



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 15, 2026 – 09:21 PM JST

PDB ID : 9WUJ / pdb_00009wuj
Title : Diguanylate cyclase Q15Z91 complex with c-di-GMP and citrate
Authors : Han, L.; Silvaggi, N.R.
Deposited on : 2025-09-18
Resolution : 1.85 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 : 1.8.5 (274361), CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

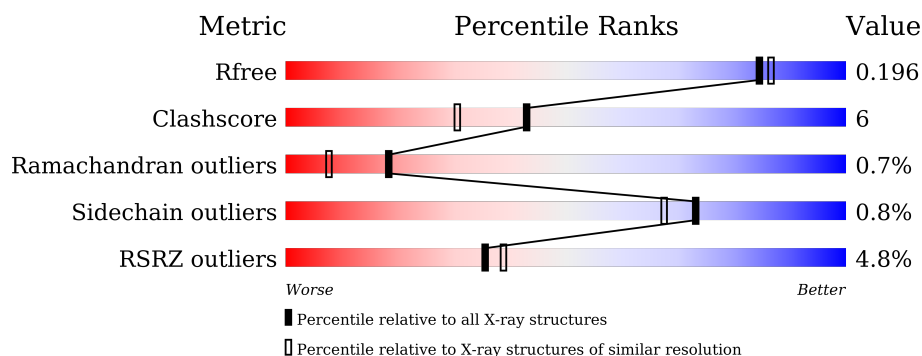
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	310	2% 90% 6% .
1	B	310	% 90% 6% .
1	C	310	13% 73% 20% . .
1	D	310	3% 85% 11% .

2 Entry composition [i](#)

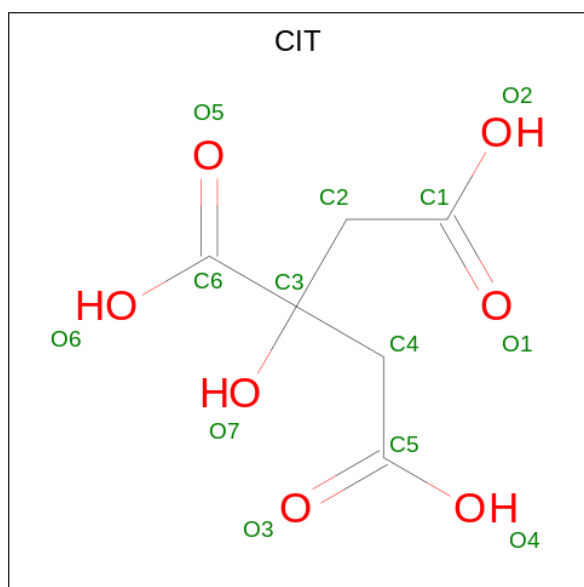
There are 6 unique types of molecules in this entry. The entry contains 20840 atoms, of which 9910 are hydrogens and 0 are deuteriums.

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 diguanylate cyclase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	300	Total	C	H	N	O	S	0	2	0
			4791	1502	2424	410	442	13			
1	B	299	Total	C	H	N	O	S	0	2	0
			4782	1499	2418	412	441	12			
1	C	297	Total	C	H	N	O	S	0	2	0
			4741	1488	2400	404	437	12			
1	D	300	Total	C	H	N	O	S	0	0	0
			4771	1496	2416	408	439	12			

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			18	6	5	7		
2	B	1	Total	C	H	O	0	0
			18	6	5	7		

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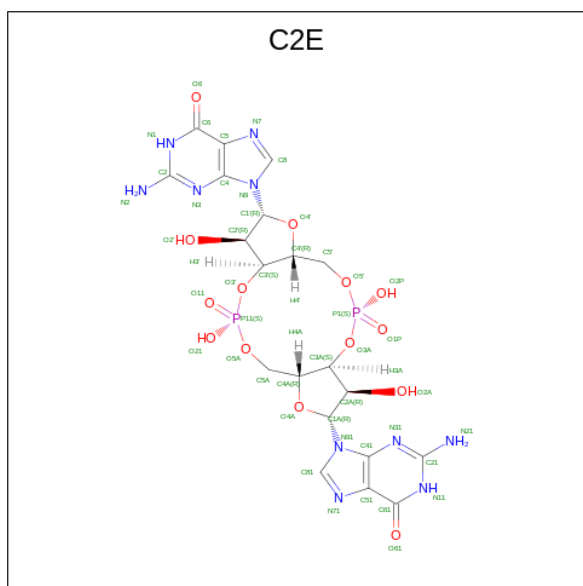
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	H	O	0	0
			18	6	5	7		
2	D	1	Total	C	H	O	0	0
			18	6	5	7		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 9,9'-[(2R,3R,3aS,5S,7aR,9R,10R,10aS,12S,14aR)-3,5,10,12-tetrahydroxy-5,12-dioxidoctahydro-2H,7H-difuro[3,2-d:3',2'-j][1,3,7,9,2,8]tetraoxadiphosphacyclododecine-2,9-diyl]bis(2-amino-1,9-dihydro-6H-purin-6-one) (CCD ID: C2E) (formula: C₂₀H₂₄N₁₀O₁₄P₂) (labeled as "Ligand of Interest" by depositor).



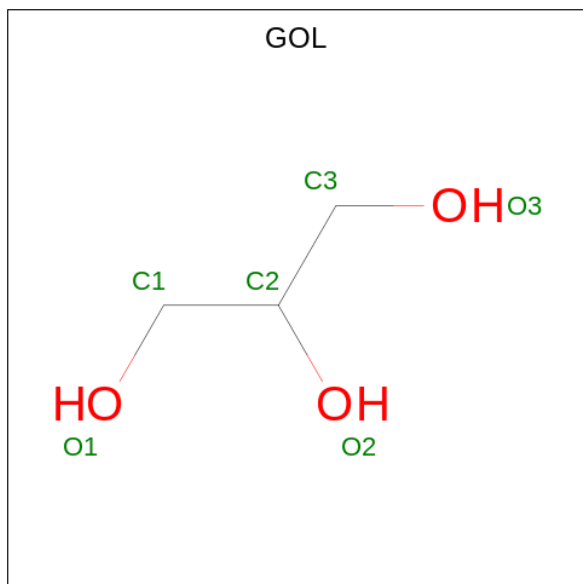
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 68	C 20	H 22	N 10	O 14	P 2	0	0
4	A	1	Total 68	C 20	H 22	N 10	O 14	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	N	O	P	
			68	20	22	10	14	2	0
4	B	1	Total	C	H	N	O	P	
			68	20	22	10	14	2	0
4	C	1	Total	C	H	N	O	P	
			68	20	22	10	14	2	0
4	C	1	Total	C	H	N	O	P	
			68	20	22	10	14	2	0
4	D	1	Total	C	H	N	O	P	
			68	20	22	10	14	2	0
4	D	1	Total	C	H	N	O	P	
			68	20	22	10	14	2	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O		
			14	3	8	3	0	0
5	A	1	Total	C	H	O		
			14	3	8	3	0	0
5	B	1	Total	C	H	O		
			14	3	8	3	0	0
5	C	1	Total	C	H	O		
			14	3	8	3	0	0
5	D	1	Total	C	H	O		
			14	3	8	3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	H	O	0	0
			14	3	8	3		
5	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	314	Total	O	0	0
			314	314		
6	B	299	Total	O	0	0
			299	299		
6	C	214	Total	O	0	0
			214	214		
6	D	210	Total	O	0	0
			210	210		

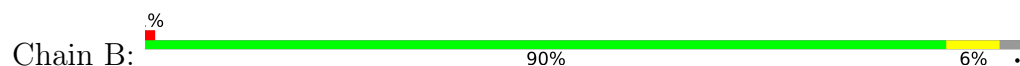
3 Residue-property plots [i](#)

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.

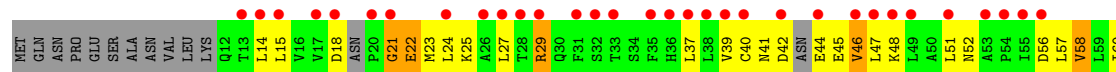
- Molecule 1: diguanylate cyclase



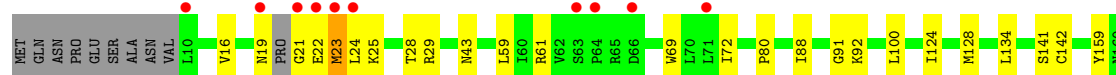
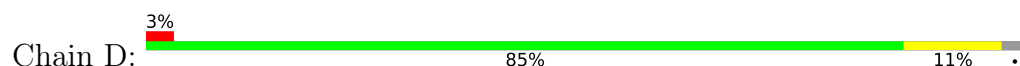
- Molecule 1: diguanylate cyclase



- Molecule 1: diguanylate cyclase



- Molecule 1: diguanylate cyclase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.08Å 115.95Å 167.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.53 – 1.85 35.53 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.5 (35.53-1.85) 99.5 (35.53-1.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 1.85Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.170 , 0.196 0.170 , 0.196	Depositor DCC
R_{free} test set	1993 reflections (1.47%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	20840	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.99% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C2E, CIT, MG, GOL

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	0/2405	0.62	0/3255
1	B	0.51	1/2402 (0.0%)	0.60	0/3251
1	C	0.44	0/2380	0.59	0/3218
1	D	0.48	0/2391	0.60	0/3233
All	All	0.49	1/9578 (0.0%)	0.60	0/12957

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	C	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	217	MET	SD-CE	-6.34	1.63	1.79

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	65	ARG	Sidechain
1	C	29	ARG	Sidechain
1	C	65	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	2367	2424	2422	15	0
1	B	2364	2418	2417	13	0
1	C	2341	2400	2398	62	0
1	D	2355	2416	2415	36	0
2	A	13	5	5	0	0
2	B	13	5	5	0	0
2	C	13	5	4	0	0
2	D	13	5	4	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	92	44	44	1	0
4	B	92	44	44	0	0
4	C	92	44	44	2	0
4	D	92	44	44	2	0
5	A	12	16	16	1	0
5	B	6	8	8	0	0
5	C	6	8	8	0	0
5	D	18	24	23	3	0
6	A	314	0	0	4	5
6	B	299	0	0	2	2
6	C	214	0	0	0	1
6	D	210	0	0	5	4
All	All	10930	9910	9901	122	6

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 6.

