



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 7, 2025 – 02:19 PM JST

PDB ID : 9U54 / pdb_00009u54
Title : Structure of Phosphopantetheine adenylyltransferase (PPAT) from Enterobacter spp. with the 17-mer expression tag bound in the substrate binding site of a neighbouring molecule at 2.10 Å resolution.
Authors : Ahmad, N.; Sharma, P.; Sharma, S.; Singh, T.P.
Deposited on : 2025-03-20
Resolution : 2.10 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)	:	2.0rc1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

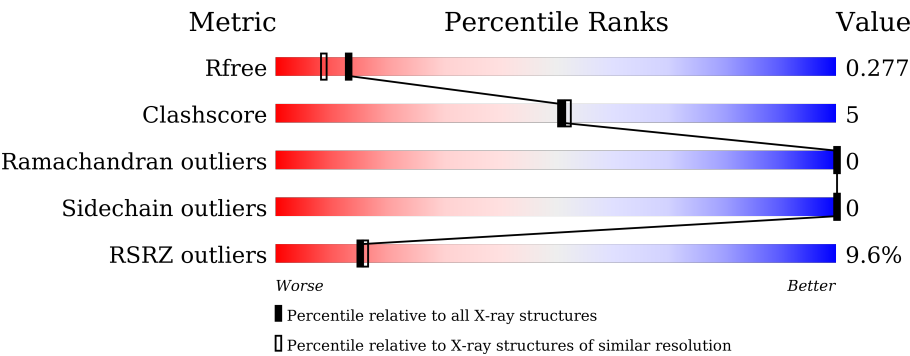
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



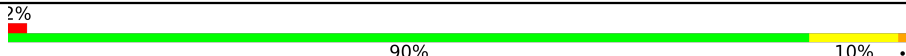
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

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	176	<div><div>6%</div><div>81%</div><div>10%</div><div>10%</div></div>
1	B	176	<div><div>%</div><div>91%</div><div>9%</div></div>
1	C	176	<div><div>26%</div><div>76%</div><div>14%</div><div>10%</div></div>
1	D	176	<div><div>15%</div><div>81%</div><div>10%</div><div>10%</div></div>
1	E	176	<div><div>3%</div><div>81%</div><div>10%</div><div>10%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	176	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a small red segment at the beginning labeled '2%', a large green segment in the middle labeled '90%', and a small yellow segment at the end labeled '10%'. A small black dot is located at the far right end of the bar.

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8279 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Phosphopantetheine adenylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	0	0
			1246	796	216	224	10			
1	B	176	Total	C	N	O	S	0	1	0
			1367	864	241	248	14			
1	C	159	Total	C	N	O	S	0	1	0
			1257	802	220	225	10			
1	D	159	Total	C	N	O	S	0	1	0
			1251	800	216	224	11			
1	E	159	Total	C	N	O	S	0	0	0
			1246	796	216	224	10			
1	F	176	Total	C	N	O	S	0	1	0
			1362	861	240	248	13			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	GLY	-	expression tag	UNP A4W515
A	-15	SER	-	expression tag	UNP A4W515
A	-14	HIS	-	expression tag	UNP A4W515
A	-13	MET	-	expression tag	UNP A4W515
A	-12	ALA	-	expression tag	UNP A4W515
A	-11	SER	-	expression tag	UNP A4W515
A	-10	MET	-	expression tag	UNP A4W515
A	-9	THR	-	expression tag	UNP A4W515
A	-8	GLY	-	expression tag	UNP A4W515
A	-7	GLY	-	expression tag	UNP A4W515
A	-6	GLN	-	expression tag	UNP A4W515
A	-5	GLN	-	expression tag	UNP A4W515
A	-4	MET	-	expression tag	UNP A4W515
A	-3	GLY	-	expression tag	UNP A4W515
A	-2	ARG	-	expression tag	UNP A4W515
A	-1	GLY	-	expression tag	UNP A4W515
A	0	SER	-	expression tag	UNP A4W515

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	GLY	-	expression tag	UNP A4W515
B	-16	SER	-	expression tag	UNP A4W515
B	-15	HIS	-	expression tag	UNP A4W515
B	-14	MET	-	expression tag	UNP A4W515
B	-13	ALA	-	expression tag	UNP A4W515
B	-12	SER	-	expression tag	UNP A4W515
B	-11	MET	-	expression tag	UNP A4W515
B	-10	THR	-	expression tag	UNP A4W515
B	-9	GLY	-	expression tag	UNP A4W515
B	-8	GLY	-	expression tag	UNP A4W515
B	-7	GLN	-	expression tag	UNP A4W515
B	-6	GLN	-	expression tag	UNP A4W515
B	-5	MET	-	expression tag	UNP A4W515
B	-4	GLY	-	expression tag	UNP A4W515
B	-3	ARG	-	expression tag	UNP A4W515
B	-2	GLY	-	expression tag	UNP A4W515
B	-1	SER	-	expression tag	UNP A4W515
C	-16	GLY	-	expression tag	UNP A4W515
C	-15	SER	-	expression tag	UNP A4W515
C	-14	HIS	-	expression tag	UNP A4W515
C	-13	MET	-	expression tag	UNP A4W515
C	-12	ALA	-	expression tag	UNP A4W515
C	-11	SER	-	expression tag	UNP A4W515
C	-10	MET	-	expression tag	UNP A4W515
C	-9	THR	-	expression tag	UNP A4W515
C	-8	GLY	-	expression tag	UNP A4W515
C	-7	GLY	-	expression tag	UNP A4W515
C	-6	GLN	-	expression tag	UNP A4W515
C	-5	GLN	-	expression tag	UNP A4W515
C	-4	MET	-	expression tag	UNP A4W515
C	-3	GLY	-	expression tag	UNP A4W515
C	-2	ARG	-	expression tag	UNP A4W515
C	-1	GLY	-	expression tag	UNP A4W515
C	0	SER	-	expression tag	UNP A4W515
D	-16	GLY	-	expression tag	UNP A4W515
D	-15	SER	-	expression tag	UNP A4W515
D	-14	HIS	-	expression tag	UNP A4W515
D	-13	MET	-	expression tag	UNP A4W515
D	-12	ALA	-	expression tag	UNP A4W515
D	-11	SER	-	expression tag	UNP A4W515
D	-10	MET	-	expression tag	UNP A4W515
D	-9	THR	-	expression tag	UNP A4W515

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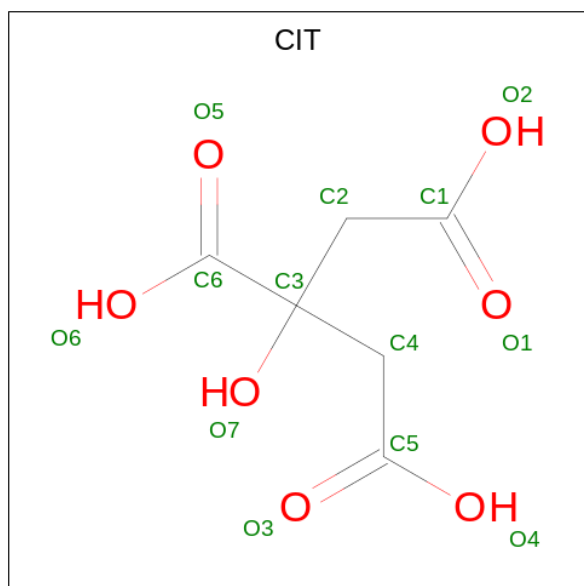
Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	GLY	-	expression tag	UNP A4W515
D	-7	GLY	-	expression tag	UNP A4W515
D	-6	GLN	-	expression tag	UNP A4W515
D	-5	GLN	-	expression tag	UNP A4W515
D	-4	MET	-	expression tag	UNP A4W515
D	-3	GLY	-	expression tag	UNP A4W515
D	-2	ARG	-	expression tag	UNP A4W515
D	-1	GLY	-	expression tag	UNP A4W515
D	0	SER	-	expression tag	UNP A4W515
E	-16	GLY	-	expression tag	UNP A4W515
E	-15	SER	-	expression tag	UNP A4W515
E	-14	HIS	-	expression tag	UNP A4W515
E	-13	MET	-	expression tag	UNP A4W515
E	-12	ALA	-	expression tag	UNP A4W515
E	-11	SER	-	expression tag	UNP A4W515
E	-10	MET	-	expression tag	UNP A4W515
E	-9	THR	-	expression tag	UNP A4W515
E	-8	GLY	-	expression tag	UNP A4W515
E	-7	GLY	-	expression tag	UNP A4W515
E	-6	GLN	-	expression tag	UNP A4W515
E	-5	GLN	-	expression tag	UNP A4W515
E	-4	MET	-	expression tag	UNP A4W515
E	-3	GLY	-	expression tag	UNP A4W515
E	-2	ARG	-	expression tag	UNP A4W515
E	-1	GLY	-	expression tag	UNP A4W515
E	0	SER	-	expression tag	UNP A4W515
F	-17	GLY	-	expression tag	UNP A4W515
F	-16	SER	-	expression tag	UNP A4W515
F	-15	HIS	-	expression tag	UNP A4W515
F	-14	MET	-	expression tag	UNP A4W515
F	-13	ALA	-	expression tag	UNP A4W515
F	-12	SER	-	expression tag	UNP A4W515
F	-11	MET	-	expression tag	UNP A4W515
F	-10	THR	-	expression tag	UNP A4W515
F	-9	GLY	-	expression tag	UNP A4W515
F	-8	GLY	-	expression tag	UNP A4W515
F	-7	GLN	-	expression tag	UNP A4W515
F	-6	GLN	-	expression tag	UNP A4W515
F	-5	MET	-	expression tag	UNP A4W515
F	-4	GLY	-	expression tag	UNP A4W515
F	-3	ARG	-	expression tag	UNP A4W515
F	-2	GLY	-	expression tag	UNP A4W515

