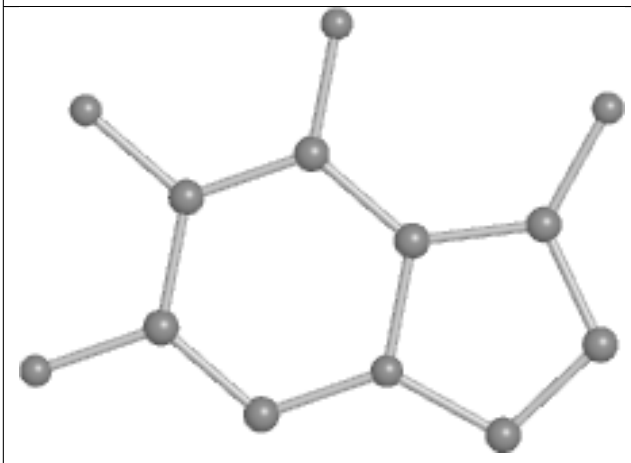
Ligand CTS B 702



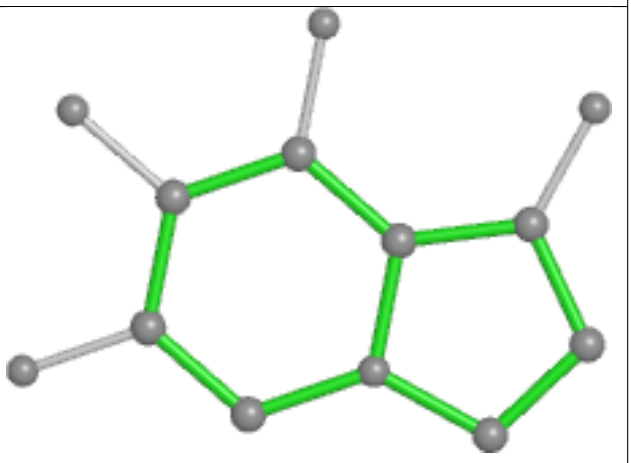
Bond lengths



Bond angles

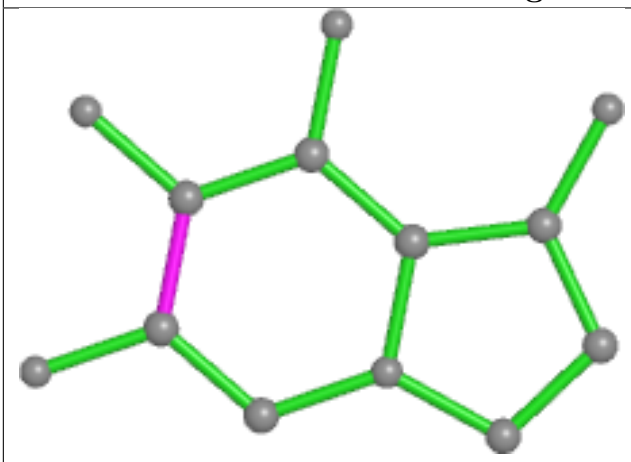


Torsions

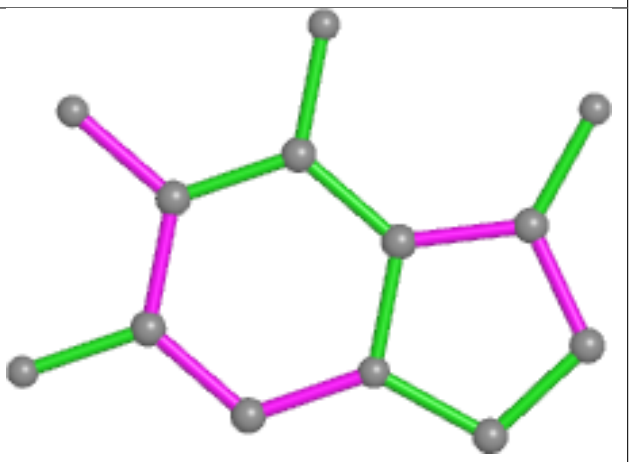


Rings

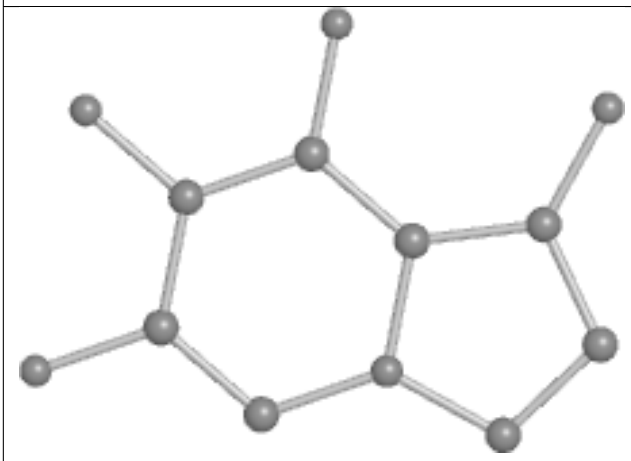
Ligand CTS A 701