All (122) 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:D:23:MET:HE1	1:D:61:ARG:NH1	1.74	1.02
1:D:23:MET:HE1	1:D:61:ARG:CZ	1.93	0.99
1:B:124:ILE:HG22	1:B:128:MET:HE2	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:MET:CE	1:D:61:ARG:NH1	2.43	0.81
1:D:23:MET:CE	1:D:61:ARG:CZ	2.64	0.76
1:C:47:LEU:O	1:C:51:LEU:HD12	1.86	0.75
1:D:43:ASN:OD1	6:D:501:HOH:O	2.05	0.74
1:B:66:ASP:OD1	6:B:501:HOH:O	2.08	0.70
1:C:140:ILE:HD12	1:D:141:SER:OG	1.92	0.69
1:C:42:ASP:O	1:C:44:GLU:N	2.25	0.69
1:C:120:LEU:HD13	1:C:124:ILE:HG12	1.76	0.68
1:A:153:MET:HG2	1:B:142:CYS:SG	2.35	0.67
1:D:182:PHE:HE2	1:D:260:VAL:HG23	1.60	0.66
1:D:124:ILE:CG2	1:D:128:MET:HE2	2.27	0.64
1:C:155:LEU:HD21	1:C:226:LEU:HB3	1.80	0.64
1:C:68:ASP:O	1:C:72:ILE:HD12	1.97	0.63
1:D:25:LYS:HE3	1:D:29:ARG:HD3	1.81	0.62
1:A:35:PHE:CE2	1:A:128:MET:HE1	2.35	0.62
1:C:72:ILE:HD12	1:C:72:ILE:H	1.64	0.62
1:C:112:GLU:HG2	1:C:115:THR:HG22	1.80	0.62
1:A:177:MET:HE1	1:A:290:VAL:HG13	1.82	0.61
1:C:79:HIS:C	1:C:83:ILE:HD11	2.26	0.61
1:A:177:MET:CE	1:A:290:VAL:HG13	2.31	0.60
1:B:124:ILE:CG2	1:B:128:MET:HE2	2.29	0.60
1:A:211:GLN:N	6:A:501:HOH:O	2.35	0.59
1:D:22:GLU:O	1:D:24:LEU:N	2.36	0.58
1:B:161[B]:ARG:NH1	6:B:508:HOH:O	2.34	0.58
1:D:24:LEU:O	1:D:28:THR:HG23	2.04	0.57
1:D:124:ILE:HG22	1:D:128:MET:HE2	1.86	0.56
1:D:80:PRO:O	6:D:502:HOH:O	2.18	0.55
1:C:56:ASP:HB3	1:C:128:MET:CE	2.37	0.55
1:D:211:GLN:HG2	4:D:403:C2E:O6	2.08	0.54
1:A:184:LYS:HE3	1:A:188:ASP:OD1	2.07	0.54
1:D:211:GLN:NE2	6:D:508:HOH:O	2.40	0.54
1:C:23:MET:HE3	1:C:92:LYS:HD3	1.88	0.54
1:C:122:ILE:CD1	1:D:100:LEU:HD22	2.38	0.54
1:C:14:LEU:C	1:C:14:LEU:HD23	2.33	0.54
1:C:65:ARG:O	1:C:66:ASP:CB	2.57	0.53
1:C:177:MET:HE2	1:C:224:GLU:OE2	2.09	0.53
1:D:59:LEU:HD21	1:D:124:ILE:HD11	1.90	0.53
1:C:177:MET:HE3	1:C:177:MET:HA	1.92	0.52
1:D:16:VAL:HG11	1:D:24:LEU:CD1	2.40	0.51
1:C:47:LEU:HG	1:C:51:LEU:HD11	1.91	0.51
1:C:87:LEU:C	1:C:88:ILE:HD12	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:68:ASP:O	1:C:72:ILE:CD1	2.60	0.50
1:C:240:ILE:HD11	4:C:403:C2E:C51	2.41	0.50
5:D:407:GOL:O1	6:D:503:HOH:O	2.20	0.50
1:C:146:LEU:O	1:C:200:LYS:HE2	2.12	0.50
1:B:35:PHE:CE1	1:B:128:MET:HE1	2.46	0.50
1:C:27:LEU:HD21	1:C:113:LEU:HD11	1.95	0.48
1:C:120:LEU:O	1:C:124:ILE:HG12	2.14	0.48
1:A:233:ASP:CG	6:A:508:HOH:O	2.57	0.48
1:C:112:GLU:HG2	1:C:115:THR:CG2	2.44	0.48
1:C:18:ASP:OD2	1:C:61:ARG:NH1	2.44	0.48
1:D:59:LEU:HD23	1:D:88:ILE:HB	1.94	0.48
1:C:24:LEU:HD12	1:C:24:LEU:O	2.14	0.48
1:C:72:ILE:HD12	1:C:72:ILE:N	2.29	0.48
1:A:134:LEU:C	1:A:134:LEU:HD23	2.39	0.47
1:C:124:ILE:O	1:C:128:MET:HG3	2.14	0.47
1:D:69:TRP:O	1:D:72:ILE:HG22	2.14	0.47
1:C:57:LEU:HD11	1:C:88:ILE:HD13	1.96	0.47
1:C:57:LEU:HB2	1:C:128:MET:HE3	1.97	0.47
1:C:14:LEU:HD22	1:C:37:LEU:HD22	1.97	0.47
1:D:240:ILE:HD11	4:D:403:C2E:C5	2.45	0.47
1:A:261:ASN:HB2	6:A:560:HOH:O	2.15	0.47
1:C:60:ILE:HB	1:C:89:LEU:HD23	1.96	0.47
1:D:61:ARG:HH11	1:D:91:GLY:HA2	1.79	0.47
1:C:23:MET:CE	1:C:92:LYS:HD3	2.45	0.46
1:A:210:LEU:HB2	5:A:406:GOL:H11	1.97	0.46
1:C:51:LEU:HD21	1:C:79:HIS:CE1	2.51	0.46
1:B:112:GLU:HG2	1:B:115:THR:CG2	2.45	0.46
1:C:69:TRP:HA	1:C:72:ILE:HD13	1.97	0.46
1:C:252:ASP:OD1	1:C:263:LYS:HD3	2.17	0.45
1:B:155:LEU:HD21	1:B:226:LEU:HB3	1.99	0.45
1:C:177:MET:CE	1:C:224:GLU:HG2	2.47	0.45
1:D:19:ASN:O	1:D:21:GLY:N	2.50	0.45
1:D:25:LYS:CE	1:D:29:ARG:HD3	2.45	0.45
1:B:112:GLU:HG2	1:B:115:THR:HG22	1.98	0.45
1:C:47:LEU:HG	1:C:51:LEU:CD1	2.47	0.45
1:C:125:ARG:NH2	1:C:126:ASN:OD1	2.50	0.44
1:C:79:HIS:O	1:C:83:ILE:CD1	2.65	0.44
1:A:239:LYS:HE2	6:A:669:HOH:O	2.18	0.44
1:C:45:GLU:O	1:C:46:VAL:C	2.60	0.43
1:D:16:VAL:HG11	1:D:24:LEU:HD11	1.99	0.43
1:C:137:LEU:HD12	1:D:134:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:ASN:HD22	1:C:41:ASN:C	2.25	0.43
1:C:70:LEU:HD13	1:C:70:LEU:C	2.44	0.43
1:B:88:ILE:HD12	1:B:124:ILE:CD1	2.49	0.43
1:C:64:PRO:O	1:C:65:ARG:HB2	2.18	0.43
1:C:65:ARG:O	1:C:66:ASP:HB2	2.17	0.43
1:C:110:PHE:CD1	1:C:110:PHE:C	2.97	0.43
1:D:124:ILE:O	1:D:128:MET:HG3	2.19	0.43
1:A:35:PHE:HE2	1:A:128:MET:HE1	1.83	0.42
1:C:29:ARG:HG2	1:C:29:ARG:HH11	1.84	0.42
1:C:56:ASP:HB3	1:C:128:MET:HE2	2.02	0.42
1:A:240:ILE:HD11	4:A:403:C2E:C51	2.49	0.42
1:C:25:LYS:O	1:C:29:ARG:N	2.48	0.42
1:C:15:LEU:O	1:C:58:VAL:HA	2.20	0.42
1:D:22:GLU:C	1:D:24:LEU:N	2.78	0.42
1:C:88:ILE:HD12	1:C:88:ILE:N	2.35	0.42
1:C:21:GLY:O	1:C:22:GLU:C	2.62	0.42
1:C:48:LYS:O	1:C:52:ASN:OD1	2.37	0.42
1:C:130:VAL:HG13	1:D:134:LEU:HD11	2.02	0.42
1:D:92:LYS:O	1:D:92:LYS:HG3	2.19	0.41
1:D:159:TYR:CD2	5:D:406:GOL:H11	2.55	0.41
1:D:177:MET:HE2	1:D:224:GLU:OE2	2.20	0.41
1:C:62:VAL:HG22	1:C:90:TYR:O	2.21	0.41
1:A:124:ILE:HD13	1:A:124:ILE:HG21	1.79	0.41
1:B:179:ASP:HB2	1:B:297:LEU:HD21	2.01	0.41
1:D:273:LEU:HD12	5:D:405:GOL:C1	2.51	0.41
1:B:163:TRP:CG	1:B:286:PRO:HB3	2.55	0.41
1:A:23:MET:HE1	1:A:61:ARG:NE	2.35	0.41
4:C:404:C2E:H4A	1:D:283:PHE:CD2	2.56	0.41
1:C:147:THR:HA	1:C:200:LYS:HG2	2.03	0.41
1:D:161:ARG:NH2	6:D:523:HOH:O	2.54	0.41
1:B:110:PHE:CD1	1:B:110:PHE:C	2.99	0.41
1:C:39:VAL:HG12	1:C:40:CYS:N	2.36	0.41
1:C:29:ARG:HH11	1:C:29:ARG:CG	2.33	0.40
1:C:71:LEU:O	1:C:75:ARG:HG2	2.20	0.40
1:D:25:LYS:HE3	1:D:29:ARG:NH1	2.35	0.40
1:C:79:HIS:O	1:C:83:ILE:HD13	2.21	0.40
1:C:37:LEU:C	1:C:37:LEU:HD13	2.46	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:610:HOH:O	6:D:617:HOH:O[4_557]	1.94	0.26
6:A:618:HOH:O	6:D:542:HOH:O[4_557]	2.04	0.16
6:B:756:HOH:O	6:C:695:HOH:O[4_557]	2.09	0.11
6:A:503:HOH:O	6:B:613:HOH:O[3_357]	2.10	0.10
6:A:674:HOH:O	6:D:617:HOH:O[4_557]	2.15	0.05
6:A:692:HOH:O	6:D:560:HOH:O[1_655]	2.19	0.01

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	300/310 (97%)	293 (98%)	6 (2%)	1 (0%)	36	25
1	B	299/310 (96%)	295 (99%)	4 (1%)	0	100	100
1	C	293/310 (94%)	282 (96%)	5 (2%)	6 (2%)	6	1
1	D	296/310 (96%)	291 (98%)	4 (1%)	1 (0%)	36	25
All	All	1188/1240 (96%)	1161 (98%)	19 (2%)	8 (1%)	18	8

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	ASP
1	C	22	GLU
1	C	66	ASP
1	D	23	MET
1	C	65	ARG
1	C	93	ASP
1	C	21	GLY
1	C	46	VAL

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	263/270 (97%)	262 (100%)	1 (0%)	84	82
1	B	262/270 (97%)	259 (99%)	3 (1%)	65	57
1	C	260/270 (96%)	256 (98%)	4 (2%)	57	47
1	D	261/270 (97%)	259 (99%)	2 (1%)	73	67
All	All	1046/1080 (97%)	1036 (99%)	10 (1%)	73	60

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

Mol	Chain	Res	Type
1	A	142	CYS
1	B	63	SER
1	B	160[A]	ASN
1	B	160[B]	ASN
1	C	58	VAL
1	C	129	GLN
1	C	143[A]	THR
1	C	143[B]	THR
1	D	142	CYS
1	D	294	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	52	ASN
1	A	78	GLN
1	A	160	ASN
1	A	171	HIS
1	A	211	GLN
1	B	192	HIS
1	C	121	ASN
1	D	129	GLN

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Mol	Chain	Res	Type
1	D	299	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 4 are monoatomic - leaving 19 for Mogul analysis.

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	CIT	B	401	3	12,12,12	1.03	0	17,17,17	1.70	2 (11%)
4	C2E	B	404	-	52,52,52	3.40	24 (46%)	80,82,82	2.87	20 (25%)
2	CIT	D	401	3	12,12,12	1.00	0	17,17,17	1.83	3 (17%)
5	GOL	B	405	-	5,5,5	0.65	0	5,5,5	1.32	1 (20%)
4	C2E	D	404	-	52,52,52	3.46	23 (44%)	80,82,82	2.72	17 (21%)
5	GOL	D	406	-	5,5,5	1.07	1 (20%)	5,5,5	0.36	0
5	GOL	D	405	-	5,5,5	1.21	0	5,5,5	1.29	1 (20%)
2	CIT	A	401	3	12,12,12	1.15	1 (8%)	17,17,17	1.62	3 (17%)
5	GOL	A	406	-	5,5,5	1.39	2 (40%)	5,5,5	0.85	0
4	C2E	C	403	-	52,52,52	3.48	25 (48%)	80,82,82	2.82	20 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	C2E	A	404	-	52,52,52	3.45	22 (42%)	80,82,82	2.77	20 (25%)
4	C2E	B	403	-	52,52,52	3.40	23 (44%)	80,82,82	2.73	17 (21%)
2	CIT	C	401	3	12,12,12	1.13	1 (8%)	17,17,17	1.91	5 (29%)
5	GOL	D	407	-	5,5,5	1.26	0	5,5,5	0.64	0
4	C2E	C	404	-	52,52,52	3.46	24 (46%)	80,82,82	2.80	17 (21%)
4	C2E	D	403	-	52,52,52	3.50	24 (46%)	80,82,82	2.84	20 (25%)
5	GOL	A	405	-	5,5,5	0.59	0	5,5,5	0.97	0
4	C2E	A	403	-	52,52,52	3.44	23 (44%)	80,82,82	2.96	24 (30%)
5	GOL	C	405	-	5,5,5	0.99	0	5,5,5	1.20	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	CIT	B	401	3	-	2/16/16/16	-
4	C2E	B	404	-	-	0/30/62/62	0/6/7/7
2	CIT	D	401	3	-	4/16/16/16	-
5	GOL	B	405	-	-	2/4/4/4	-
4	C2E	D	404	-	-	0/30/62/62	0/6/7/7
5	GOL	D	406	-	-	2/4/4/4	-
5	GOL	D	405	-	-	1/4/4/4	-
2	CIT	A	401	3	-	0/16/16/16	-
5	GOL	A	406	-	-	0/4/4/4	-
4	C2E	C	403	-	-	0/30/62/62	0/6/7/7
4	C2E	A	404	-	-	0/30/62/62	0/6/7/7
4	C2E	B	403	-	-	0/30/62/62	0/6/7/7
2	CIT	C	401	3	-	8/16/16/16	-
5	GOL	D	407	-	-	4/4/4/4	-
4	C2E	C	404	-	-	0/30/62/62	0/6/7/7
4	C2E	D	403	-	-	0/30/62/62	0/6/7/7
5	GOL	A	405	-	-	0/4/4/4	-
4	C2E	A	403	-	-	2/30/62/62	0/6/7/7
5	GOL	C	405	-	-	4/4/4/4	-