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-1	SER	-	expression tag	UNP A4W515

- 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 O 13 6 7	0	0
2	B	1	Total C O 13 6 7	0	0
2	C	1	Total C O 13 6 7	0	0
2	D	1	Total C O 13 6 7	0	0
2	E	1	Total C O 13 6 7	0	0
2	F	1	Total C O 13 6 7	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	91	Total O 91 91	0	0
3	B	120	Total O 120 120	0	0

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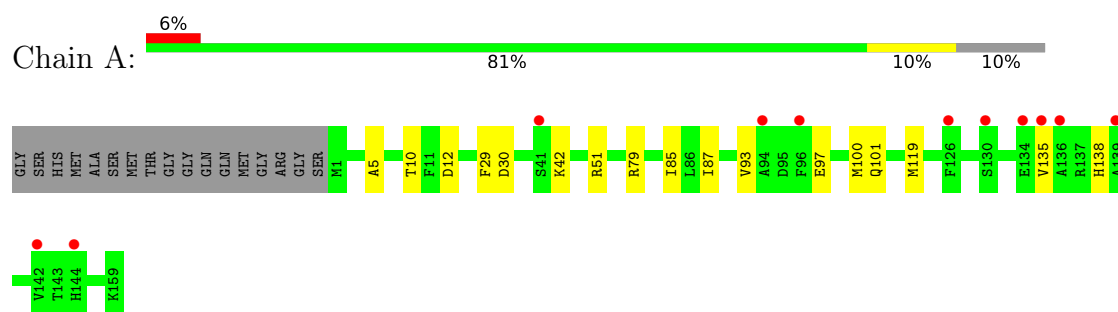
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	22	Total 22	O 22	0	0
3	D	30	Total 30	O 30	0	0
3	E	80	Total 80	O 80	0	0
3	F	129	Total 129	O 129	0	0

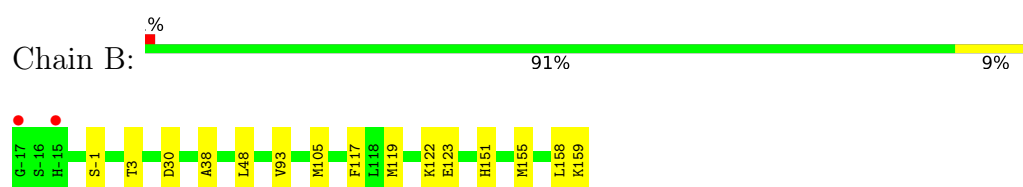
3 Residue-property plots [i](#)

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.

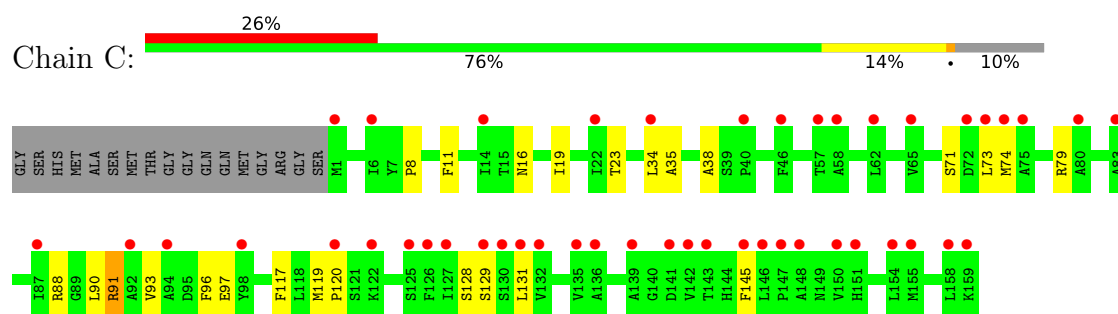
- Molecule 1: Phosphopantetheine adenylyltransferase



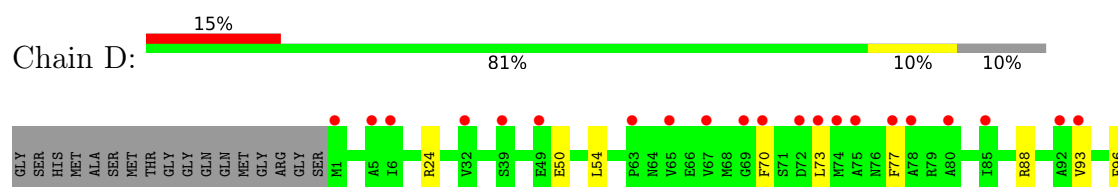
- Molecule 1: Phosphopantetheine adenylyltransferase



- Molecule 1: Phosphopantetheine adenylyltransferase

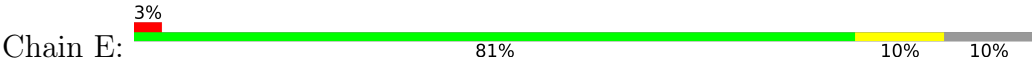


- Molecule 1: Phosphopantetheine adenylyltransferase

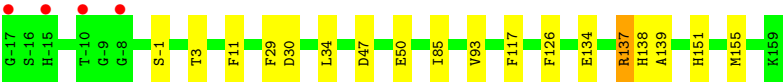
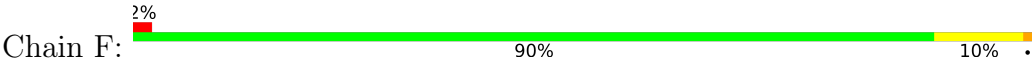




● Molecule 1: Phosphopantetheine adenylyltransferase



● Molecule 1: Phosphopantetheine adenylyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.31Å 78.68Å 106.80Å 90.00° 93.25° 90.00°	Depositor
Resolution (Å)	43.33 – 2.10 43.33 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (43.33-2.10) 98.7 (43.33-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.224 , 0.278 0.230 , 0.277	Depositor DCC
R_{free} test set	1325 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.004 for 1/2*h+3/2*k,1/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8279	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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: CIT

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	0.40	0/1273	0.86	0/1722
1	B	0.39	0/1395	0.80	0/1881
1	C	0.30	0/1284	0.67	0/1736
1	D	0.32	0/1281	0.67	0/1733
1	E	0.38	0/1273	0.82	0/1722
1	F	0.39	0/1393	0.80	0/1879
All	All	0.37	0/7899	0.78	0/10673