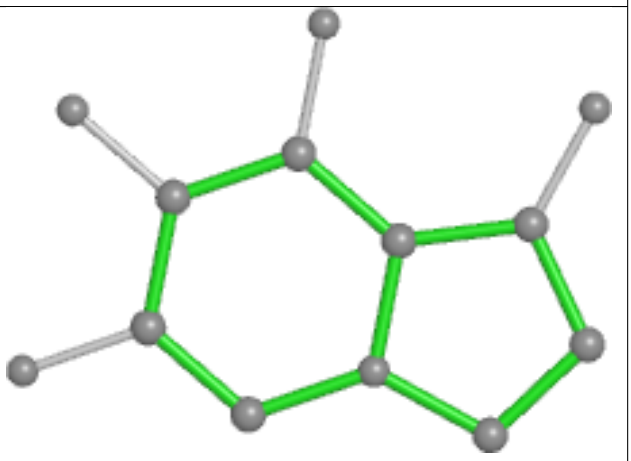
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	0.33	11 (1%) 69 71	11, 27, 49, 70	2 (0%)
1	B	659/678 (97%)	1.07	135 (20%) 3 3	14, 35, 64, 88	2 (0%)
1	C	659/678 (97%)	0.29	8 (1%) 76 79	17, 27, 44, 60	1 (0%)
All	All	1977/2034 (97%)	0.57	154 (7%) 20 19	11, 29, 55, 88	5 (0%)