All (193) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	C2E	C5-C4	12.09	1.73	1.38
4	A	404	C2E	C5-C4	11.67	1.72	1.38
4	D	404	C2E	C5-C4	11.61	1.71	1.38
4	B	404	C2E	C5-C4	11.55	1.71	1.38
4	D	403	C2E	C5-C4	11.48	1.71	1.38
4	B	403	C2E	C5-C4	11.44	1.71	1.38
4	C	403	C2E	C5-C4	11.39	1.71	1.38
4	C	404	C2E	C5-C4	11.38	1.71	1.38
4	D	403	C2E	C5-N7	-8.21	1.23	1.39
4	C	404	C2E	C5-N7	-8.17	1.23	1.39
4	C	403	C2E	C5-N7	-8.02	1.23	1.39
4	A	404	C2E	C8-N7	-7.98	1.10	1.32
4	C	404	C2E	C8-N7	-7.86	1.10	1.32
4	D	403	C2E	C8-N7	-7.79	1.10	1.32
4	D	404	C2E	C8-N7	-7.76	1.10	1.32
4	A	404	C2E	C5-N7	-7.67	1.24	1.39
4	B	403	C2E	C5-N7	-7.42	1.24	1.39
4	D	404	C2E	C5-N7	-7.40	1.24	1.39
4	A	403	C2E	O61-C61	7.39	1.37	1.23
4	A	403	C2E	C5-N7	-7.35	1.24	1.39
4	B	403	C2E	C8-N7	-7.30	1.12	1.32
4	B	404	C2E	C8-N7	-7.25	1.12	1.32
4	D	404	C2E	O61-C61	7.22	1.37	1.23
4	D	403	C2E	O6-C6	7.11	1.37	1.23
4	C	404	C2E	O61-C61	7.10	1.37	1.23
4	C	403	C2E	O61-C61	7.07	1.37	1.23
4	D	403	C2E	C2-N3	-7.07	1.15	1.33
4	A	403	C2E	C8-N7	-7.03	1.12	1.32
4	D	404	C2E	O6-C6	7.02	1.36	1.23
4	B	403	C2E	O61-C61	6.93	1.36	1.23
4	A	404	C2E	O61-C61	6.85	1.36	1.23
4	B	404	C2E	C5-N7	-6.77	1.25	1.39
4	C	403	C2E	C8-N7	-6.67	1.13	1.32
4	A	404	C2E	C2-N3	-6.67	1.16	1.33
4	C	404	C2E	O6-C6	6.66	1.36	1.23
4	C	403	C2E	C2-N3	-6.43	1.17	1.33
4	B	403	C2E	O6-C6	6.41	1.35	1.23
4	D	403	C2E	O61-C61	6.36	1.35	1.23
4	B	404	C2E	O61-C61	6.32	1.35	1.23
4	A	404	C2E	O6-C6	6.23	1.35	1.23
4	D	404	C2E	C2-N3	-6.20	1.18	1.33
4	C	403	C2E	O6-C6	6.13	1.35	1.23
4	B	404	C2E	O6-C6	6.09	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	404	C2E	C2-N3	-5.98	1.18	1.33
4	A	403	C2E	C2-N3	-5.90	1.18	1.33
4	C	404	C2E	C2-N3	-5.74	1.19	1.33
4	B	403	C2E	C4-N9	5.73	1.53	1.38
4	B	403	C2E	C2-N3	-5.57	1.19	1.33
4	A	403	C2E	O6-C6	5.55	1.34	1.23
4	C	403	C2E	C4-N9	5.43	1.52	1.38
4	B	404	C2E	C4-N9	5.34	1.52	1.38
4	D	404	C2E	C4-N9	5.31	1.51	1.38
4	C	404	C2E	C2-N2	5.12	1.46	1.34
4	A	403	C2E	C51-N71	5.03	1.48	1.39
4	C	404	C2E	C4-N9	5.01	1.51	1.38
4	A	403	C2E	C4-N9	4.95	1.51	1.38
4	C	404	C2E	C5-C6	4.86	1.62	1.44
4	A	404	C2E	C4-N9	4.86	1.50	1.38
4	D	403	C2E	C4-N9	4.83	1.50	1.38
4	B	404	C2E	C5-C6	4.77	1.62	1.44
4	D	404	C2E	C5-C6	4.67	1.61	1.44
4	C	403	C2E	C5-C6	4.64	1.61	1.44
4	B	403	C2E	C5-C6	4.62	1.61	1.44
4	A	403	C2E	C5-C6	4.60	1.61	1.44
4	C	403	C2E	C2-N2	4.46	1.44	1.34
4	D	403	C2E	C5-C6	4.38	1.60	1.44
4	A	404	C2E	C2-N2	4.36	1.44	1.34
4	D	403	C2E	C2'-C3'	-4.35	1.43	1.52
4	C	403	C2E	C21-N21	4.34	1.44	1.34
4	D	404	C2E	C2-N2	4.33	1.44	1.34
4	B	403	C2E	C8-N9	-4.30	1.27	1.37
4	A	404	C2E	C5-C6	4.28	1.60	1.44
4	A	403	C2E	C2-N2	4.27	1.44	1.34
4	C	403	C2E	C51-N71	4.15	1.47	1.39
4	B	403	C2E	C21-N31	4.12	1.43	1.33
4	B	404	C2E	C21-N21	4.09	1.43	1.34
4	B	404	C2E	C21-N31	4.03	1.42	1.33
4	A	403	C2E	C21-N11	3.91	1.47	1.37
4	A	404	C2E	C2'-C3'	-3.89	1.44	1.52
4	B	404	C2E	C21-N11	3.89	1.47	1.37
4	B	403	C2E	C21-N21	3.88	1.43	1.34
4	C	403	C2E	C2'-C3'	-3.83	1.44	1.52
4	C	404	C2E	C21-N31	3.83	1.42	1.33
4	B	403	C2E	C21-N11	3.82	1.47	1.37
4	C	403	C2E	C21-N11	3.81	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	C2E	C51-N71	3.78	1.46	1.39
4	D	404	C2E	C2'-C3'	-3.77	1.44	1.52
4	A	404	C2E	C21-N31	3.76	1.42	1.33
4	D	403	C2E	C21-N31	3.76	1.42	1.33
4	C	403	C2E	C21-N31	3.72	1.42	1.33
4	A	403	C2E	C8-N9	-3.71	1.29	1.37
4	C	404	C2E	C21-N21	3.70	1.43	1.34
4	B	404	C2E	C2-N2	3.70	1.43	1.34
4	A	404	C2E	C8-N9	-3.69	1.29	1.37
4	D	403	C2E	C51-N71	3.68	1.46	1.39
4	B	404	C2E	C2'-C3'	-3.68	1.44	1.52
4	D	403	C2E	C21-N11	3.68	1.46	1.37
4	D	403	C2E	C21-N21	3.67	1.42	1.34
4	D	403	C2E	C2-N2	3.67	1.42	1.34
4	A	403	C2E	C21-N31	3.62	1.41	1.33
4	D	404	C2E	C21-N21	3.60	1.42	1.34
4	A	404	C2E	C21-N11	3.60	1.46	1.37
4	A	404	C2E	C61-N11	-3.52	1.32	1.38
4	C	403	C2E	C8-N9	-3.47	1.29	1.37
4	D	404	C2E	C21-N31	3.45	1.41	1.33
4	C	404	C2E	C2'-C3'	-3.44	1.45	1.52
4	A	403	C2E	C2'-C3'	-3.39	1.45	1.52
4	C	404	C2E	C51-N71	3.39	1.45	1.39
4	D	403	C2E	C8-N9	-3.36	1.30	1.37
4	A	403	C2E	C2A-C3A	-3.35	1.45	1.52
4	D	404	C2E	C8-N9	-3.34	1.30	1.37
4	D	404	C2E	C51-N71	3.32	1.45	1.39
4	B	404	C2E	O4'-C1'	3.32	1.49	1.42
4	C	404	C2E	C21-N11	3.28	1.45	1.37
4	C	403	C2E	O4'-C1'	3.21	1.49	1.42
4	D	404	C2E	O4'-C1'	3.18	1.49	1.42
4	B	404	C2E	C2-N1	-3.17	1.29	1.37
4	B	404	C2E	O4A-C1A	3.16	1.49	1.42
4	B	404	C2E	C51-N71	3.16	1.45	1.39
4	A	404	C2E	C21-N21	3.14	1.41	1.34
4	C	404	C2E	C8-N9	-3.13	1.30	1.37
4	A	403	C2E	O4'-C1'	3.11	1.49	1.42
4	A	403	C2E	C21-N21	3.10	1.41	1.34
4	B	403	C2E	C2'-C3'	-3.05	1.46	1.52
4	C	403	C2E	O4A-C1A	3.05	1.49	1.42
4	D	404	C2E	C21-N11	3.02	1.45	1.37
4	B	404	C2E	C8-N9	-3.01	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	403	C2E	O4'-C1'	2.97	1.49	1.42
4	B	403	C2E	C51-N71	2.93	1.44	1.39
4	B	403	C2E	O4'-C4'	2.92	1.51	1.45
4	B	403	C2E	C2-N2	2.88	1.41	1.34
4	B	404	C2E	C2'-C1'	-2.88	1.44	1.53
4	D	403	C2E	C2A-C3A	-2.87	1.46	1.52
4	D	404	C2E	O4A-C1A	2.86	1.48	1.42
4	D	403	C2E	C2-N1	-2.84	1.30	1.37
4	B	403	C2E	C2A-C3A	-2.80	1.46	1.52
4	B	404	C2E	C4-N3	-2.77	1.27	1.34
4	D	403	C2E	C1'-N9	-2.77	1.39	1.47
4	A	404	C2E	O4'-C4'	2.72	1.51	1.45
4	B	404	C2E	C1'-N9	-2.69	1.39	1.47
4	B	403	C2E	C2'-C1'	-2.68	1.44	1.53
4	C	403	C2E	C2-N1	-2.68	1.31	1.37
4	D	403	C2E	O4A-C1A	2.66	1.48	1.42
4	C	404	C2E	O4A-C1A	2.66	1.48	1.42
4	C	404	C2E	O4'-C1'	2.65	1.48	1.42
4	D	404	C2E	C2-N1	-2.64	1.31	1.37
4	D	403	C2E	C4-N3	-2.63	1.28	1.34
4	D	403	C2E	O4'-C4'	2.60	1.50	1.45
4	A	404	C2E	C1'-N9	-2.59	1.40	1.47
4	A	403	C2E	C81-N91	-2.58	1.31	1.37
4	C	403	C2E	O4'-C4'	2.58	1.50	1.45
4	C	404	C2E	C2-N1	-2.58	1.31	1.37
4	C	403	C2E	C2A-C3A	-2.57	1.47	1.52
4	D	403	C2E	O4'-C1'	2.56	1.48	1.42
4	B	404	C2E	C61-N11	-2.54	1.34	1.38
4	A	403	C2E	C2-N1	-2.51	1.31	1.37
4	D	404	C2E	C81-N91	-2.51	1.32	1.37
4	B	404	C2E	C2A-C3A	-2.50	1.47	1.52
4	C	403	C2E	C81-N91	-2.50	1.32	1.37
4	A	404	C2E	C2-N1	-2.47	1.31	1.37
4	B	403	C2E	O4A-C1A	2.46	1.47	1.42
4	A	403	C2E	C2'-C1'	-2.43	1.45	1.53
4	A	404	C2E	O4A-C1A	2.42	1.47	1.42
4	D	404	C2E	O4'-C4'	2.40	1.50	1.45
4	B	403	C2E	C2-N1	-2.39	1.31	1.37
2	A	401	CIT	C3-C6	-2.39	1.50	1.53
4	C	404	C2E	C41-N91	-2.38	1.31	1.38
4	C	404	C2E	O4'-C4'	2.35	1.50	1.45
4	A	403	C2E	O4A-C1A	2.34	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	C2E	C41-N91	-2.34	1.32	1.38
4	D	403	C2E	C61-N11	-2.34	1.34	1.38
4	B	403	C2E	C61-N11	-2.33	1.34	1.38
4	C	403	C2E	C2'-C1'	-2.27	1.46	1.53
4	D	404	C2E	C1'-N9	-2.24	1.41	1.47
4	D	403	C2E	C41-N91	-2.24	1.32	1.38
4	D	404	C2E	P11-O21	-2.18	1.45	1.55
4	C	404	C2E	C1'-N9	-2.18	1.41	1.47
4	A	403	C2E	O4'-C4'	2.15	1.49	1.45
4	C	404	C2E	C81-N91	-2.14	1.32	1.37
4	A	404	C2E	O4'-C1'	2.14	1.47	1.42
5	A	406	GOL	C1-C2	2.12	1.60	1.51
4	B	403	C2E	C41-N91	-2.12	1.32	1.38
5	A	406	GOL	C3-C2	2.11	1.60	1.51
4	C	404	C2E	C61-N11	-2.10	1.34	1.38
4	C	403	C2E	C61-N11	-2.08	1.35	1.38
2	C	401	CIT	O7-C3	2.08	1.47	1.43
5	D	406	GOL	C3-C2	2.08	1.60	1.51
4	C	404	C2E	C2A-C3A	-2.05	1.48	1.52
4	D	404	C2E	C41-N91	-2.04	1.32	1.38
4	A	403	C2E	O2'-C2'	2.03	1.47	1.43
4	C	403	C2E	C41-N91	-2.02	1.32	1.38
4	B	404	C2E	C81-N91	-2.02	1.33	1.37
4	C	403	C2E	C4-N3	-2.00	1.29	1.34