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	1
1	D	0	1
1	F	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	79	ARG	Sidechain
1	C	91	ARG	Sidechain
1	D	107	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	F	137	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	1246	0	1260	16	0
1	B	1367	0	1373	13	0
1	C	1257	0	1272	23	0
1	D	1251	0	1269	17	0
1	E	1246	0	1260	16	0
1	F	1362	0	1370	17	0
2	A	13	0	5	1	0
2	B	13	0	5	1	0
2	C	13	0	5	0	0
2	D	13	0	5	0	0
2	E	13	0	5	0	0
2	F	13	0	5	1	0
3	A	91	0	0	2	0
3	B	120	0	0	2	0
3	C	22	0	0	1	0
3	D	30	0	0	0	0
3	E	80	0	0	2	0
3	F	129	0	0	3	0
All	All	8279	0	7834	80	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (80) 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:C:93:VAL:HG13	1:D:93:VAL:HG13	1.51	0.93
1:C:93:VAL:CG1	1:D:93:VAL:HG13	2.16	0.76
1:E:29:PHE:CE1	1:E:85:ILE:HD13	2.32	0.64
2:F:201:CIT:H21	3:F:370:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105[B]:MET:SD	1:C:131:LEU:HD11	2.41	0.61
2:B:201:CIT:H21	3:B:380:HOH:O	2.01	0.60
1:C:79[B]:ARG:NH1	3:C:303:HOH:O	2.34	0.60
1:B:158:LEU:O	1:B:159:LYS:HB2	2.02	0.60
1:B:123:GLU:HG3	3:B:378:HOH:O	2.02	0.58
1:F:134:GLU:OE1	1:F:137:ARG:NH1	2.36	0.58
1:A:29:PHE:HE2	1:A:87:ILE:HD11	1.68	0.58
1:C:119:MET:HG3	1:D:117:PHE:CE2	2.39	0.57
1:A:93:VAL:HG13	1:B:93:VAL:HG13	1.85	0.57
1:E:141:ASP:OD1	1:E:143:THR:HG23	2.04	0.57
1:F:29:PHE:CE1	1:F:85:ILE:HD13	2.41	0.56
1:C:97:GLU:HG2	1:D:93:VAL:HG21	1.87	0.56
1:C:90:LEU:O	1:C:120:PRO:HD3	2.07	0.54
1:C:93:VAL:HG22	1:D:96:PHE:HD2	1.74	0.53
1:D:70:PHE:HB2	1:D:77:PHE:CD1	2.45	0.51
1:A:30:ASP:HA	1:B:-1:SER:HB2	1.92	0.51
1:F:137:ARG:NH2	3:F:304:HOH:O	2.44	0.51
1:C:16:ASN:CG	1:C:145:PHE:O	2.49	0.51
1:A:119:MET:HG3	1:B:117:PHE:CE1	2.46	0.51
1:F:11:PHE:CZ	1:F:34:LEU:HD11	2.46	0.50
2:A:201:CIT:H21	3:A:312:HOH:O	2.12	0.50
1:B:3:THR:O	1:B:30:ASP:HB2	2.12	0.49
1:E:30:ASP:HA	1:F:-1[A]:SER:HB3	1.93	0.49
1:E:107:ARG:NH1	3:E:301:HOH:O	2.34	0.49
1:C:88:ARG:HB2	1:C:117:PHE:CD1	2.48	0.49
1:E:107:ARG:NE	3:E:308:HOH:O	2.46	0.49
1:E:58:ALA:O	1:E:61:HIS:CE1	2.66	0.49
1:A:135:VAL:HG13	1:D:109:LEU:HD21	1.95	0.49
1:D:88:ARG:NH2	1:D:99:GLU:OE2	2.45	0.49
1:F:3:THR:HB	1:F:85:ILE:HD12	1.95	0.48
1:A:42:LYS:NZ	3:A:306:HOH:O	2.47	0.48
1:B:151:HIS:O	1:B:155:MET:HG2	2.13	0.48
1:A:100:MET:HA	1:B:119:MET:SD	2.54	0.48
1:C:128:SER:O	1:C:129:SER:C	2.52	0.48
1:E:58:ALA:O	1:E:61:HIS:HE1	1.96	0.48
1:E:93:VAL:HG13	1:F:93:VAL:HG13	1.96	0.47
1:E:30:ASP:HA	1:F:-1[B]:SER:HB2	1.96	0.47
1:C:128:SER:O	1:C:131:LEU:N	2.48	0.47
1:C:96:PHE:HD2	1:D:93:VAL:HG22	1.79	0.47
1:F:138:HIS:O	1:F:139:ALA:HB3	2.14	0.47
1:C:8:PRO:HA	1:C:35:ALA:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:MET:O	1:C:74:MET:SD	2.73	0.47
1:A:12:ASP:HB2	1:A:51:ARG:HD3	1.96	0.47
1:D:88:ARG:HB2	1:D:117:PHE:CD1	2.50	0.47
1:C:73:LEU:HD13	1:E:138:HIS:HB2	1.97	0.46
1:C:91:ARG:HG2	1:C:120:PRO:HG3	1.97	0.46
1:E:29:PHE:CE2	1:E:87:ILE:HD11	2.51	0.46
1:C:128:SER:O	1:C:131:LEU:HB3	2.16	0.45
1:C:93:VAL:CG1	1:D:93:VAL:CG1	2.91	0.45
1:B:38:ALA:CB	1:B:48:LEU:HD22	2.47	0.45
1:C:19:ILE:O	1:C:23:THR:OG1	2.22	0.45
1:D:128:SER:O	1:D:132:VAL:HG23	2.16	0.45
1:A:29:PHE:CE2	1:A:87:ILE:HD11	2.50	0.45
1:D:50:GLU:O	1:D:54:LEU:HG	2.18	0.44
1:F:134:GLU:O	1:F:138:HIS:HD2	2.01	0.44
1:A:97:GLU:OE2	1:F:93:VAL:HB	2.17	0.43
1:C:38:ALA:HB3	1:C:71:SER:HB3	1.99	0.43
1:A:100:MET:HB2	1:B:119:MET:HE2	2.01	0.43
1:D:132:VAL:HG11	1:D:146:LEU:HD21	2.01	0.43
1:E:117:PHE:HB2	1:F:117:PHE:HB2	2.00	0.42
1:B:105[A]:MET:HE2	1:C:131:LEU:HD21	2.01	0.42
1:E:4:LYS:HE2	1:E:33:ILE:HD11	2.02	0.42
1:A:97:GLU:OE2	1:F:93:VAL:N	2.52	0.42
1:A:138:HIS:HB2	1:D:73:LEU:HG	2.02	0.42
1:F:151:HIS:O	1:F:155:MET:HG2	2.20	0.42
1:B:122:LYS:HG3	3:F:384:HOH:O	2.19	0.42
1:E:2:SER:HA	1:E:30:ASP:OD2	2.20	0.42
1:A:10:THR:O	1:A:51:ARG:HD2	2.19	0.41
1:A:101:GLN:NE2	1:F:126:PHE:O	2.48	0.41
1:F:47:ASP:OD1	1:F:50:GLU:HG3	2.21	0.41
1:C:11:PHE:CE1	1:C:34:LEU:HD11	2.55	0.41
1:D:126:PHE:HE2	1:E:122:LYS:HE2	1.85	0.41
1:E:5:ALA:HA	1:E:85:ILE:O	2.21	0.41
1:A:5:ALA:HA	1:A:85:ILE:O	2.21	0.40
1:F:3:THR:O	1:F:30:ASP:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	157/176 (89%)	155 (99%)	2 (1%)	0	100	100
1	B	175/176 (99%)	169 (97%)	6 (3%)	0	100	100
1	C	158/176 (90%)	150 (95%)	8 (5%)	0	100	100
1	D	158/176 (90%)	153 (97%)	5 (3%)	0	100	100
1	E	157/176 (89%)	153 (98%)	4 (2%)	0	100	100
1	F	175/176 (99%)	168 (96%)	7 (4%)	0	100	100
All	All	980/1056 (93%)	948 (97%)	32 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	134/145 (92%)	134 (100%)	0	100	100
1	B	146/145 (101%)	146 (100%)	0	100	100
1	C	135/145 (93%)	135 (100%)	0	100	100
1	D	135/145 (93%)	135 (100%)	0	100	100
1	E	134/145 (92%)	134 (100%)	0	100	100
1	F	146/145 (101%)	146 (100%)	0	100	100
All	All	830/870 (95%)	830 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	-7	GLN
1	B	144	HIS
1	C	61	HIS
1	D	82	GLN
1	F	-6	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](#)

6 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	CIT	D	201	-	12,12,12	1.10	0	17,17,17	1.28	2 (11%)
2	CIT	C	201	-	12,12,12	1.15	1 (8%)	17,17,17	1.27	2 (11%)
2	CIT	E	201	-	12,12,12	1.18	1 (8%)	17,17,17	1.53	2 (11%)
2	CIT	F	201	-	12,12,12	1.28	1 (8%)	17,17,17	1.19	2 (11%)
2	CIT	B	201	-	12,12,12	1.25	0	17,17,17	1.37	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CIT	A	201	-	12,12,12	1.15	1 (8%)	17,17,17	1.33	2 (11%)