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	101	TYR	5.4
1	B	298	VAL	4.7
1	B	406	LEU	4.7
1	B	409	ALA	4.6
1	B	672	ILE	4.3
1	B	564	TYR	4.1
1	B	533	THR	4.1
1	B	504	ILE	4.0
1	B	562	LEU	4.0
1	B	678	VAL	3.8
1	B	532	TYR	3.8
1	B	662	TRP	3.8
1	C	504	ILE	3.7
1	B	657	VAL	3.7
1	B	596	TYR	3.6
1	C	672	ILE	3.6
1	B	569	ILE	3.6
1	B	428	VAL	3.6
1	B	40	TYR	3.5
1	B	522	SER	3.5
1	B	567	THR	3.5
1	B	477	ILE	3.5
1	B	58	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	525	VAL	3.4
1	B	408	GLY	3.4
1	A	672	ILE	3.3
1	B	614	ILE	3.3
1	B	661	ASN	3.3
1	B	639	GLY	3.3
1	B	517	LEU	3.3
1	B	635	ALA	3.2
1	B	473	TRP	3.2
1	B	23	HIS	3.2
1	B	427	LEU	3.2
1	B	592	SER	3.1
1	B	589	LEU	3.1
1	B	474	ALA	3.1
1	B	523	ASN	3.1
1	B	570	PRO	3.1
1	B	531	SER	3.1
1	A	504	ILE	3.0
1	B	302	PRO	3.0
1	B	563	LYS	3.0
1	B	677	PHE	3.0
1	B	304	ALA	3.0
1	B	599	PHE	3.0
1	A	152	GLN	3.0
1	B	660	LYS	3.0
1	B	566	GLN	2.9
1	B	680	THR	2.9
1	B	101	TYR	2.9
1	B	598	TRP	2.9
1	B	611	PHE	2.9
1	C	150	ASN	2.8
1	B	143	ILE	2.8
1	B	502	GLY	2.8
1	B	582	PHE	2.8
1	B	586	TYR	2.8
1	C	648	ALA	2.8
1	A	23	HIS	2.8
1	B	381	ILE	2.7
1	B	34	PRO	2.7
1	B	574	THR	2.7
1	B	39	TYR	2.7
1	A	103	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	434	TRP	2.7
1	B	613	VAL	2.7
1	B	665	LEU	2.7
1	B	558	ILE	2.7
1	C	647	ALA	2.7
1	B	603	TYR	2.7
1	B	658	LEU	2.6
1	B	647	ALA	2.6
1	B	476	ASN	2.6
1	B	503	VAL	2.6
1	B	565	TYR	2.6
1	B	604	GLN	2.6
1	B	552	ILE	2.6
1	B	373	ASP	2.6
1	B	617	CYS	2.5
1	B	608	ASN	2.5
1	B	285	MET	2.5
1	C	649	GLY	2.5
1	C	127	ALA	2.5
1	B	619	GLY	2.5
1	B	654	VAL	2.5
1	B	303	GLN	2.5
1	B	585	LEU	2.5
1	B	537	ILE	2.5
1	B	431	ASP	2.5
1	B	56	GLU	2.5
1	B	372	LEU	2.4
1	B	584	LEU	2.4
1	B	30	SER	2.4
1	B	621	THR	2.4
1	B	605	PRO	2.4
1	B	106	TYR	2.4
1	B	594	GLN	2.4
1	B	500	VAL	2.4
1	B	607	LEU	2.4
1	B	679	LEU	2.4
1	B	659	PRO	2.4
1	B	355	LEU	2.4
1	B	593	ASP	2.4
1	B	323	THR	2.3
1	B	609	PRO	2.3
1	B	505	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	301	ASP	2.3
1	B	643	LEU	2.3
1	B	499	THR	2.3
1	B	571	GLN	2.3
1	B	57	PRO	2.3
1	B	572	SER	2.3
1	B	648	ALA	2.3
1	A	503	VAL	2.3
1	B	632	VAL	2.3
1	B	651	ILE	2.3
1	B	561	ASP	2.2
1	B	606	ASN	2.2
1	B	60	VAL	2.2
1	A	563	LYS	2.2
1	B	27	TRP	2.2
1	B	430	GLY	2.2
1	B	296	ILE	2.2
1	B	597	HIS	2.2
1	B	646	ASP	2.2
1	B	529	HIS	2.2
1	B	595	ALA	2.2
1	B	100	THR	2.2
1	B	526	THR	2.2
1	B	98	VAL	2.2
1	C	503	VAL	2.2
1	B	31	ALA	2.1
1	B	527	ARG	2.1
1	B	475	GLU	2.1
1	B	636	VAL	2.1
1	A	498	ALA	2.1
1	B	543	ASN	2.1
1	A	100	THR	2.1
1	B	410	PHE	2.1
1	B	640	PHE	2.1
1	B	41	GLY	2.1
1	B	546	ALA	2.1
1	B	587	SER	2.1
1	B	591	ASP	2.1
1	B	498	ALA	2.0
1	A	182	THR	2.0
1	B	581	ILE	2.0
1	B	663	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	423	TRP	2.0
1	B	560	ARG	2.0
1	B	64	VAL	2.0
1	B	422	ALA	2.0
1	B	666	THR	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 monosaccharides in this entry.

6.4 Ligands (i)

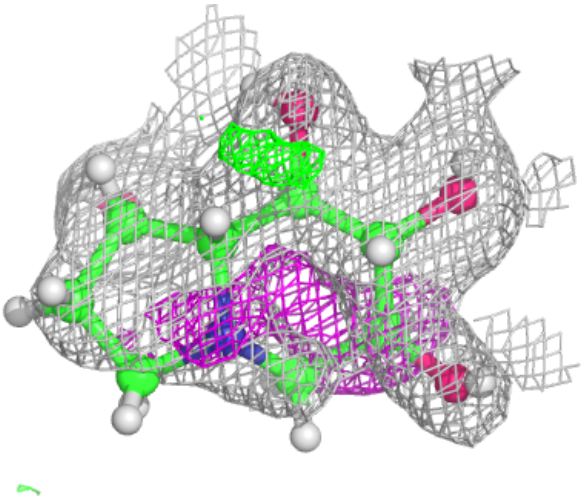
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