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	C2E	C6-C5-N7	12.52	153.53	130.25
4	D	403	C2E	C6-C5-N7	12.39	153.28	130.25
4	A	403	C2E	C6-C5-N7	11.83	152.24	130.25
4	B	404	C2E	C6-C5-C4	-11.59	100.95	118.77
4	A	404	C2E	C6-C5-N7	11.50	151.64	130.25
4	D	403	C2E	C6-C5-C4	-11.46	101.15	118.77
4	D	404	C2E	C6-C5-N7	11.40	151.44	130.25
4	C	404	C2E	C6-C5-N7	11.20	151.08	130.25
4	A	403	C2E	C6-C5-C4	-11.08	101.73	118.77
4	C	403	C2E	C6-C5-N7	10.95	150.62	130.25
4	C	403	C2E	C6-C5-C4	-10.95	101.92	118.77
4	C	404	C2E	C6-C5-C4	-10.74	102.25	118.77
4	B	403	C2E	C6-C5-N7	10.68	150.10	130.25
4	A	404	C2E	C6-C5-C4	-10.53	102.57	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	404	C2E	C6-C5-C4	-10.25	103.00	118.77
4	B	403	C2E	C6-C5-C4	-10.16	103.14	118.77
4	C	404	C2E	N9-C4-N3	9.13	144.28	125.94
4	B	403	C2E	C5-C4-N9	-8.88	89.51	105.63
4	A	403	C2E	N9-C4-N3	8.78	143.58	125.94
4	D	404	C2E	N9-C4-N3	8.78	143.57	125.94
4	B	403	C2E	N9-C4-N3	8.71	143.44	125.94
4	C	404	C2E	C5-C4-N9	-8.70	89.85	105.63
4	A	404	C2E	N9-C4-N3	8.65	143.30	125.94
4	A	403	C2E	C5-C4-N9	-8.51	90.20	105.63
4	A	404	C2E	C5-C4-N9	-8.46	90.27	105.63
4	C	403	C2E	C5-C4-N9	-8.46	90.28	105.63
4	C	403	C2E	N9-C4-N3	8.42	142.85	125.94
4	D	404	C2E	C5-C4-N9	-8.39	90.40	105.63
4	D	403	C2E	C5-C4-N9	-8.32	90.54	105.63
4	B	404	C2E	C5-C4-N9	-8.24	90.67	105.63
4	B	404	C2E	N9-C4-N3	7.98	141.96	125.94
4	D	403	C2E	N9-C4-N3	7.96	141.91	125.94
4	D	403	C2E	C8-N7-C5	6.54	116.08	104.24
4	B	404	C2E	C8-N7-C5	6.51	116.03	104.24
4	D	404	C2E	C8-N7-C5	6.43	115.88	104.24
4	C	404	C2E	C8-N7-C5	6.16	115.38	104.24
4	A	404	C2E	C8-N7-C5	5.82	114.77	104.24
4	B	403	C2E	C8-N7-C5	5.55	114.29	104.24
4	A	403	C2E	C8-N7-C5	5.54	114.27	104.24
4	C	403	C2E	O6-C6-N1	5.31	130.30	120.12
4	C	403	C2E	C8-N7-C5	5.19	113.64	104.24
4	C	404	C2E	C2-N3-C4	5.07	121.33	112.30
4	A	403	C2E	O6-C6-C5	-5.05	113.20	126.60
4	C	403	C2E	O6-C6-C5	-4.96	113.44	126.60
4	A	403	C2E	C21-N11-C61	-4.79	116.36	125.10
4	D	403	C2E	C2-N3-C4	4.65	120.59	112.30
2	B	401	CIT	O6-C6-C3	4.62	121.08	113.05
4	B	403	C2E	O6-C6-N1	4.57	128.88	120.12
2	D	401	CIT	O6-C6-C3	4.57	120.99	113.05
4	A	403	C2E	O6-C6-N1	4.57	128.87	120.12
2	C	401	CIT	O6-C6-C3	4.54	120.94	113.05
4	C	403	C2E	C2-N3-C4	4.54	120.38	112.30
4	D	404	C2E	C2-N3-C4	4.45	120.22	112.30
4	A	404	C2E	C2-N3-C4	4.42	120.17	112.30
4	B	403	C2E	O6-C6-C5	-4.38	114.98	126.60
4	A	403	C2E	C81-N91-C41	4.35	114.33	106.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	C2E	C2-N3-C4	4.32	120.00	112.30
4	B	404	C2E	C1'-N9-C4	-4.28	113.80	126.50
4	C	403	C2E	C4'-O4'-C1'	-4.24	100.12	109.47
4	A	404	C2E	N9-C8-N7	4.22	121.34	113.39
4	A	403	C2E	C2-N3-C4	4.20	119.78	112.30
4	C	404	C2E	O6-C6-C5	-4.17	115.54	126.60
4	A	404	C2E	C21-N11-C61	-4.09	117.63	125.10
4	D	403	C2E	C21-N11-C61	-4.02	117.78	125.10
4	C	403	C2E	N9-C8-N7	3.94	120.82	113.39
4	A	403	C2E	N9-C8-N7	3.94	120.82	113.39
4	B	403	C2E	N9-C8-N7	3.94	120.81	113.39
4	B	404	C2E	C21-N11-C61	-3.85	118.08	125.10
4	B	404	C2E	O6-C6-C5	-3.79	116.54	126.60
4	C	404	C2E	O6-C6-N1	3.70	127.21	120.12
4	B	403	C2E	C4'-O4'-C1'	-3.67	101.38	109.47
4	B	404	C2E	C1'-N9-C8	3.66	137.12	126.70
4	B	403	C2E	N1-C2-N3	3.64	130.12	123.32
4	C	404	C2E	C21-N11-C61	-3.63	118.49	125.10
4	C	403	C2E	C1'-N9-C4	-3.62	115.75	126.50
4	D	404	C2E	C21-N11-C61	-3.59	118.56	125.10
4	C	403	C2E	C81-N91-C41	3.58	112.86	106.05
4	D	404	C2E	N9-C8-N7	3.53	120.05	113.39
4	A	404	C2E	O6-C6-C5	-3.51	117.29	126.60
2	A	401	CIT	O6-C6-C3	3.46	119.06	113.05
4	D	403	C2E	C81-N91-C41	3.45	112.62	106.05
4	D	403	C2E	N9-C8-N7	3.42	119.84	113.39
4	C	404	C2E	N9-C8-N7	3.42	119.83	113.39
4	C	403	C2E	C1'-N9-C8	3.40	136.38	126.70
2	C	401	CIT	O7-C3-C6	3.38	113.60	108.86
4	B	404	C2E	C4'-O4'-C1'	-3.37	102.03	109.47
4	B	403	C2E	C81-N91-C41	3.34	112.41	106.05
4	D	403	C2E	N2-C2-N3	-3.33	113.26	119.73
4	C	404	C2E	C81-N91-C41	3.32	112.36	106.05
4	B	404	C2E	C4-C5-N7	-3.29	105.51	110.72
4	D	404	C2E	C4-C5-N7	-3.28	105.52	110.72
4	D	403	C2E	C4-C5-N7	-3.28	105.54	110.72
4	B	403	C2E	C21-N11-C61	-3.27	119.14	125.10
4	A	404	C2E	O6-C6-N1	3.22	126.30	120.12
4	A	403	C2E	C4'-O4'-C1'	-3.20	102.42	109.47
4	A	403	C2E	C1'-N9-C4	-3.16	117.12	126.50
4	D	403	C2E	C1'-N9-C4	-3.14	117.17	126.50
4	A	404	C2E	C4-C5-N7	-3.14	105.75	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	C2E	C81-N91-C41	3.11	111.96	106.05
4	B	403	C2E	C1'-N9-C4	-3.10	117.29	126.50
4	B	403	C2E	C2-N3-C4	3.06	117.75	112.30
2	A	401	CIT	C2-C3-C6	-3.05	103.54	110.11
4	C	403	C2E	C21-N11-C61	-3.05	119.55	125.10
4	A	403	C2E	C51-C61-N11	3.04	120.90	113.19
4	A	404	C2E	C51-C61-N11	3.02	120.86	113.19
4	A	403	C2E	N1-C2-N3	3.02	128.96	123.32
4	A	403	C2E	C4-C5-N7	-2.97	106.01	110.72
4	D	404	C2E	N1-C2-N3	2.97	128.87	123.32
4	B	404	C2E	O6-C6-N1	2.96	125.79	120.12
4	B	404	C2E	N9-C8-N7	2.95	118.95	113.39
4	D	403	C2E	C51-C61-N11	2.94	120.65	113.19
4	D	404	C2E	C51-C61-N11	2.93	120.64	113.19
4	D	403	C2E	O6-C6-C5	-2.89	118.92	126.60
4	C	404	C2E	C51-C61-N11	2.89	120.53	113.19
4	D	404	C2E	O6-C6-C5	-2.89	118.94	126.60
4	D	403	C2E	C1'-N9-C8	2.85	134.81	126.70
4	B	404	C2E	N1-C2-N3	2.85	128.64	123.32
4	A	404	C2E	N2-C2-N3	-2.84	114.20	119.73
4	A	404	C2E	N1-C2-N3	2.81	128.56	123.32
2	C	401	CIT	C2-C3-C6	-2.80	104.08	110.11
4	D	404	C2E	C81-N91-C41	2.80	111.38	106.05
4	A	404	C2E	C81-N91-C41	2.77	111.33	106.05
4	C	404	C2E	C4'-O4'-C1'	-2.75	103.40	109.47
4	B	404	C2E	C51-C61-N11	2.65	119.92	113.19
4	A	403	C2E	C1'-N9-C8	2.62	134.14	126.70
4	B	404	C2E	C4A-O4A-C1A	-2.61	103.71	109.47
4	C	404	C2E	C4-C5-N7	-2.61	106.60	110.72
2	C	401	CIT	O4-C5-C4	2.57	122.61	114.35
4	A	403	C2E	C61-C51-N71	2.57	135.02	130.25
4	D	404	C2E	O6-C6-N1	2.56	125.03	120.12
4	C	403	C2E	C51-C61-N11	2.56	119.68	113.19
4	A	404	C2E	C4'-O4'-C1'	-2.55	103.85	109.47
4	B	403	C2E	C4-C5-N7	-2.52	106.72	110.72
4	B	403	C2E	C1'-N9-C8	2.49	133.79	126.70
4	A	403	C2E	C1A-N91-C41	-2.49	119.10	126.50
2	D	401	CIT	O4-C5-C4	2.48	122.31	114.35
4	B	403	C2E	C51-C61-N11	2.46	119.44	113.19
4	D	404	C2E	C3A-C2A-C1A	2.45	105.32	99.89
4	C	404	C2E	C1'-N9-C4	-2.40	119.37	126.50
4	A	403	C2E	C41-C51-N71	-2.37	106.96	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	403	C2E	C3'-C2'-C1'	2.37	105.14	99.89
2	C	401	CIT	O4-C5-O3	-2.35	117.45	123.30
5	D	405	GOL	C3-C2-C1	-2.33	102.63	111.70
4	D	404	C2E	C1'-N9-C4	-2.31	119.63	126.50
4	A	404	C2E	C3'-C2'-C1'	2.27	104.91	99.89
4	D	403	C2E	N1-C2-N3	2.26	127.55	123.32
4	C	403	C2E	O3'-P11-O11	-2.25	101.01	109.47
4	A	403	C2E	N2-C2-N3	-2.24	115.38	119.73
4	D	403	C2E	O6-C6-N1	2.22	124.38	120.12
5	B	405	GOL	C3-C2-C1	-2.18	103.23	111.70
4	A	403	C2E	C2A-C1A-N91	2.18	119.38	113.22
4	C	404	C2E	C3A-C2A-C1A	2.17	104.70	99.89
4	A	404	C2E	C81-N71-C51	-2.16	100.33	104.24
4	C	403	C2E	O4'-C1'-C2'	2.15	111.33	106.64
4	D	403	C2E	O2'-C2'-C1'	-2.15	102.83	110.02
4	A	403	C2E	O61-C61-C51	-2.14	120.92	126.60
4	A	403	C2E	N91-C81-N71	-2.14	109.36	113.39
4	C	403	C2E	N1-C2-N3	2.12	127.28	123.32
4	C	404	C2E	N1-C2-N3	2.11	127.26	123.32
4	D	404	C2E	N2-C2-N3	-2.10	115.65	119.73
2	B	401	CIT	O5-C6-C3	-2.09	119.29	122.25
4	B	404	C2E	N2-C2-N3	-2.09	115.67	119.73
2	D	401	CIT	O7-C3-C6	2.08	111.79	108.86
4	A	404	C2E	O3A-P1-O1P	-2.08	101.67	109.47
4	D	403	C2E	C4'-O4'-C1'	-2.08	104.89	109.47
4	C	403	C2E	C4-C5-N7	-2.06	107.46	110.72
4	C	403	C2E	O61-C61-C51	-2.05	121.16	126.60
4	B	404	C2E	O61-C61-C51	-2.02	121.23	126.60
2	A	401	CIT	O4-C5-C4	2.02	120.83	114.35
4	A	404	C2E	C1'-N9-C4	-2.00	120.56	126.50

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	CIT	O7-C3-C6-O6
2	D	401	CIT	O7-C3-C6-O5
2	D	401	CIT	O7-C3-C6-O6
2	D	401	CIT	C4-C3-C6-O5
2	D	401	CIT	C4-C3-C6-O6
5	B	405	GOL	O1-C1-C2-C3
5	C	405	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	D	407	GOL	C1-C2-C3-O3
5	D	406	GOL	C1-C2-C3-O3
5	D	407	GOL	O1-C1-C2-C3
2	C	401	CIT	C4-C3-C6-O5
2	C	401	CIT	C4-C3-C6-O6
5	B	405	GOL	O1-C1-C2-O2
5	C	405	GOL	O1-C1-C2-O2
5	D	406	GOL	O2-C2-C3-O3
2	C	401	CIT	O7-C3-C6-O5
5	D	407	GOL	O2-C2-C3-O3
5	C	405	GOL	O2-C2-C3-O3
5	D	405	GOL	O2-C2-C3-O3
2	C	401	CIT	C2-C3-C6-O5
2	C	401	CIT	C2-C3-C6-O6
4	A	403	C2E	O4A-C4A-C5A-O5A
2	C	401	CIT	C3-C4-C5-O4
2	C	401	CIT	C3-C4-C5-O3
5	D	407	GOL	O1-C1-C2-O2
5	C	405	GOL	C1-C2-C3-O3
2	B	401	CIT	O1-C1-C2-C3
4	A	403	C2E	C5A-O5A-P11-O11
2	B	401	CIT	O2-C1-C2-C3

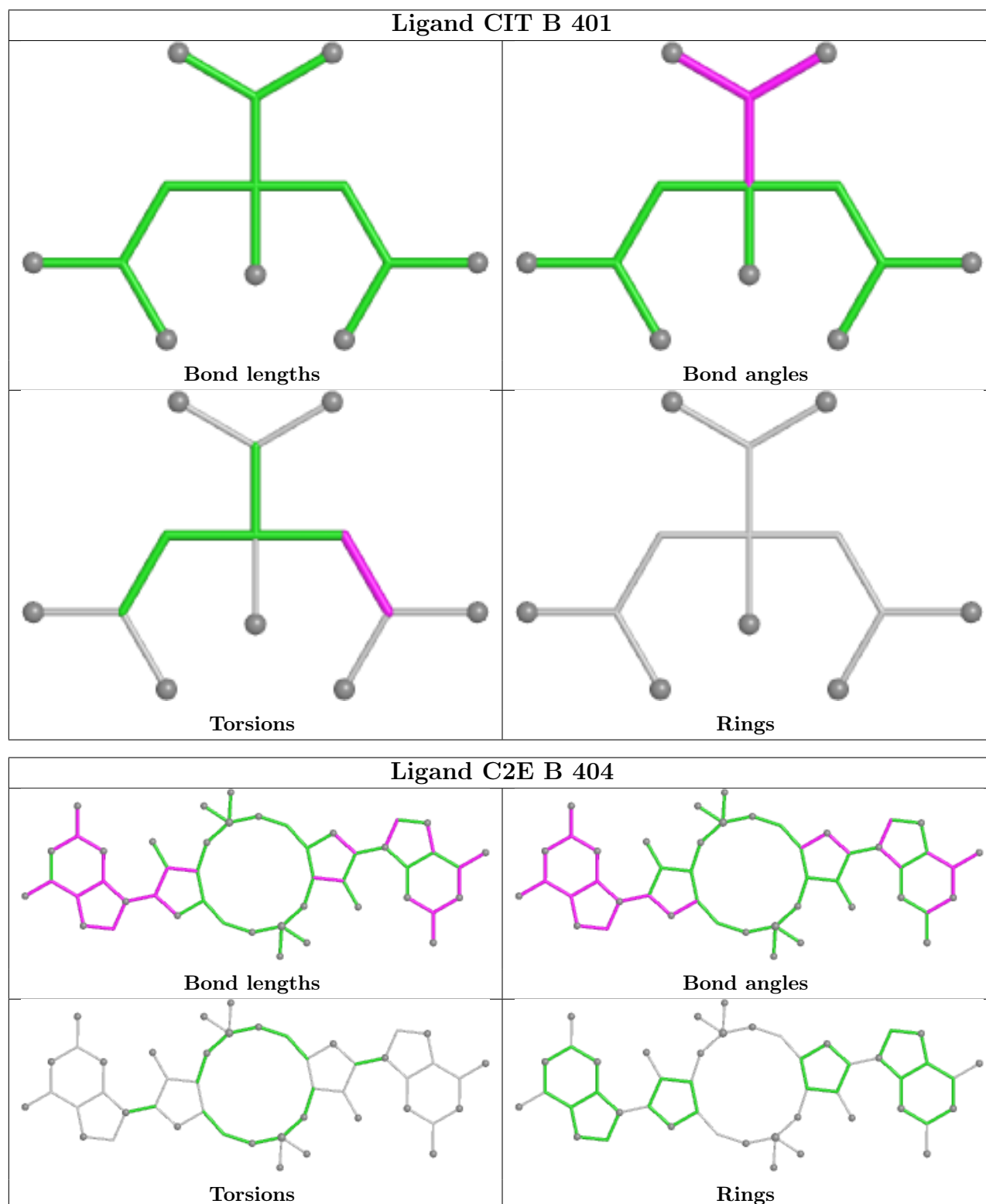
There are no ring outliers.

8 monomers are involved in 9 short contacts:

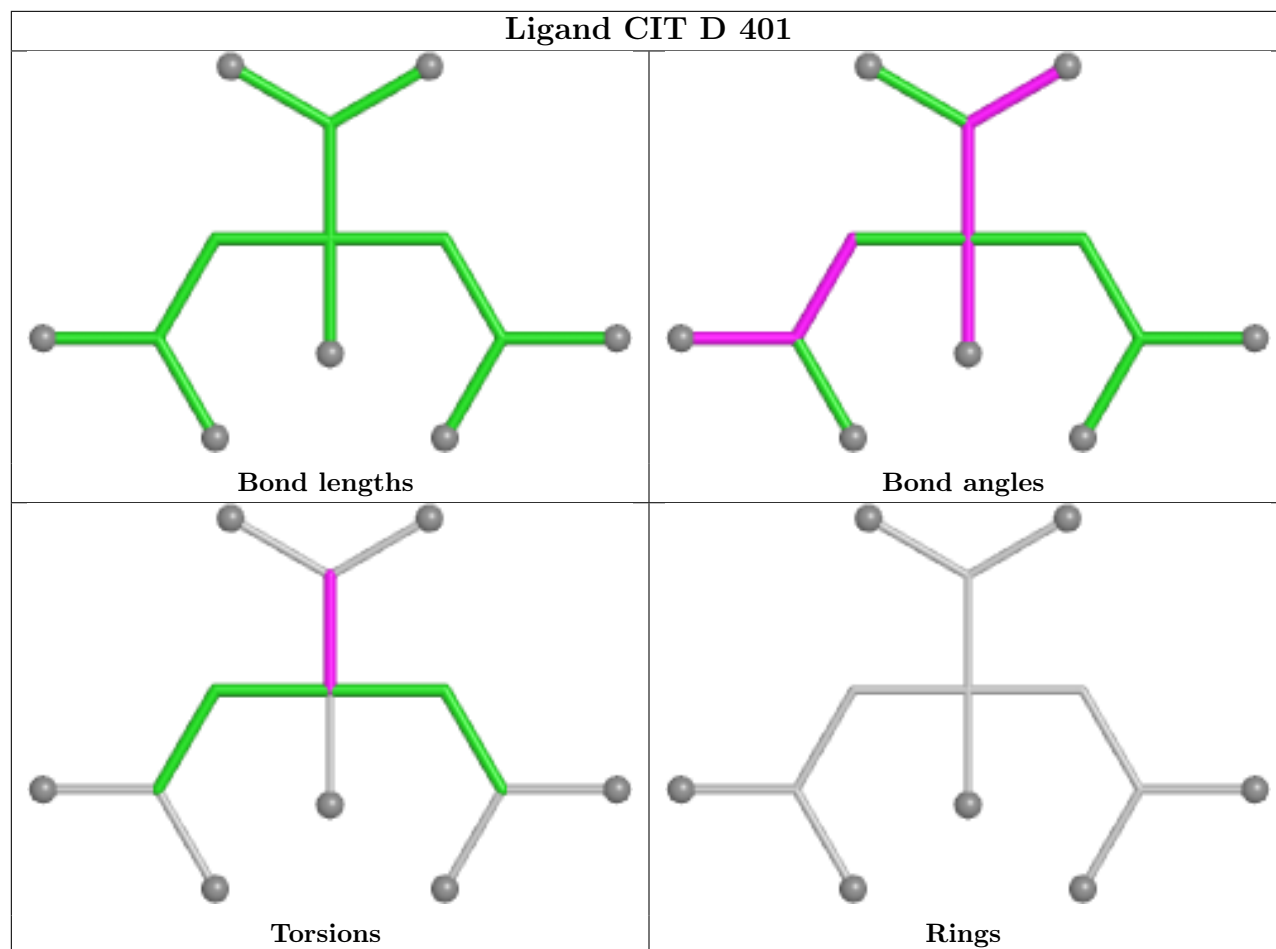
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	406	GOL	1	0
5	D	405	GOL	1	0
5	A	406	GOL	1	0
4	C	403	C2E	1	0
5	D	407	GOL	1	0
4	C	404	C2E	1	0
4	D	403	C2E	2	0
4	A	403	C2E	1	0