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	D	201	-	-	9/16/16/16	-
2	CIT	C	201	-	-	6/16/16/16	-
2	CIT	E	201	-	-	8/16/16/16	-
2	CIT	F	201	-	-	8/16/16/16	-
2	CIT	B	201	-	-	8/16/16/16	-
2	CIT	A	201	-	-	8/16/16/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	CIT	C3-C6	2.44	1.55	1.53
2	F	201	CIT	C3-C6	2.37	1.55	1.53
2	A	201	CIT	C3-C6	2.26	1.55	1.53
2	C	201	CIT	C3-C6	2.25	1.55	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	201	CIT	O5-C6-C3	-4.17	116.35	122.25
2	D	201	CIT	O5-C6-C3	-3.45	117.36	122.25
2	A	201	CIT	O5-C6-C3	-3.39	117.45	122.25
2	E	201	CIT	O6-C6-C3	3.29	118.77	113.05
2	C	201	CIT	O5-C6-C3	-3.29	117.60	122.25
2	B	201	CIT	O5-C6-C3	-3.28	117.60	122.25
2	A	201	CIT	O6-C6-C3	2.86	118.01	113.05
2	F	201	CIT	O5-C6-C3	-2.70	118.42	122.25
2	C	201	CIT	O6-C6-C3	2.58	117.53	113.05
2	F	201	CIT	C3-C4-C5	2.45	119.74	113.81
2	D	201	CIT	O6-C6-C3	2.36	117.14	113.05
2	B	201	CIT	O6-C6-C3	2.29	117.02	113.05
2	B	201	CIT	C3-C4-C5	2.28	119.35	113.81

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	CIT	C2-C3-C6-O5
2	A	201	CIT	C2-C3-C6-O6
2	A	201	CIT	O7-C3-C6-O5
2	A	201	CIT	O7-C3-C6-O6
2	B	201	CIT	C1-C2-C3-C4
2	B	201	CIT	C1-C2-C3-C6
2	B	201	CIT	C2-C3-C6-O5
2	B	201	CIT	C2-C3-C6-O6
2	B	201	CIT	O7-C3-C6-O5
2	B	201	CIT	O7-C3-C6-O6
2	C	201	CIT	C1-C2-C3-O7
2	C	201	CIT	C1-C2-C3-C4
2	C	201	CIT	C1-C2-C3-C6
2	C	201	CIT	C2-C3-C4-C5
2	C	201	CIT	O7-C3-C4-C5
2	C	201	CIT	C6-C3-C4-C5
2	D	201	CIT	C1-C2-C3-C4
2	D	201	CIT	C1-C2-C3-C6
2	D	201	CIT	C2-C3-C6-O5
2	D	201	CIT	C2-C3-C6-O6
2	D	201	CIT	O7-C3-C6-O5
2	D	201	CIT	O7-C3-C6-O6
2	E	201	CIT	C2-C3-C6-O5
2	E	201	CIT	C2-C3-C6-O6
2	E	201	CIT	O7-C3-C6-O5
2	E	201	CIT	O7-C3-C6-O6
2	F	201	CIT	C1-C2-C3-O7
2	F	201	CIT	C1-C2-C3-C4
2	F	201	CIT	C1-C2-C3-C6
2	F	201	CIT	C2-C3-C6-O5
2	F	201	CIT	C2-C3-C6-O6
2	F	201	CIT	O7-C3-C6-O5
2	F	201	CIT	O7-C3-C6-O6
2	A	201	CIT	C1-C2-C3-C6
2	E	201	CIT	C1-C2-C3-C4
2	E	201	CIT	C1-C2-C3-C6
2	A	201	CIT	C1-C2-C3-C4
2	D	201	CIT	C1-C2-C3-O7
2	D	201	CIT	O7-C3-C4-C5
2	F	201	CIT	O7-C3-C4-C5

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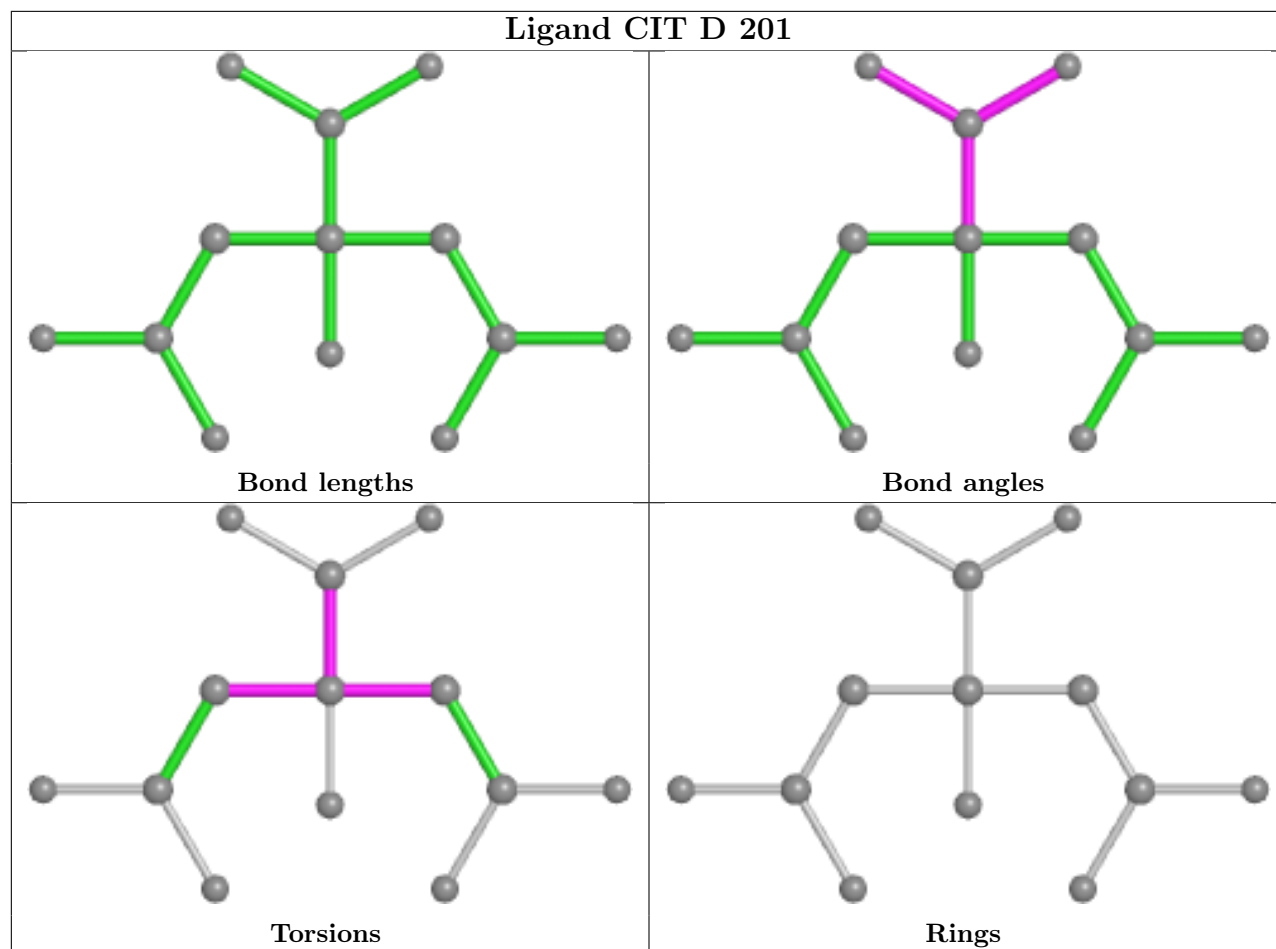
Mol	Chain	Res	Type	Atoms
2	B	201	CIT	C1-C2-C3-O7
2	E	201	CIT	C1-C2-C3-O7
2	A	201	CIT	C1-C2-C3-O7
2	E	201	CIT	O7-C3-C4-C5
2	A	201	CIT	O7-C3-C4-C5
2	B	201	CIT	O7-C3-C4-C5
2	D	201	CIT	C4-C3-C6-O6