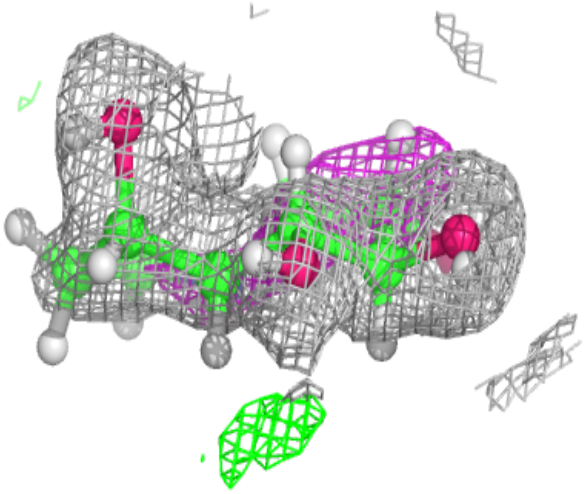
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CTS	B	702	13/13	0.84	0.14	30,39,44,45	4
2	CTS	A	702	13/13	0.87	0.15	21,30,36,37	4
2	CTS	C	702	13/13	0.87	0.14	21,30,36,37	4
3	EDO	C	704	4/4	0.88	0.13	28,31,33,33	2
3	EDO	A	704	4/4	0.89	0.12	30,36,36,39	2
3	EDO	C	705	4/4	0.89	0.12	30,36,37,39	2
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

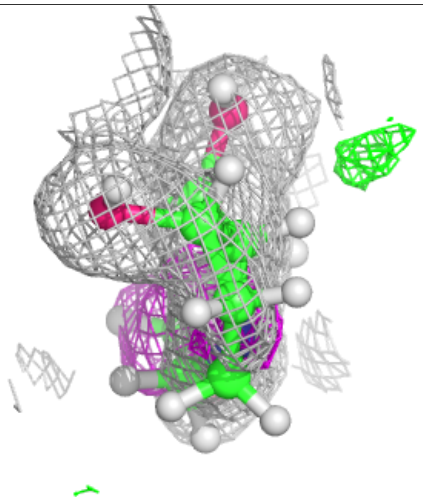
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