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 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

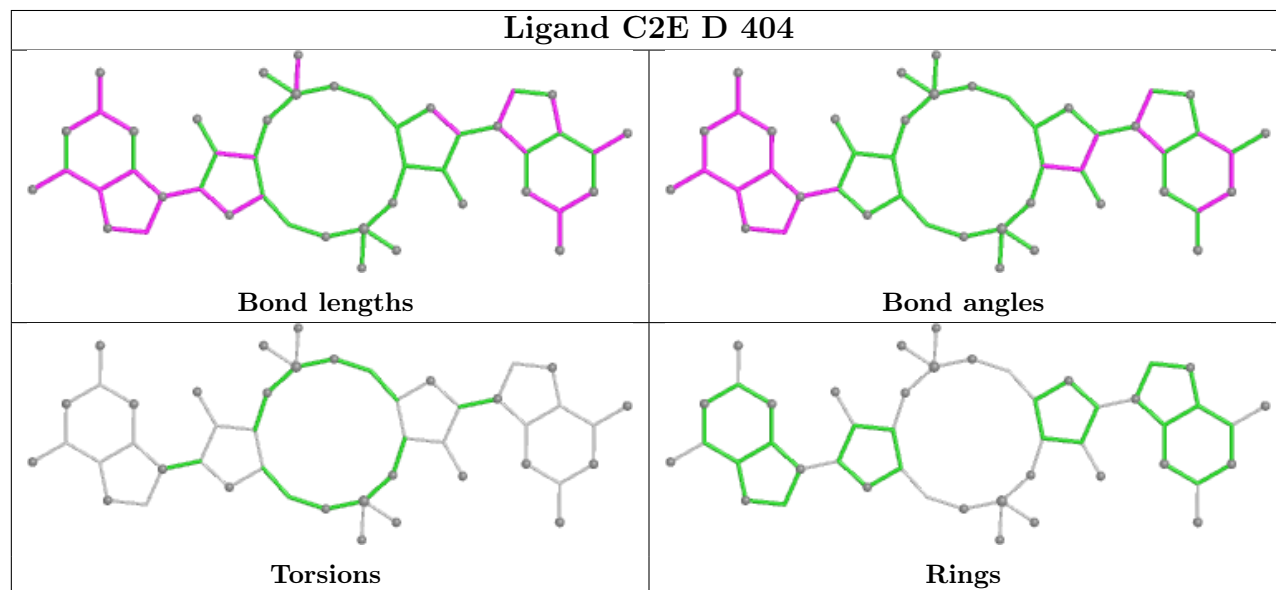
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