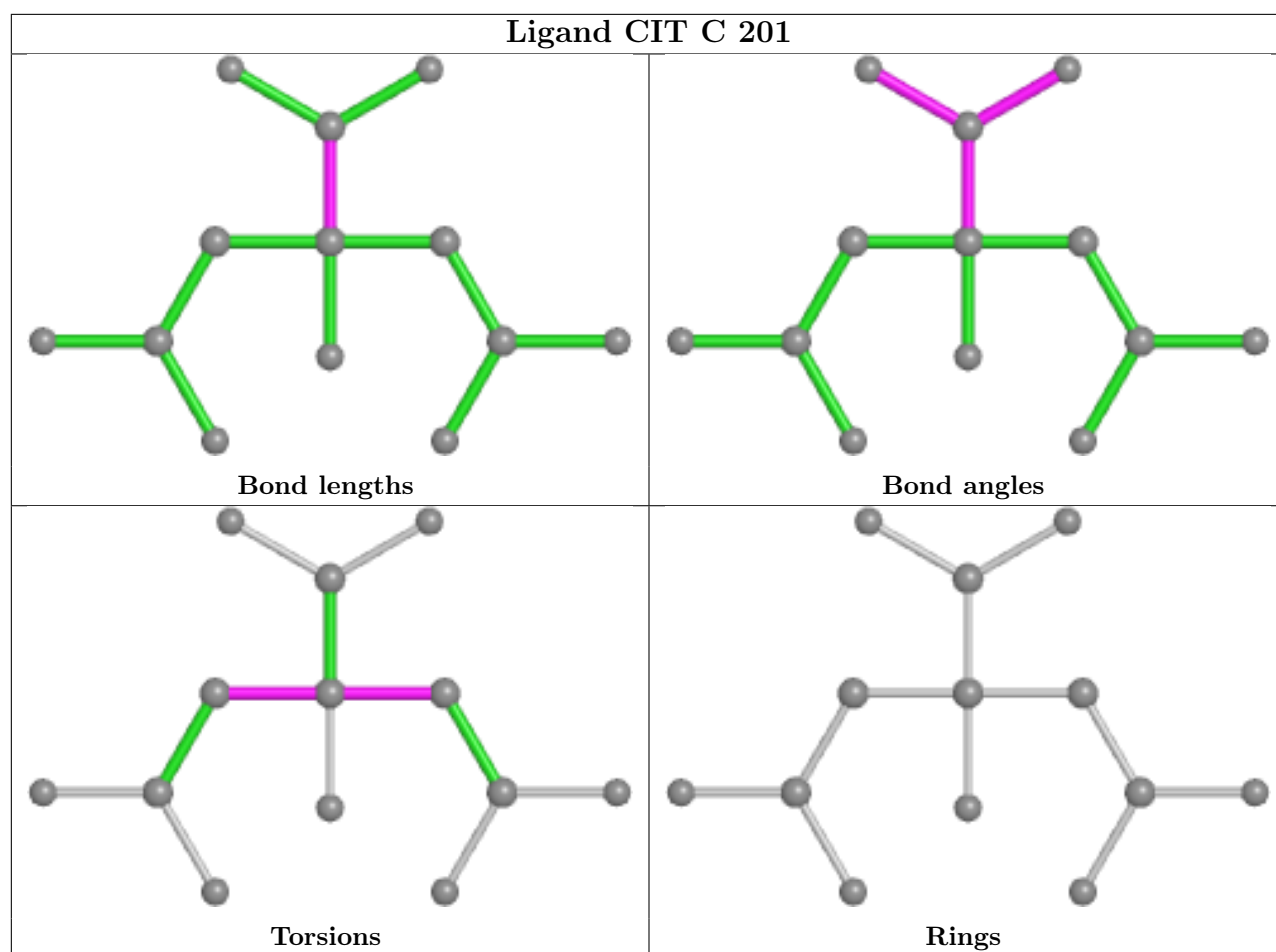
There are no ring outliers.

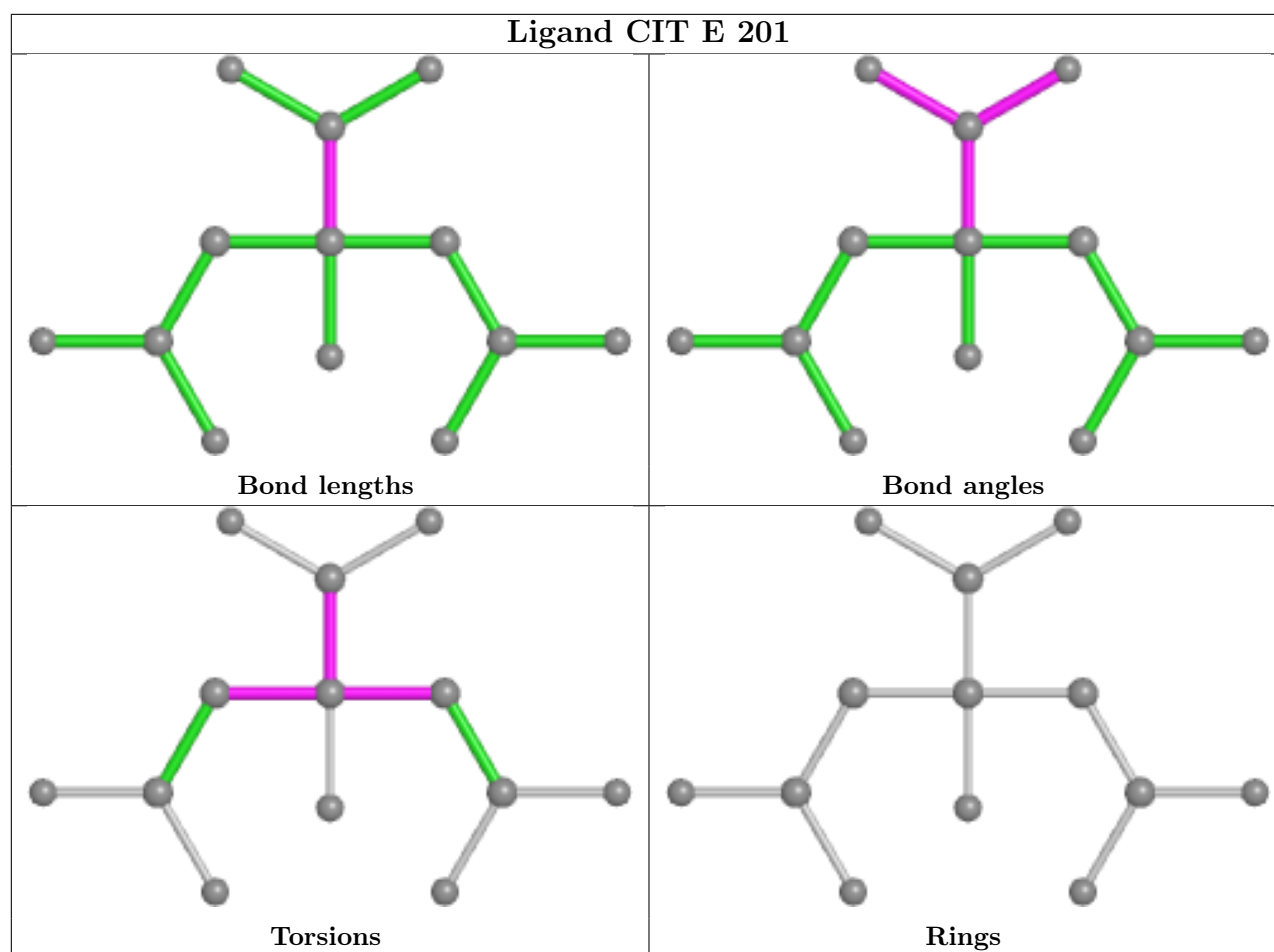
3 monomers are involved in 3 short contacts:

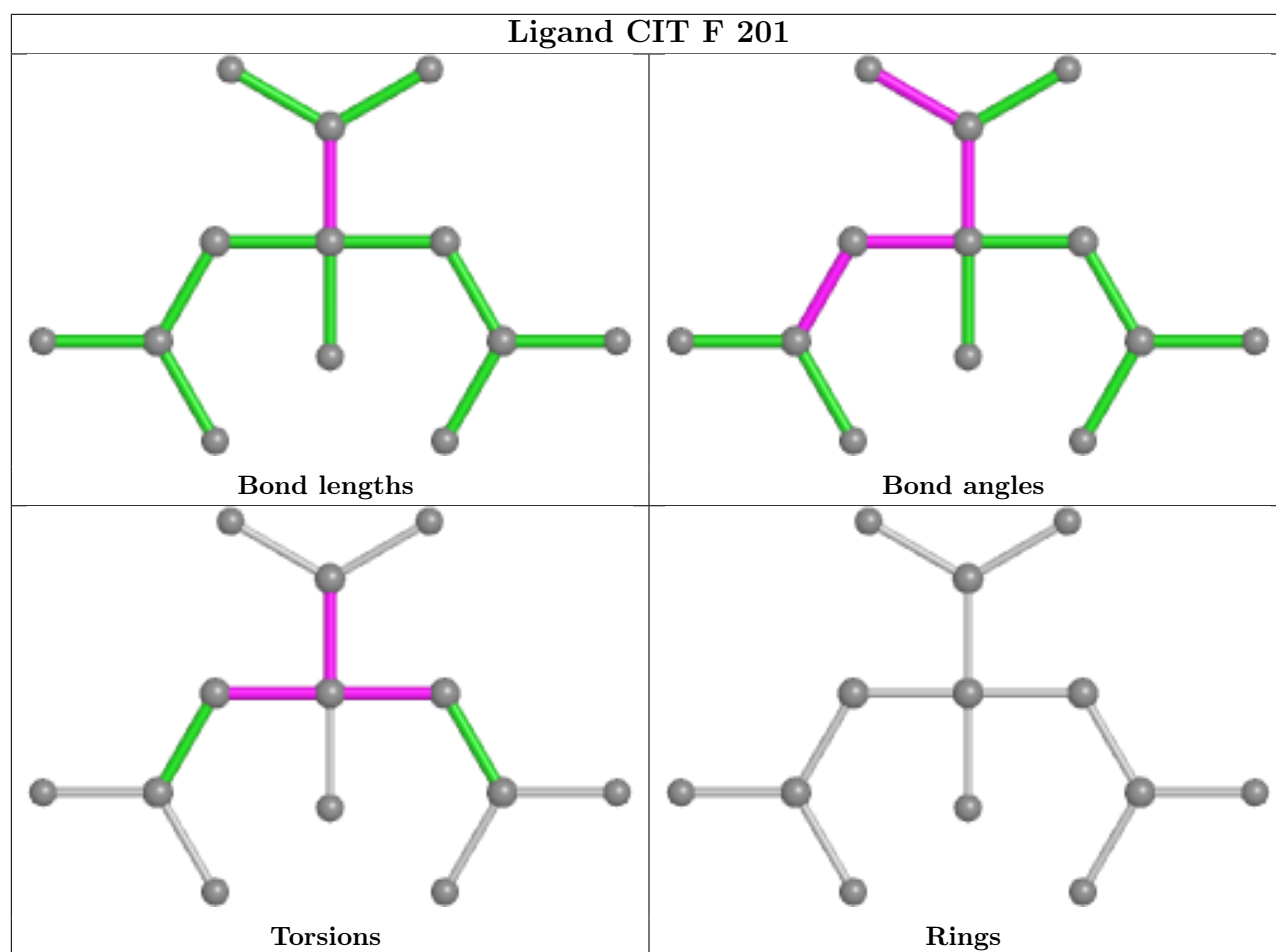
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	201	CIT	1	0
2	B	201	CIT	1	0
2	A	201	CIT	1	0