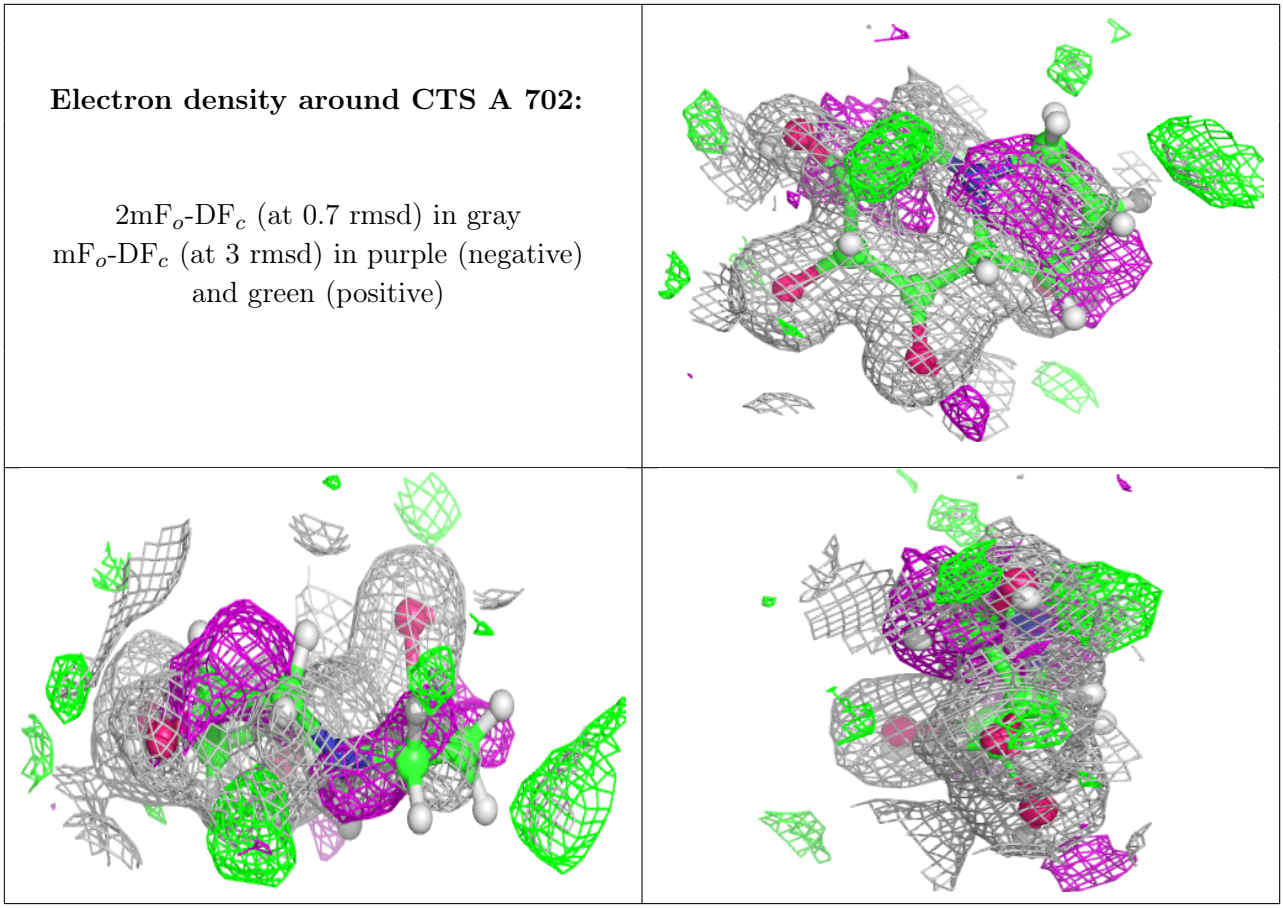






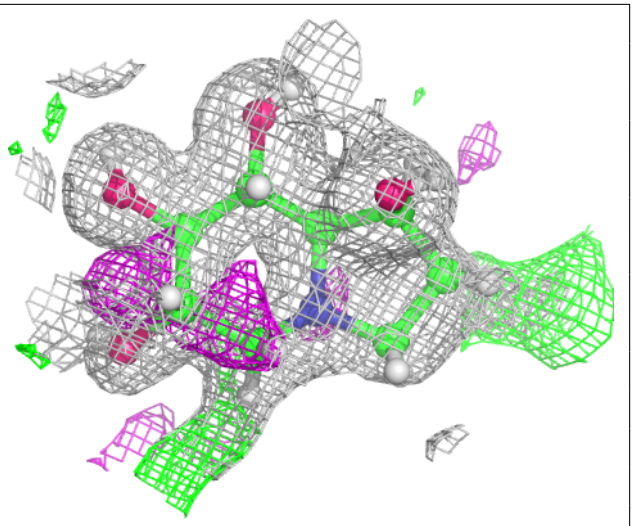
Electron density around CTS A 702:

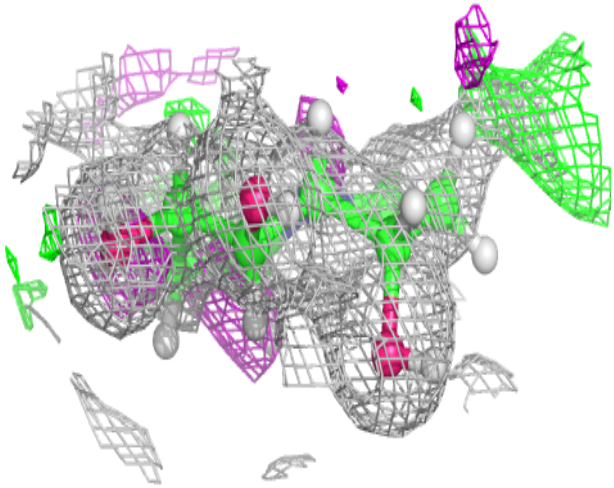
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