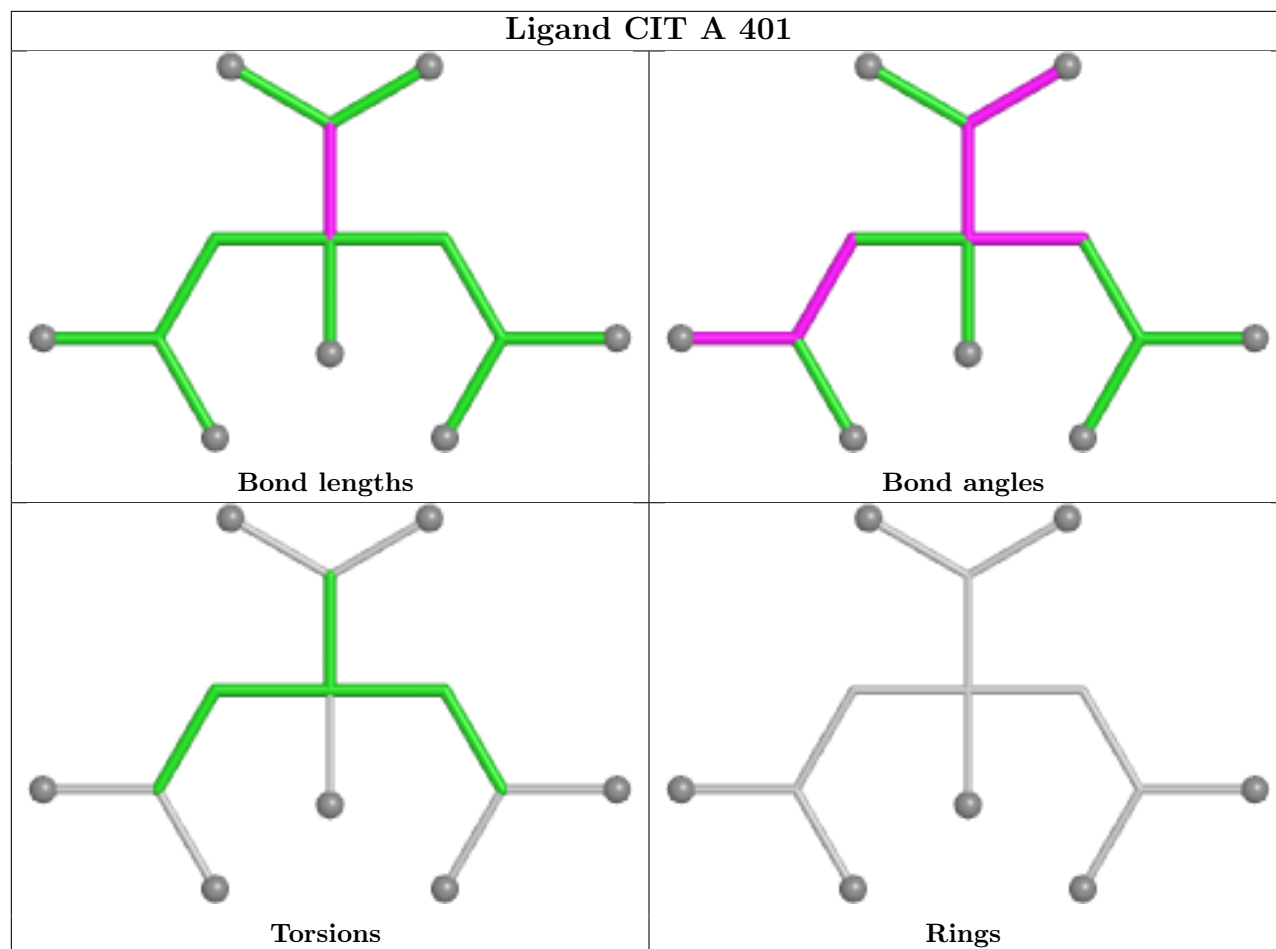
Ligand CIT D 401



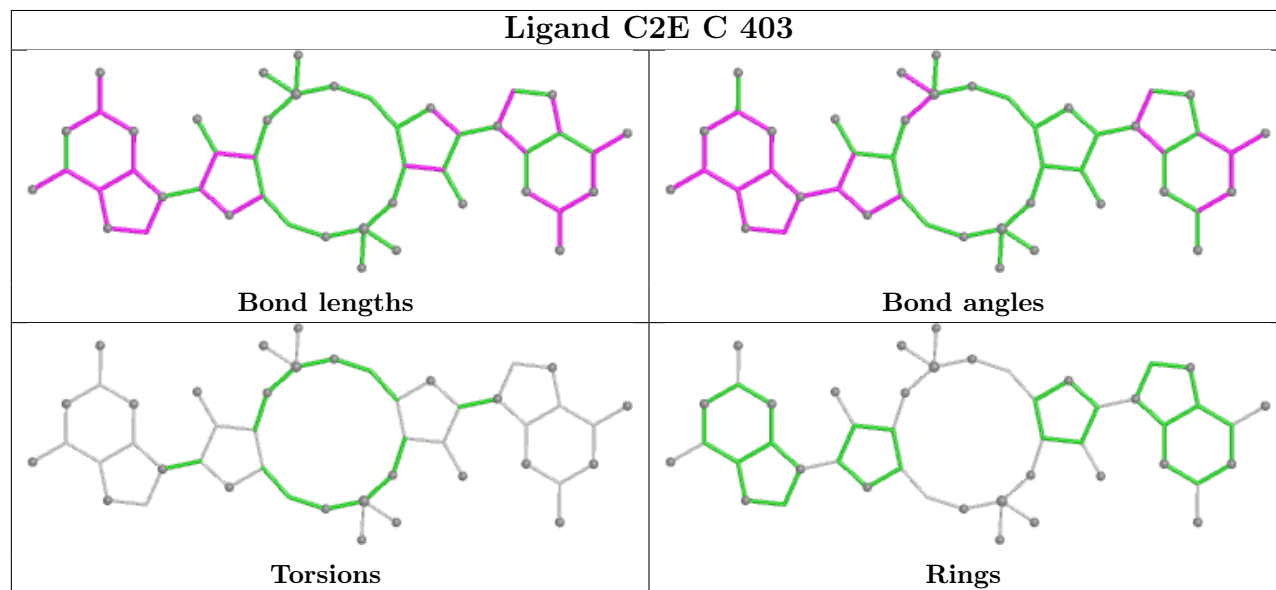
Ligand C2E D 404



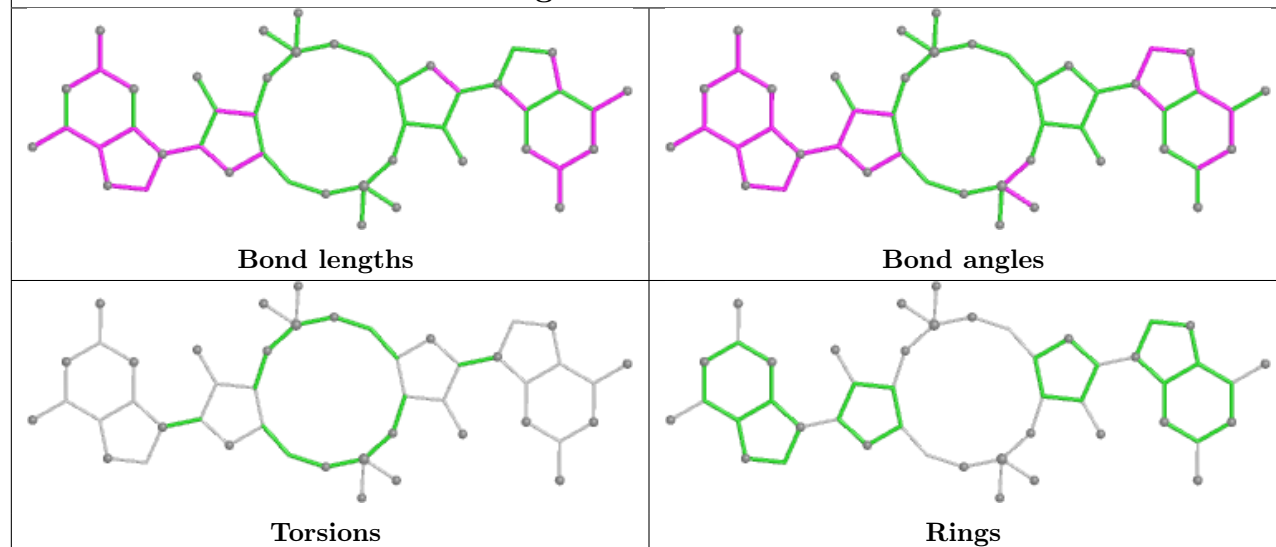
Ligand CIT A 401



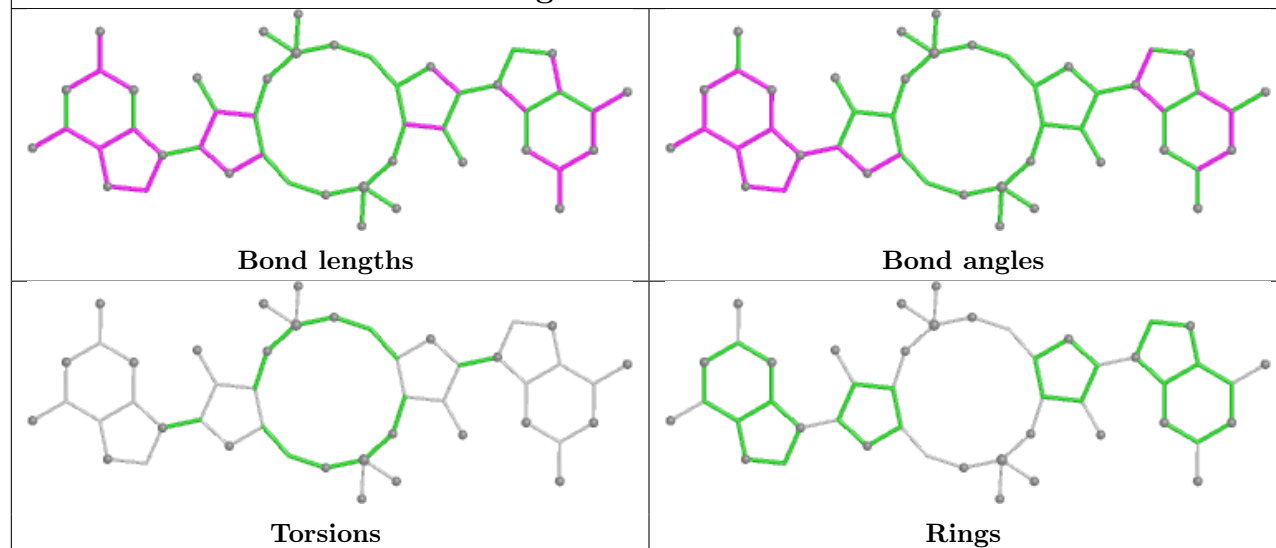
Ligand C2E C 403

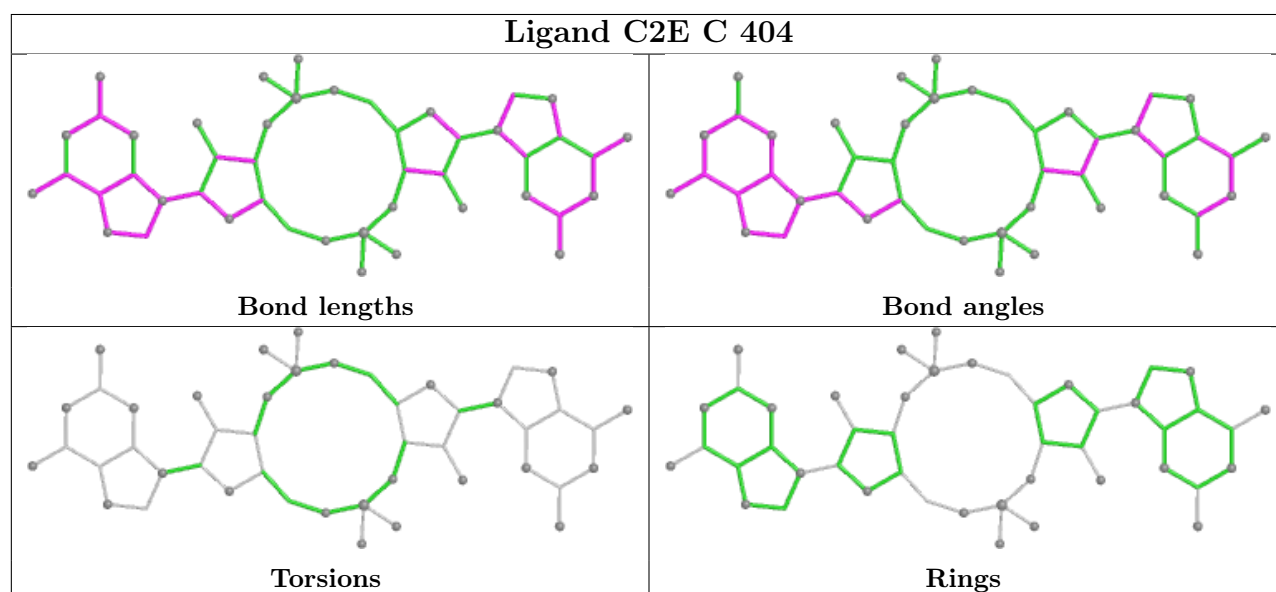
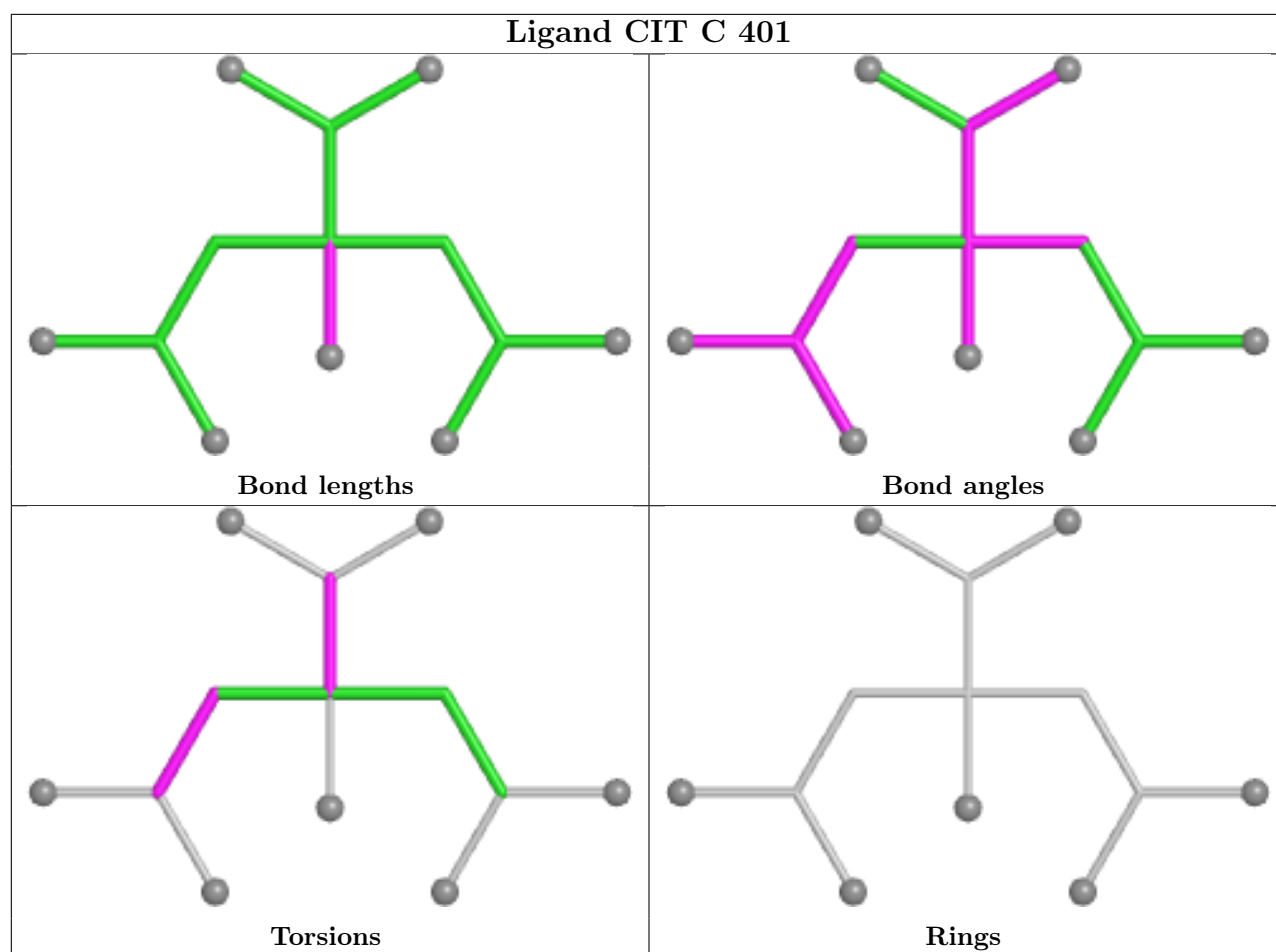


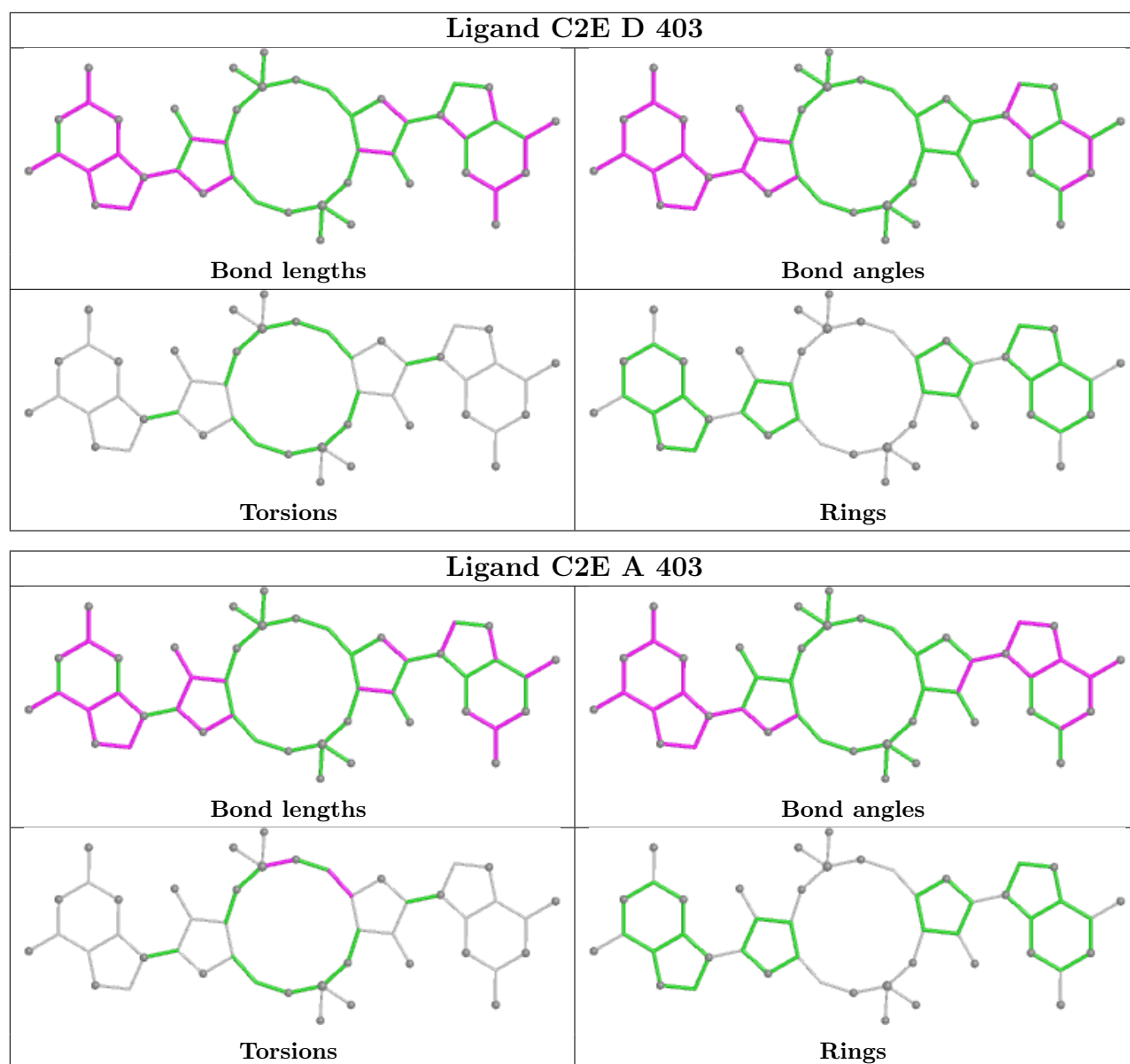
Ligand C2E A 404



Ligand C2E B 403







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	300/310 (96%)	-0.31	5 (1%) 69 73	13, 29, 59, 102	2 (0%)
1	B	299/310 (96%)	-0.28	3 (1%) 79 83	12, 31, 59, 91	2 (0%)
1	C	297/310 (95%)	0.42	40 (13%) 7 6	14, 38, 98, 174	2 (0%)
1	D	300/310 (96%)	0.07	10 (3%) 49 53	19, 37, 66, 103	0
All	All	1196/1240 (96%)	-0.03	58 (4%) 35 39	12, 34, 79, 174	6 (0%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	21	GLY	4.1
1	C	46	VAL	4.0
1	C	47	LEU	4.0
1	C	27	LEU	3.8
1	D	10	LEU	3.8
1	C	64	PRO	3.7
1	C	20	PRO	3.7
1	C	29	ARG	3.7
1	C	21	GLY	3.6
1	C	31	PHE	3.6
1	D	24	LEU	3.4
1	D	23	MET	3.4
1	C	62	VAL	3.3
1	C	81	LEU	3.3
1	A	281	HIS	3.2
1	C	38	LEU	3.2
1	C	35	PHE	3.2
1	C	54	PRO	3.1
1	C	37	LEU	3.1
1	B	64	PRO	3.1
1	C	14	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	13	THR	3.0
1	C	33	THR	2.9
1	C	32	SER	2.8
1	C	39	VAL	2.8
1	C	65	ARG	2.8
1	C	24	LEU	2.8
1	C	55	ILE	2.8
1	C	83	ILE	2.8
1	D	63	SER	2.7
1	C	49	LEU	2.7
1	D	64	PRO	2.7
1	C	51	LEU	2.7
1	A	20	PRO	2.6
1	D	19	ASN	2.6
1	A	21	GLY	2.6
1	C	26	ALA	2.5
1	C	18	ASP	2.5
1	C	56	ASP	2.5
1	C	36	HIS	2.4
1	C	44	GLU	2.4
1	D	22	GLU	2.3
1	C	15	LEU	2.3
1	D	66	ASP	2.3
1	B	37	LEU	2.2
1	C	42	ASP	2.2
1	B	281	HIS	2.2
1	A	65	ARG	2.2
1	C	17	VAL	2.2
1	C	28	THR	2.2
1	D	71	LEU	2.1
1	A	22	GLU	2.1
1	C	63	SER	2.1
1	C	40	CYS	2.1
1	C	48	LYS	2.1
1	C	281	HIS	2.1
1	C	80	PRO	2.0
1	C	53	ALA	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