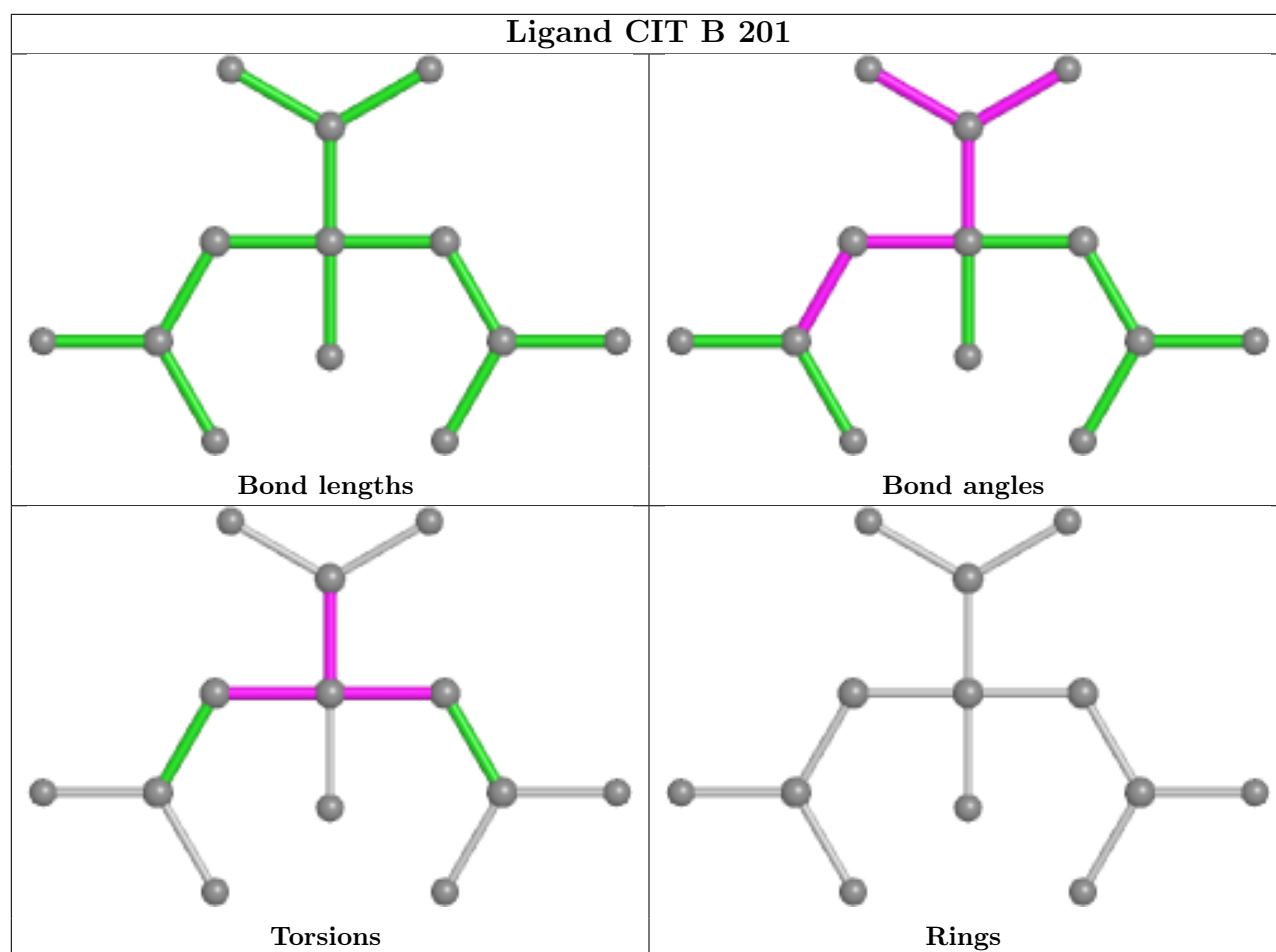
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