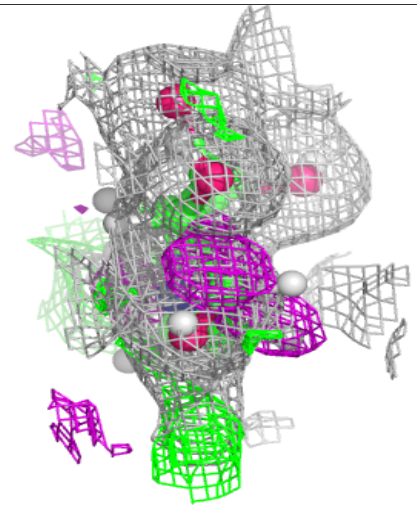


Electron density around CTS C 702:

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

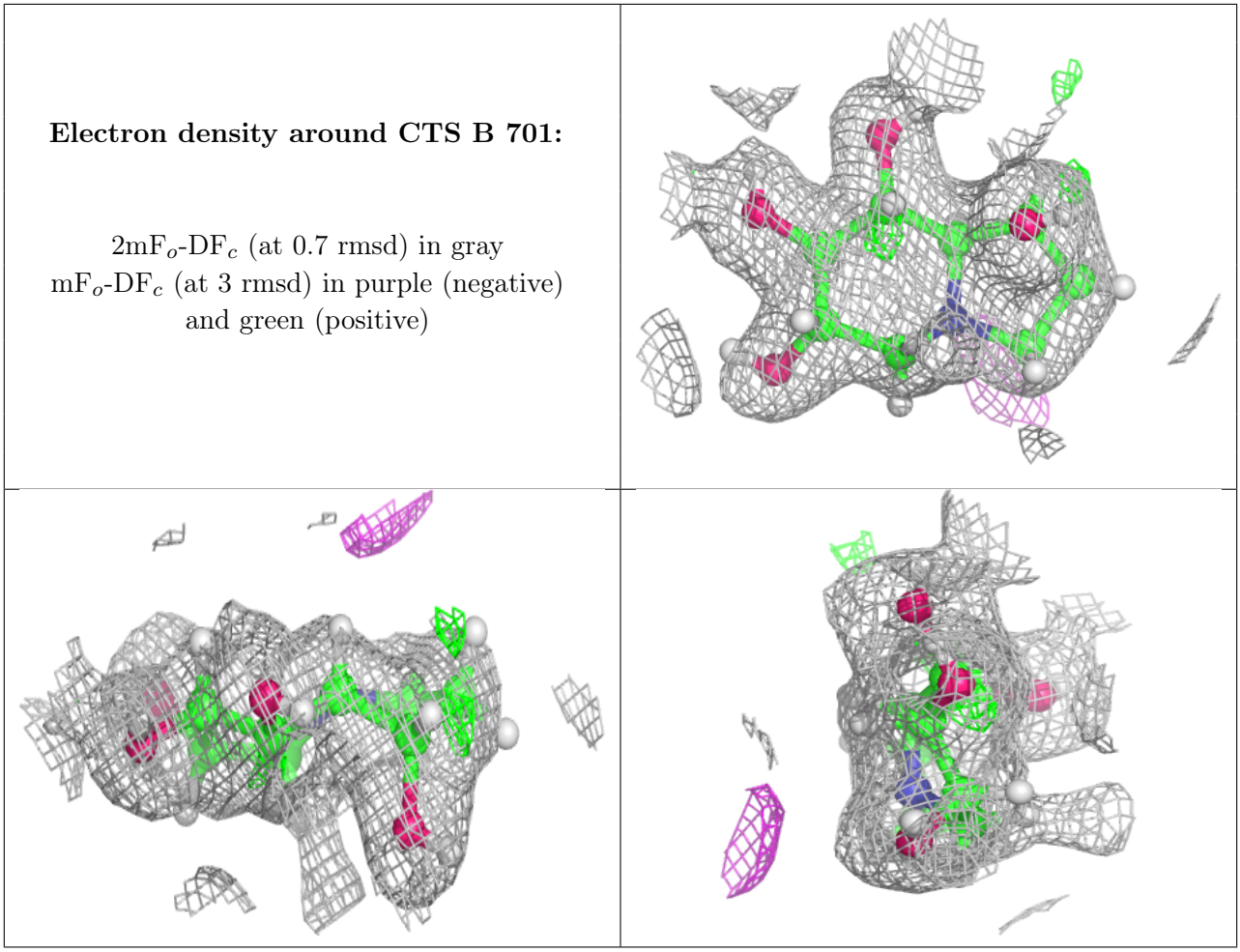






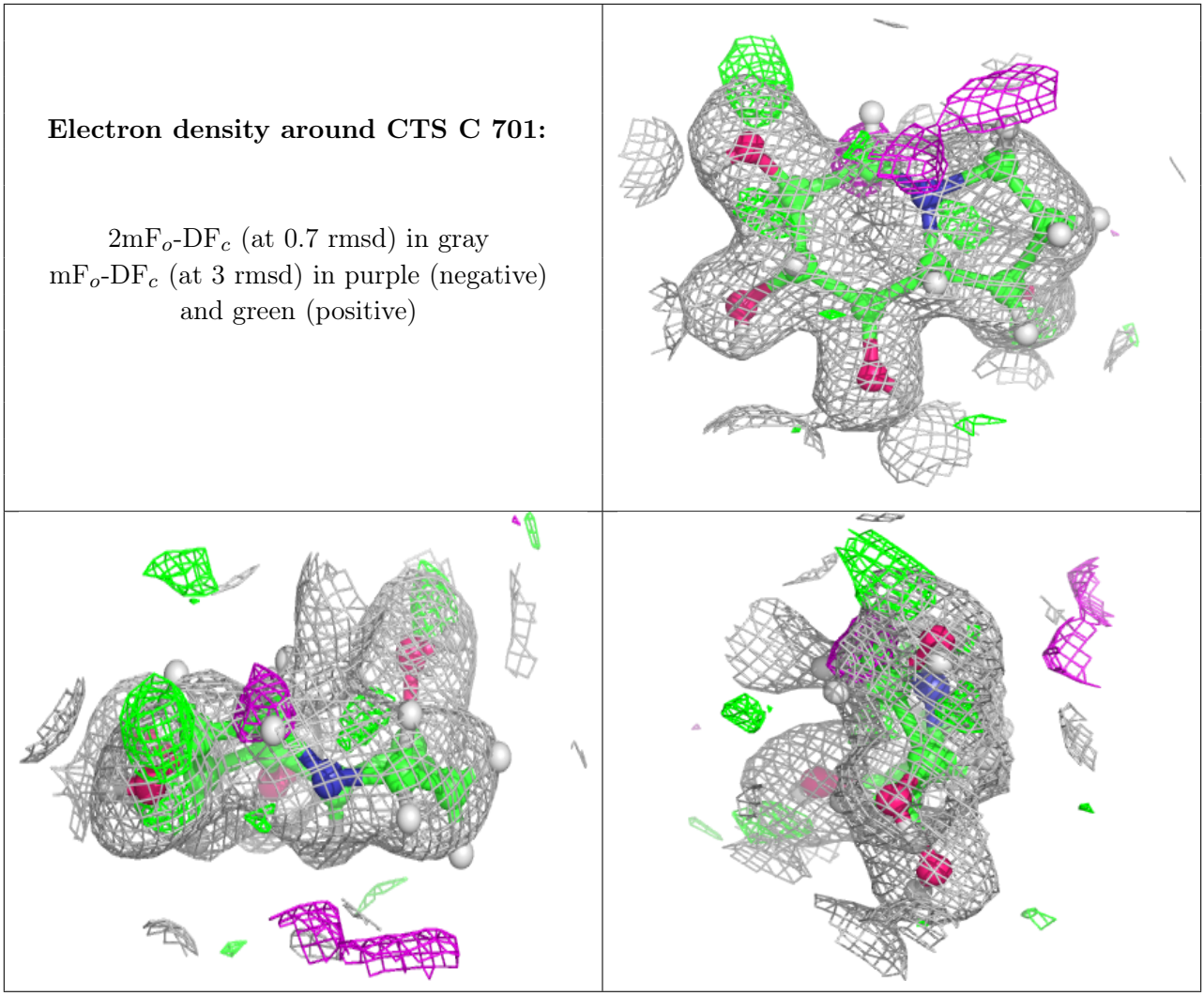
Electron density around CTS B 701:

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



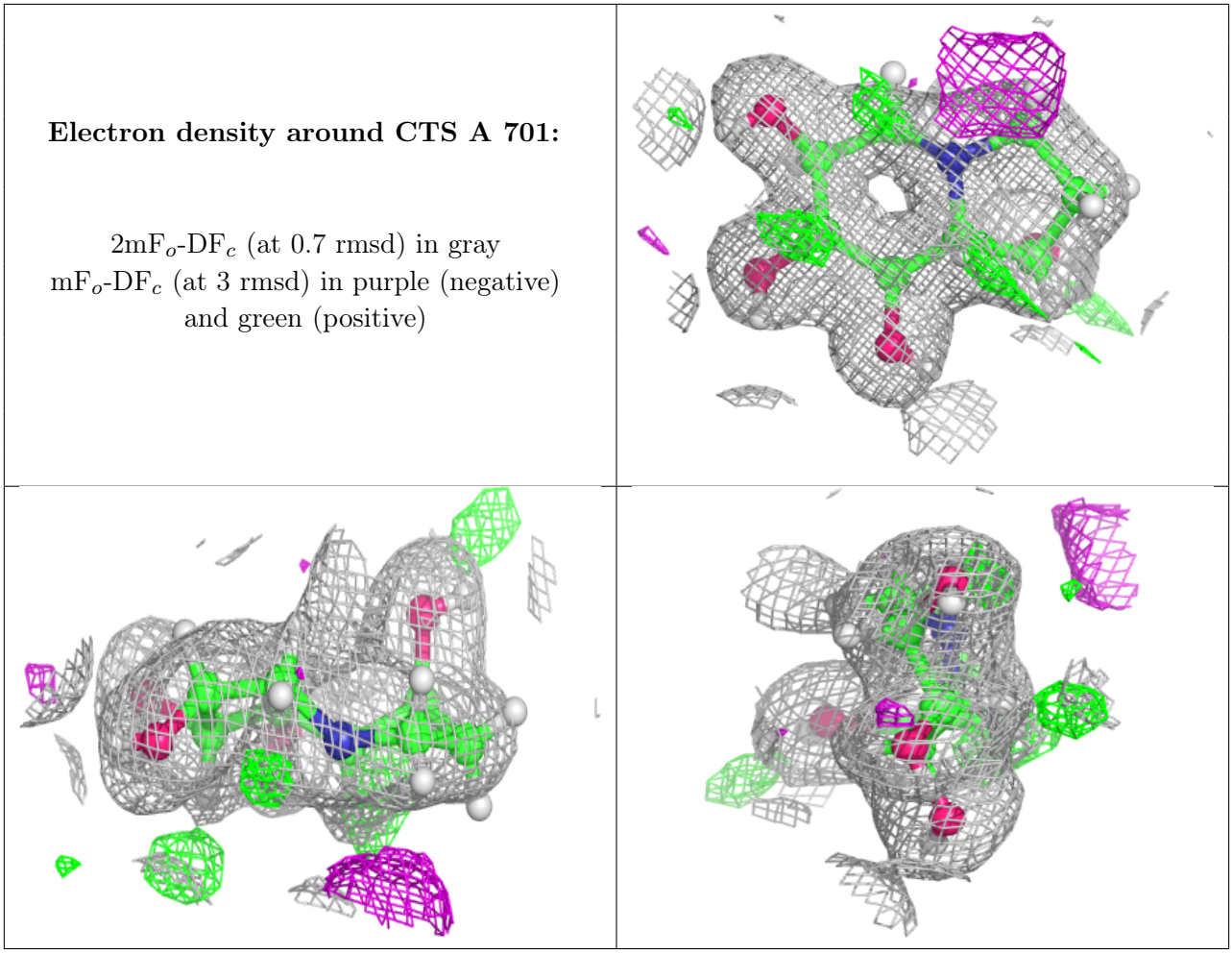
Electron density around CTS C 701:

$2mF_o$-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

There are no such residues in this entry.