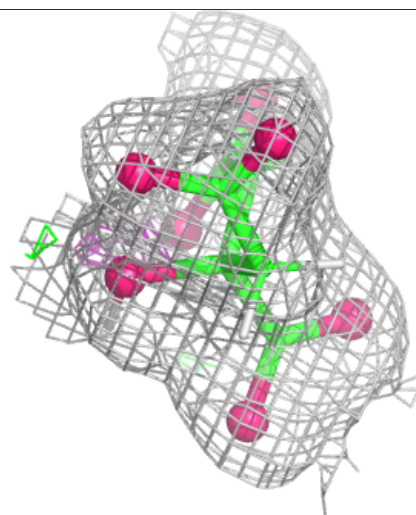
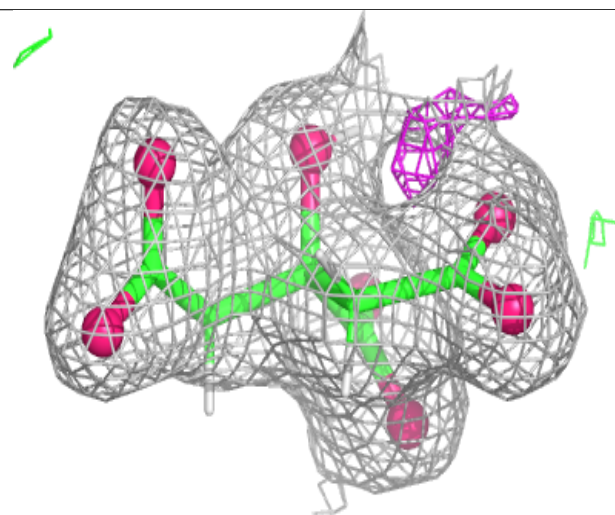
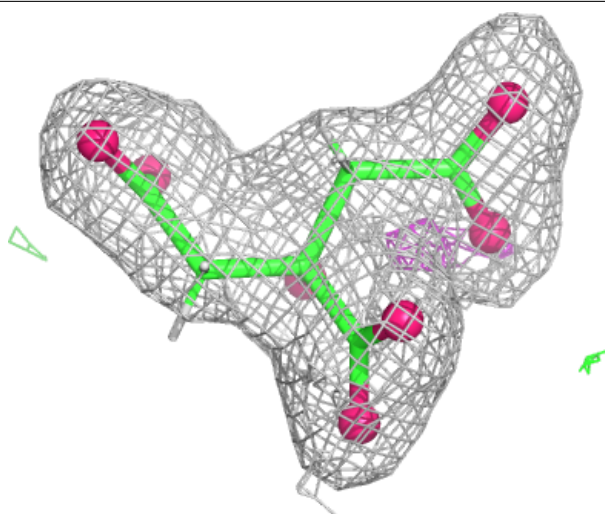
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	A	406	6/6	0.81	0.16	39,60,67,73	0
5	GOL	D	407	6/6	0.84	0.15	35,45,63,68	0
5	GOL	D	406	6/6	0.85	0.12	44,54,58,65	0
5	GOL	A	405	6/6	0.86	0.14	30,49,59,70	0
5	GOL	B	405	6/6	0.90	0.10	28,46,55,63	0
5	GOL	D	405	6/6	0.91	0.10	32,39,54,58	0
2	CIT	D	401	13/13	0.93	0.07	27,38,51,54	0
5	GOL	C	405	6/6	0.94	0.09	30,46,56,59	0
2	CIT	C	401	13/13	0.94	0.07	26,38,45,50	0
2	CIT	B	401	13/13	0.95	0.07	23,30,39,49	0
4	C2E	D	403	46/46	0.97	0.05	18,25,34,38	0
2	CIT	A	401	13/13	0.97	0.06	20,30,41,44	0
3	MG	C	402	1/1	0.97	0.05	28,28,28,28	0
3	MG	D	402	1/1	0.97	0.09	27,27,27,27	0
4	C2E	D	404	46/46	0.98	0.05	18,23,31,33	0
4	C2E	A	403	46/46	0.98	0.05	15,22,28,30	0
4	C2E	A	404	46/46	0.98	0.05	17,22,29,33	0
4	C2E	B	403	46/46	0.98	0.05	15,22,28,32	0
4	C2E	B	404	46/46	0.98	0.04	16,21,29,32	0
4	C2E	C	403	46/46	0.98	0.05	15,22,28,31	0
4	C2E	C	404	46/46	0.98	0.05	16,21,29,31	0
3	MG	A	402	1/1	0.98	0.03	24,24,24,24	0
3	MG	B	402	1/1	0.99	0.04	22,22,22,22	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.

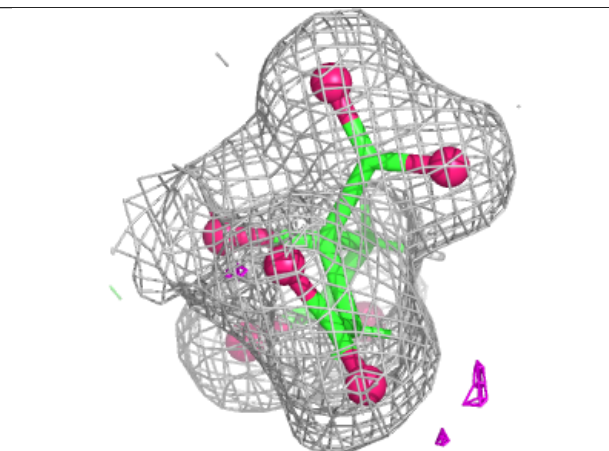
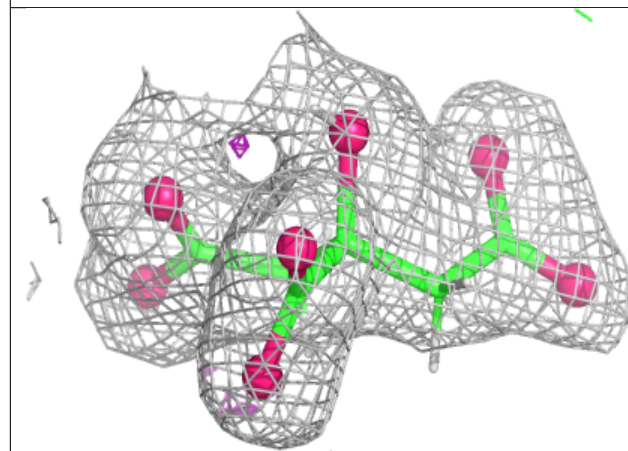
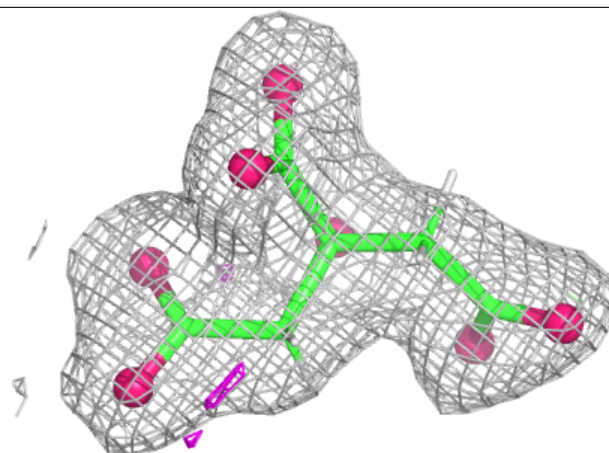
Electron density around CIT D 401:

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



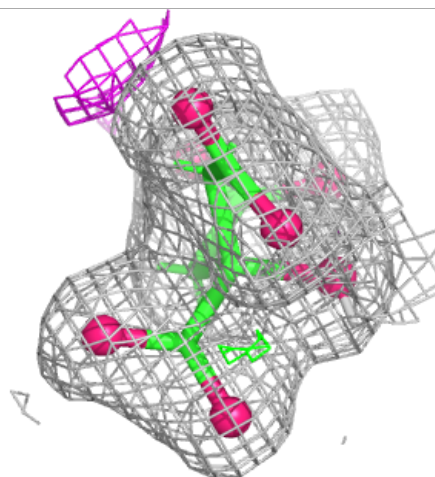
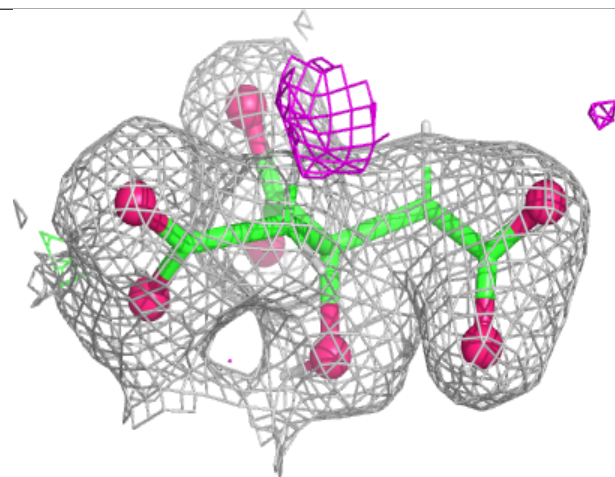
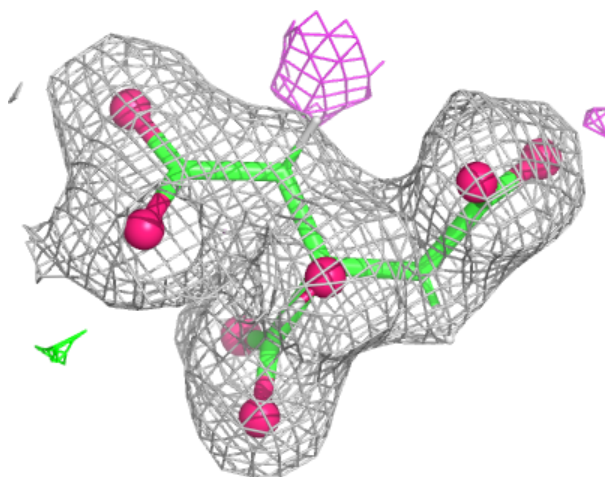
Electron density around CIT C 401:

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and green (positive)



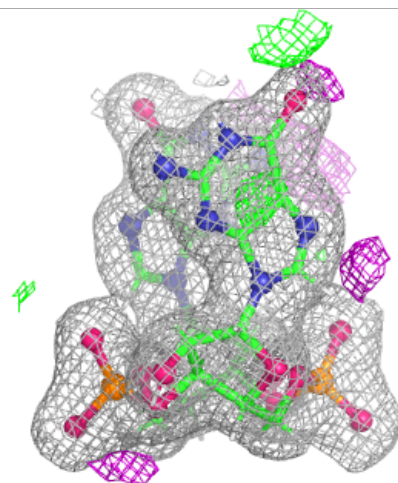
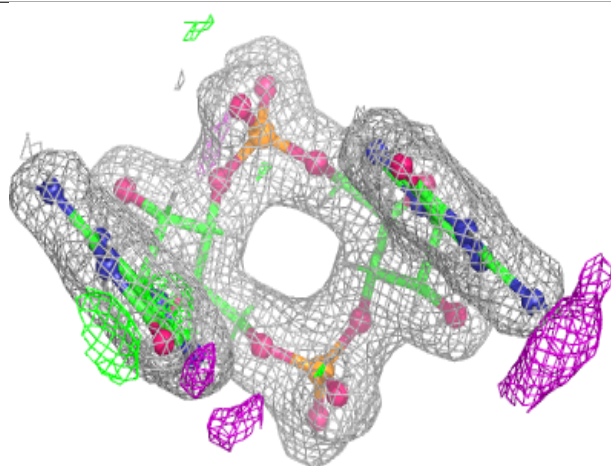
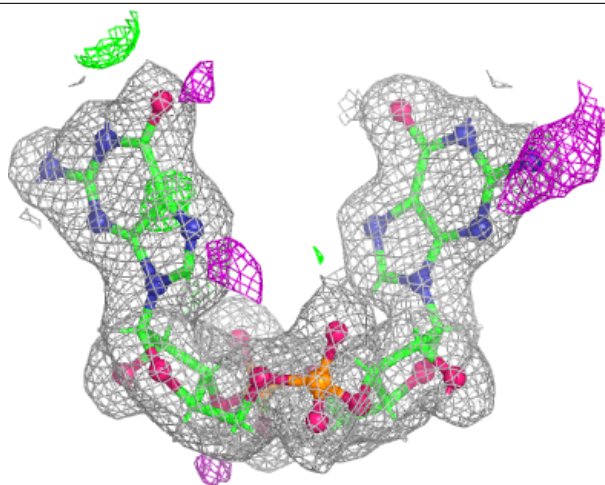
Electron density around CIT B 401:

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



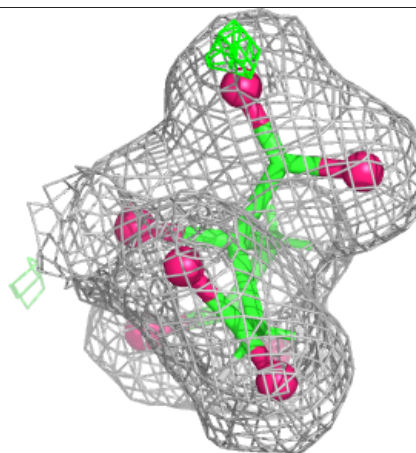
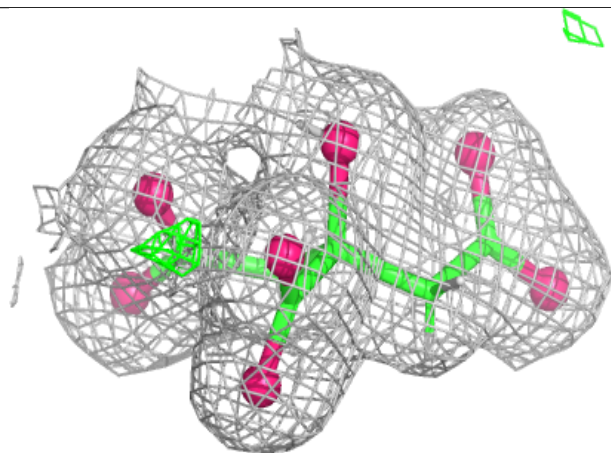
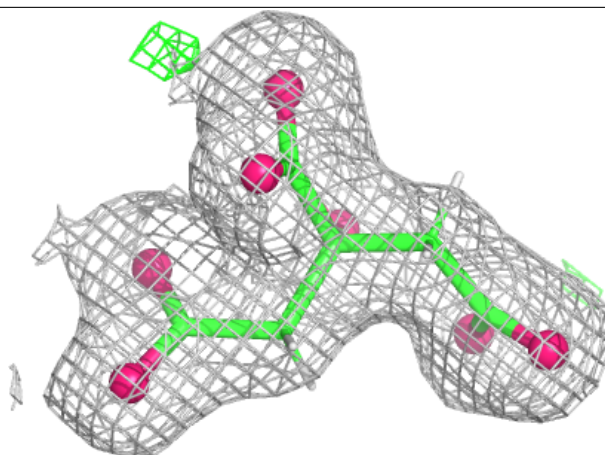
Electron density around C2E D 403:

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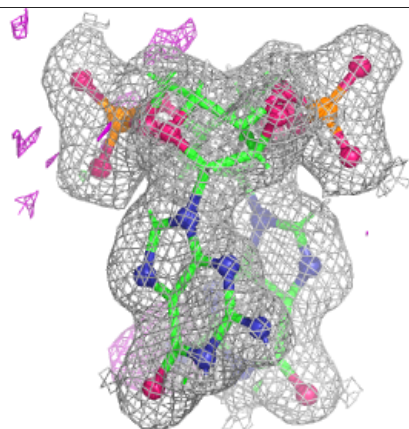
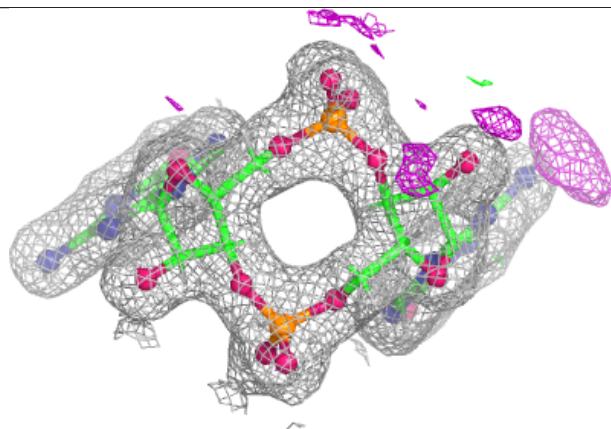
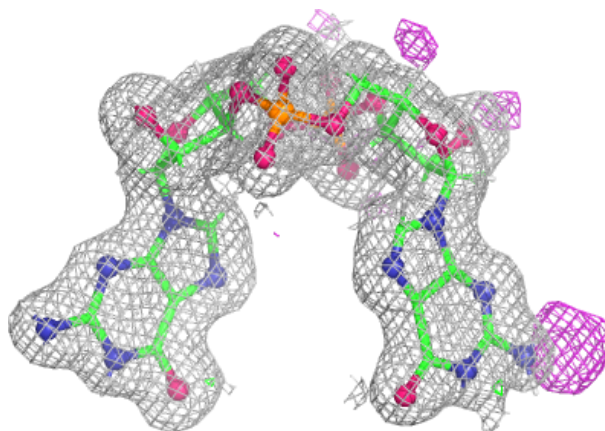
Electron density around CIT A 401:

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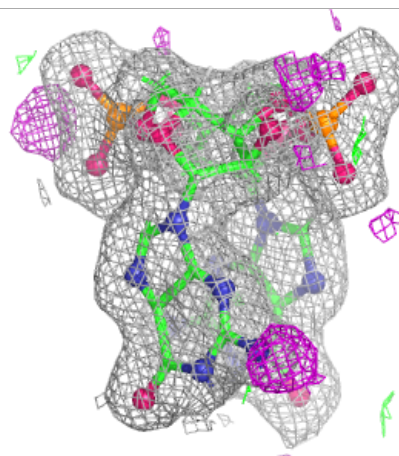
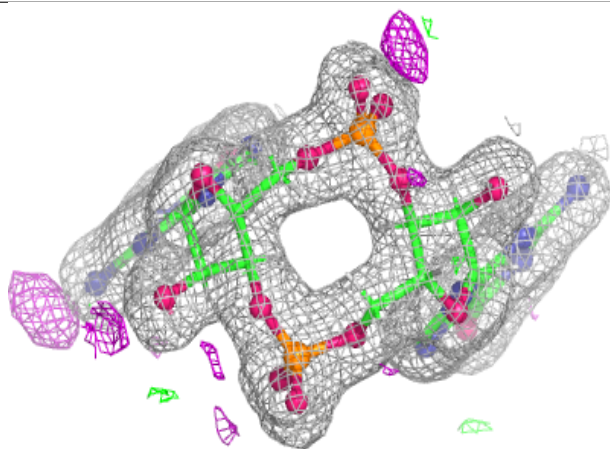
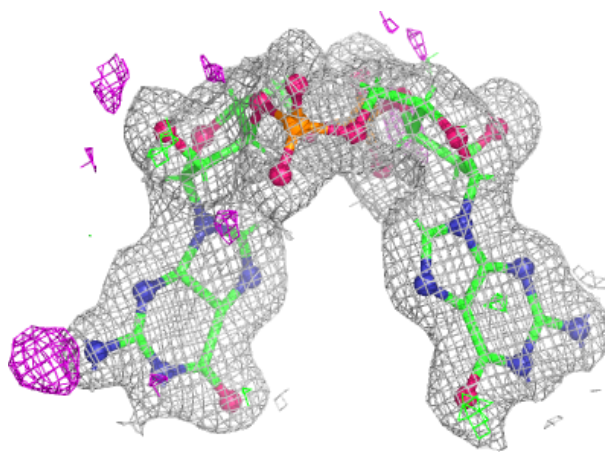
Electron density around C2E D 404:

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and green (positive)



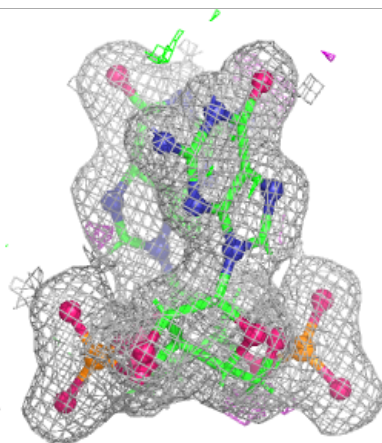
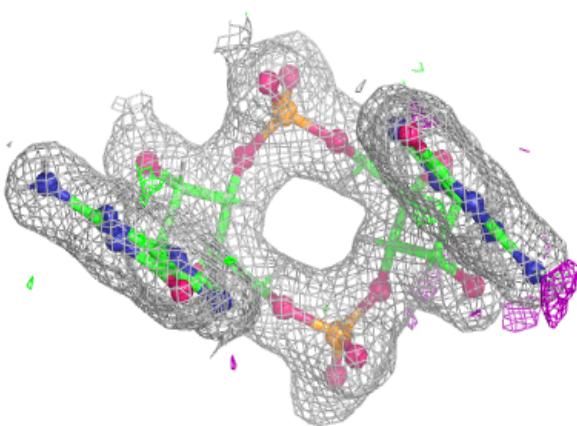
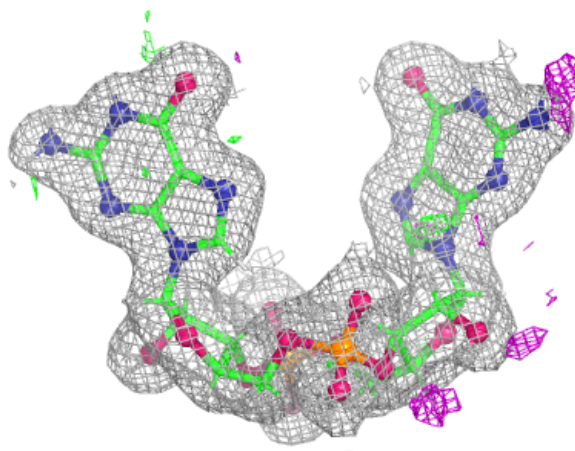
Electron density around C2E A 403:

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



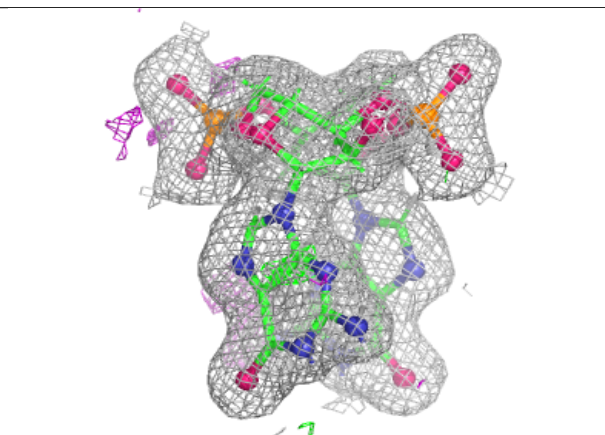
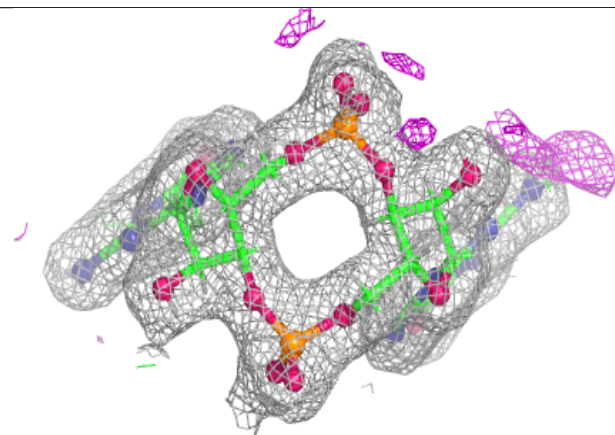
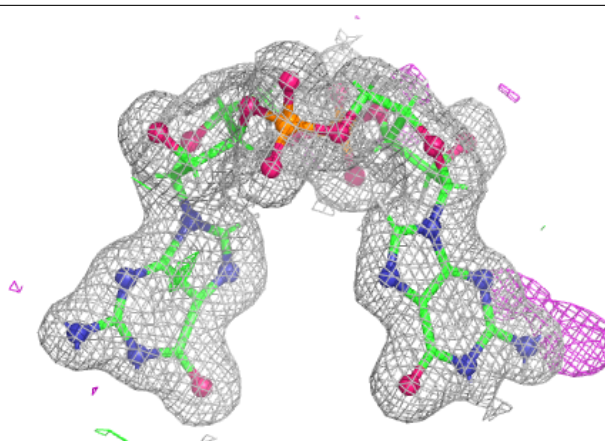
Electron density around C2E A 404:

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



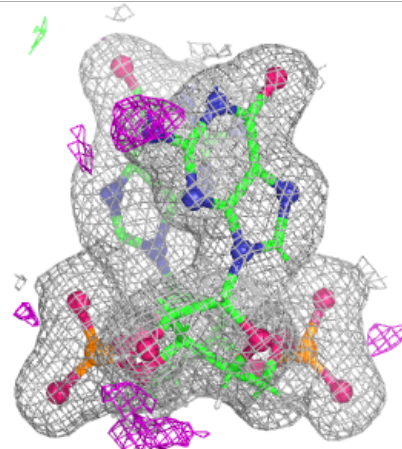
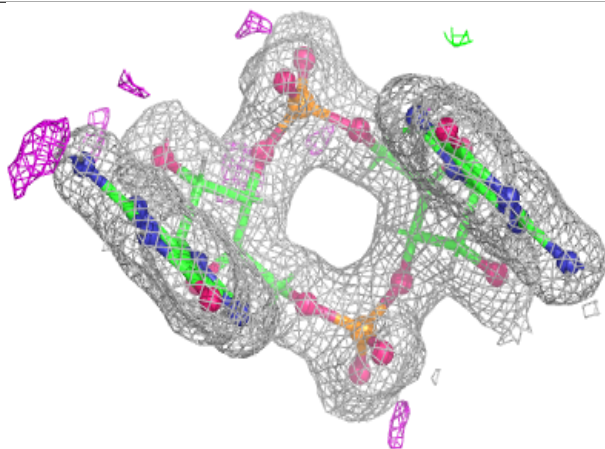
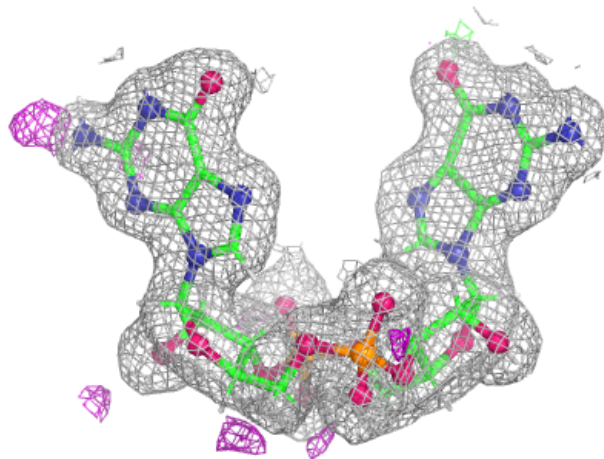
Electron density around C2E B 403:

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and green (positive)



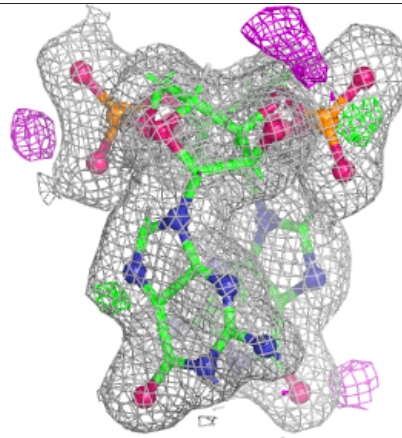
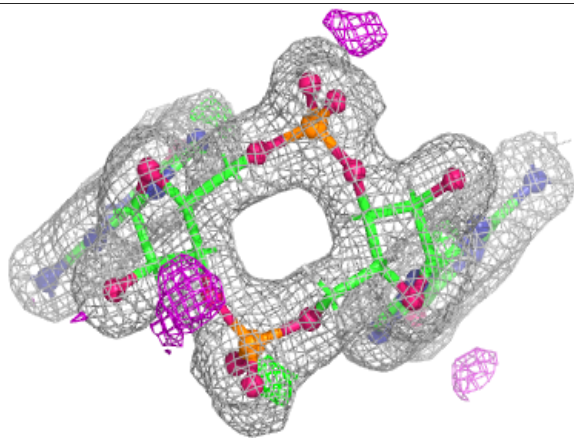
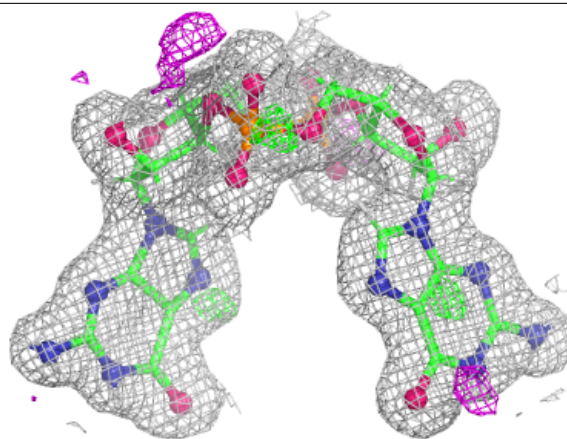
Electron density around C2E B 404:

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and green (positive)



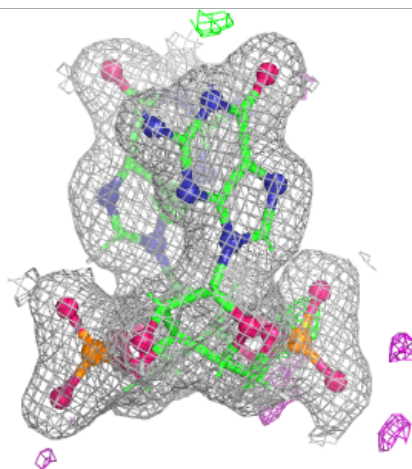
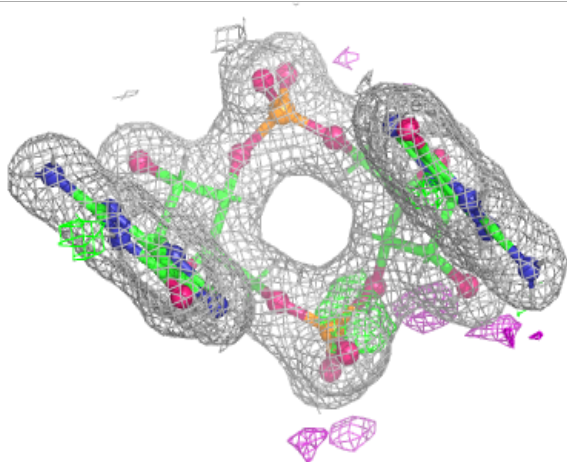
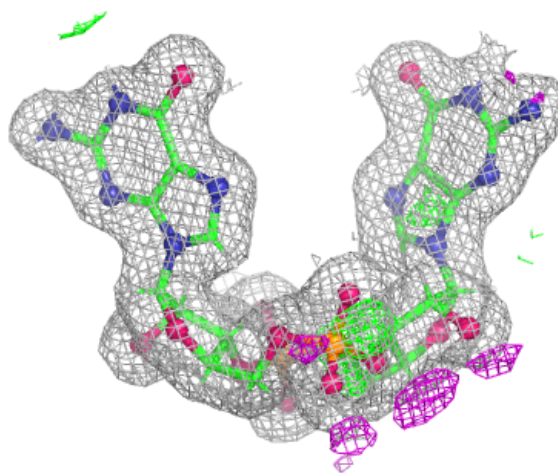
Electron density around C2E C 403:

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



Electron density around C2E C 404:

$2mF_o-DF_c$ (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.