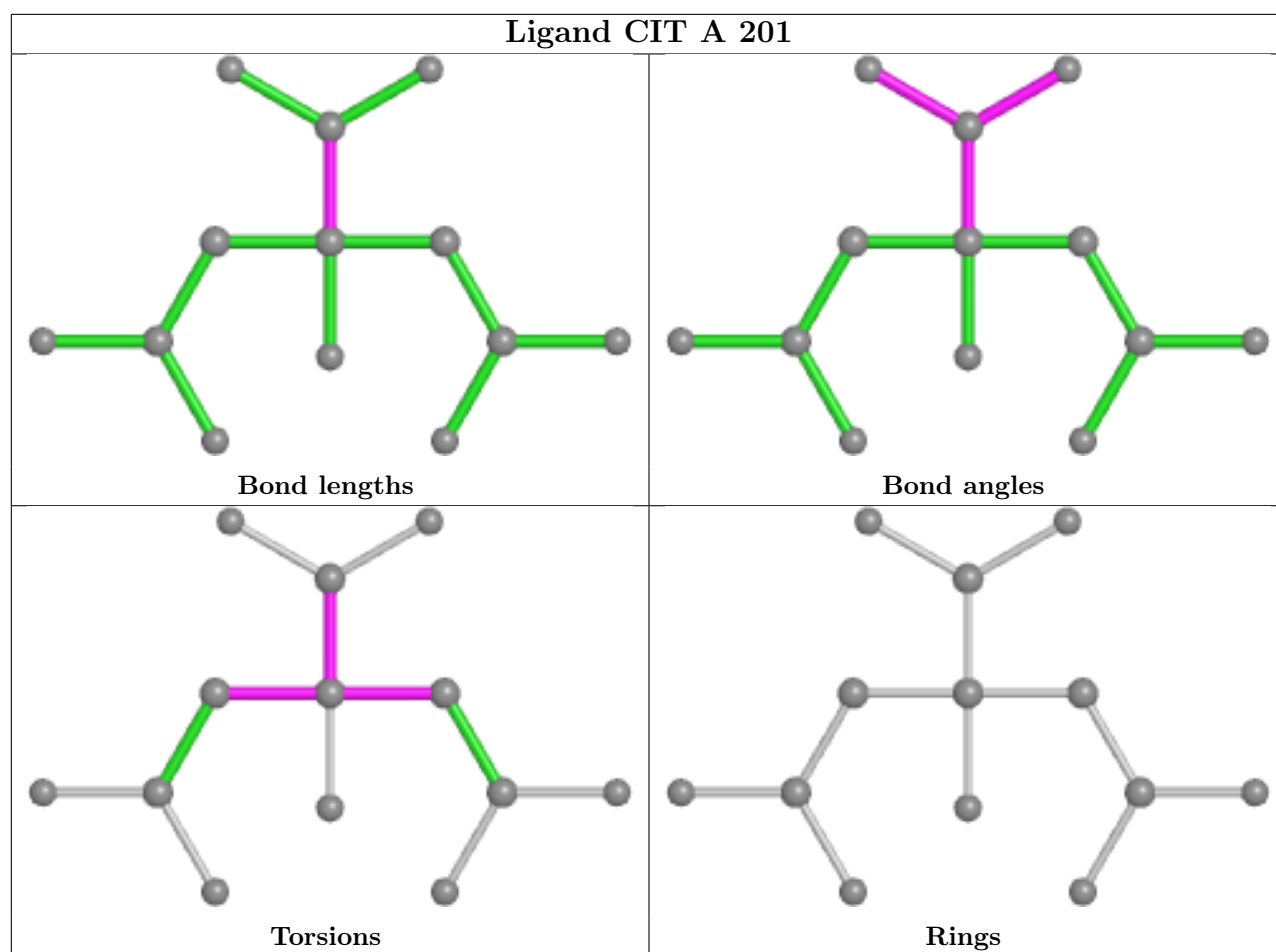












5.7 Other polymers [i](#)

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	159/176 (90%)	0.40	11 (6%) 24 26	25, 38, 69, 106	0
1	B	176/176 (100%)	0.26	2 (1%) 77 78	20, 37, 69, 93	1 (0%)
1	C	159/176 (90%)	1.59	46 (28%) 1 1	29, 79, 115, 131	1 (0%)
1	D	159/176 (90%)	1.18	26 (16%) 5 6	35, 65, 98, 123	1 (0%)
1	E	159/176 (90%)	0.47	6 (3%) 44 47	27, 41, 75, 98	0
1	F	176/176 (100%)	0.25	4 (2%) 61 63	24, 36, 63, 130	1 (0%)
All	All	988/1056 (93%)	0.68	95 (9%) 15 16	20, 49, 99, 131	4 (0%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	131	LEU	5.6
1	D	74	MET	5.3
1	C	127	ILE	4.4
1	C	135	VAL	4.2
1	D	73	LEU	4.0
1	D	6	ILE	4.0
1	D	70	PHE	3.9
1	C	74	MET	3.8
1	D	75	ALA	3.8
1	D	78	ALA	3.8
1	F	-17	GLY	3.8
1	C	126	PHE	3.6
1	F	-15	HIS	3.6
1	D	113	LEU	3.6
1	C	142	VAL	3.5
1	C	98	TYR	3.4
1	C	154	LEU	3.3
1	D	85	ILE	3.2
1	A	130	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	-8	GLY	3.1
1	C	158	LEU	3.0
1	B	-17	GLY	3.0
1	C	136	ALA	3.0
1	B	-15	HIS	2.9
1	C	120	PRO	2.9
1	D	63	PRO	2.8
1	C	73	LEU	2.8
1	D	109	LEU	2.8
1	C	147	PRO	2.8
1	C	139	ALA	2.7
1	A	139	ALA	2.7
1	D	77	PHE	2.7
1	C	6	ILE	2.7
1	E	159	LYS	2.7
1	C	1	MET	2.7
1	C	83	ALA	2.7
1	C	146	LEU	2.6
1	C	151	HIS	2.6
1	D	69	GLY	2.5
1	E	121	SER	2.5
1	C	62	LEU	2.5
1	C	150	VAL	2.5
1	D	102	LEU	2.5
1	C	75	ALA	2.5
1	C	92	ALA	2.5
1	C	132	VAL	2.5
1	D	67	VAL	2.5
1	C	129	SER	2.4
1	E	127	ILE	2.4
1	C	58	ALA	2.4
1	C	141	ASP	2.4
1	D	92	ALA	2.4
1	C	145	PHE	2.4
1	D	110	MET	2.4
1	C	143	THR	2.3
1	C	22	ILE	2.3
1	C	148	ALA	2.3
1	C	155	MET	2.3
1	D	80	ALA	2.3
1	E	74	MET	2.3
1	D	72	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	126	PHE	2.3
1	C	125	SER	2.3
1	C	130	SER	2.3
1	E	96	PHE	2.2
1	A	136	ALA	2.2
1	C	94	ALA	2.2
1	C	14	ILE	2.2
1	C	57	THR	2.2
1	F	-10	THR	2.2
1	A	41	SER	2.2
1	D	39	SER	2.2
1	D	93	VAL	2.2
1	C	46	PHE	2.2
1	A	94	ALA	2.2
1	C	122	LYS	2.2
1	D	1	MET	2.2
1	A	134	GLU	2.1
1	C	87	ILE	2.1
1	D	127	ILE	2.1
1	C	80	ALA	2.1
1	C	40	PRO	2.1
1	A	96	PHE	2.1
1	D	49	GLU	2.1
1	C	65	VAL	2.1
1	D	65	VAL	2.1
1	A	144	HIS	2.1
1	C	159	LYS	2.0
1	A	135	VAL	2.0
1	A	142	VAL	2.0
1	D	32	VAL	2.0
1	C	34	LEU	2.0
1	E	158	LEU	2.0
1	D	5	ALA	2.0
1	C	72	ASP	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 [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

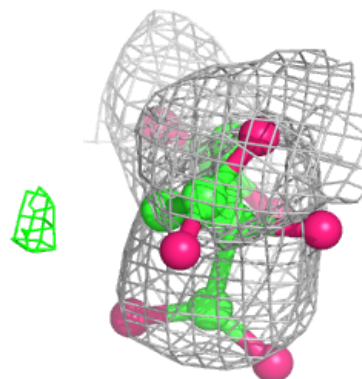
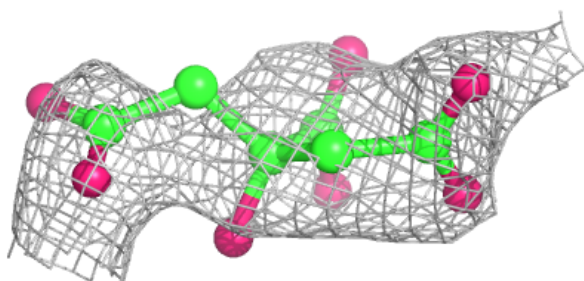
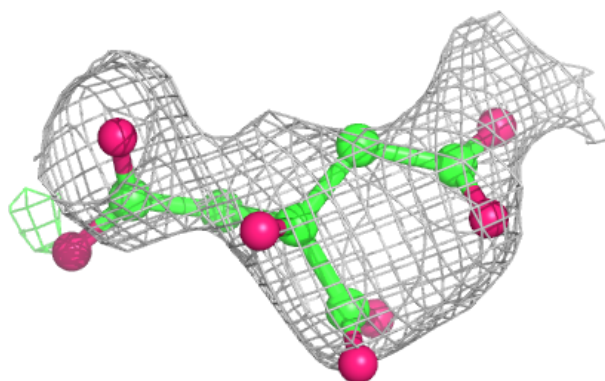
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	CIT	C	201	13/13	0.75	0.14	66,77,84,84	13
2	CIT	D	201	13/13	0.76	0.14	62,67,77,78	13
2	CIT	B	201	13/13	0.77	0.14	39,52,58,60	0
2	CIT	F	201	13/13	0.84	0.12	38,54,59,67	0
2	CIT	E	201	13/13	0.85	0.11	52,64,68,69	0
2	CIT	A	201	13/13	0.88	0.10	40,56,66,71	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.

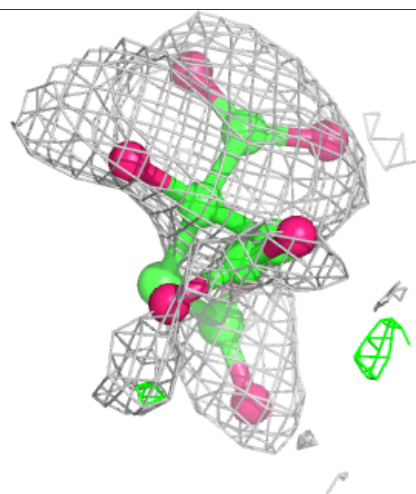
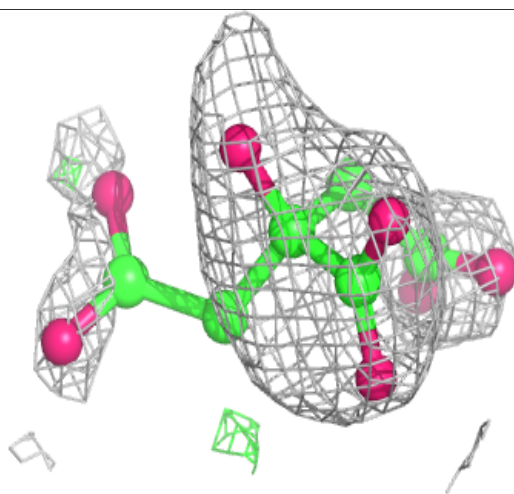
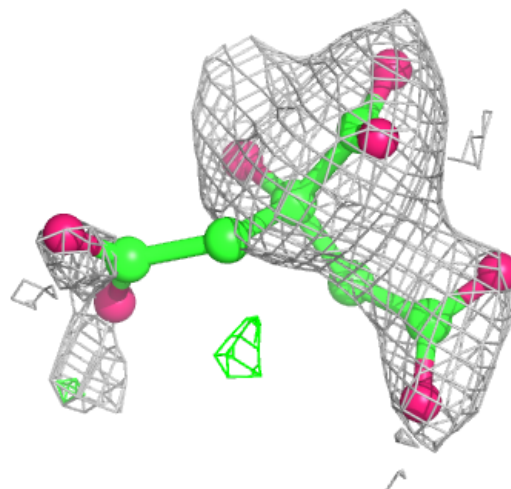
Electron density around CIT C 201:

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



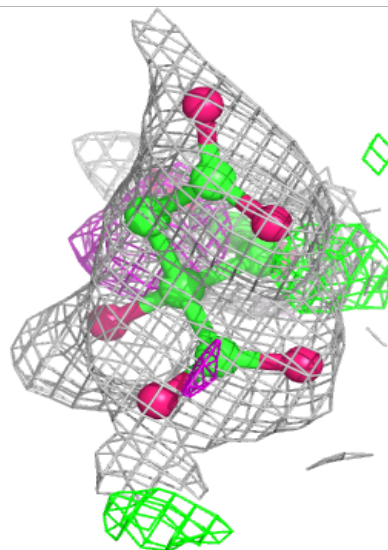
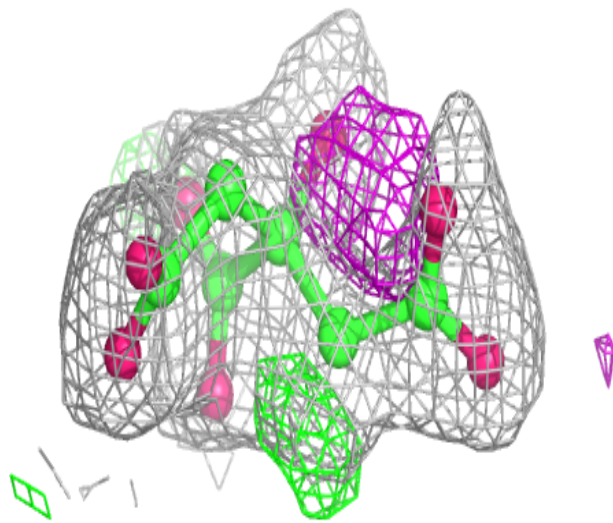
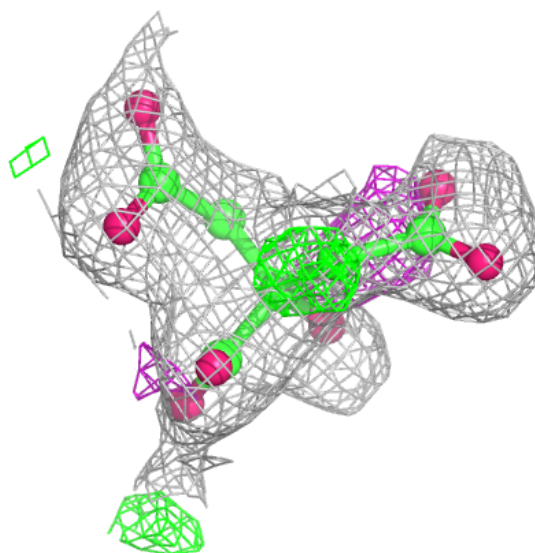
Electron density around CIT D 201:

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



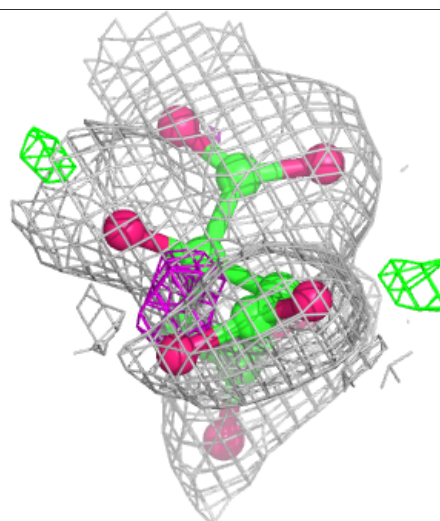
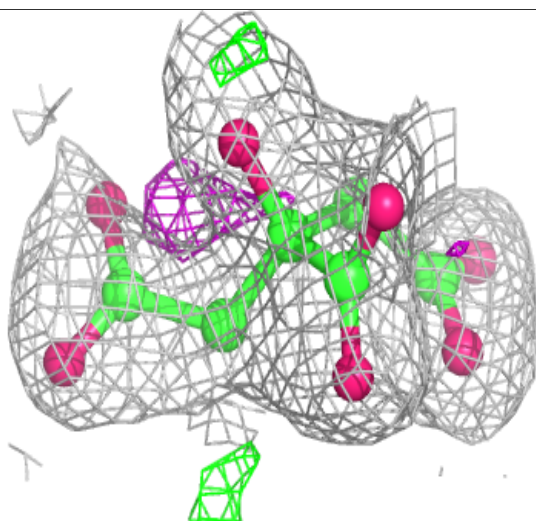
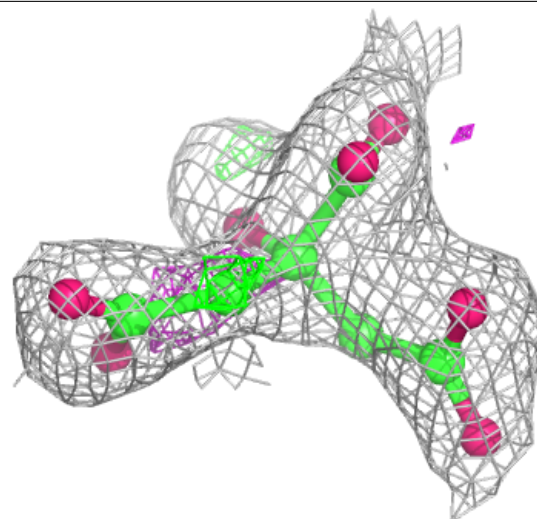
Electron density around CIT B 201:

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



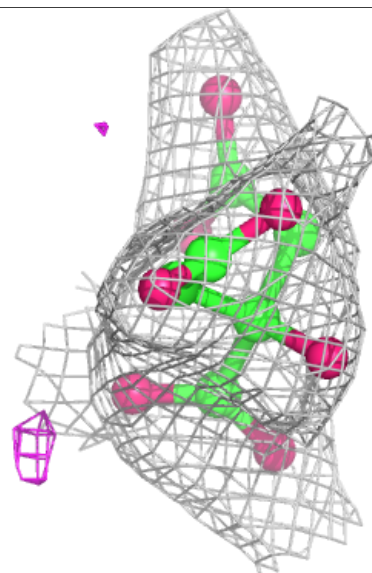
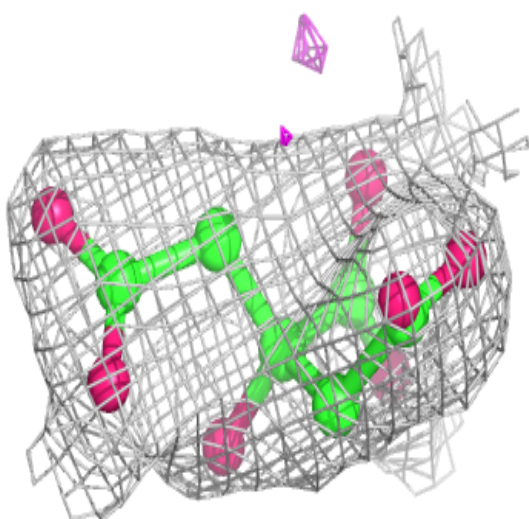
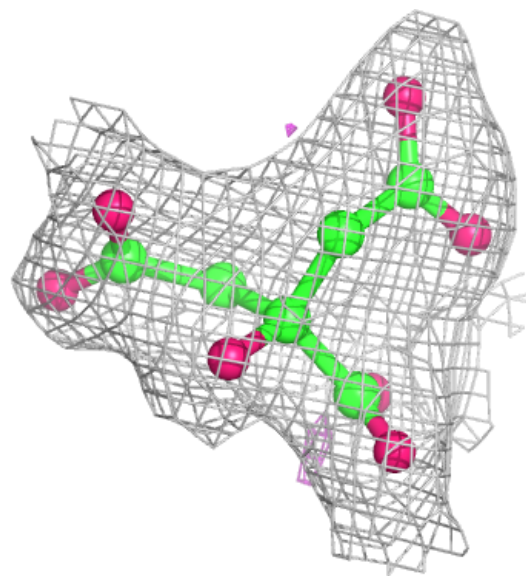
Electron density around CIT F 201:

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



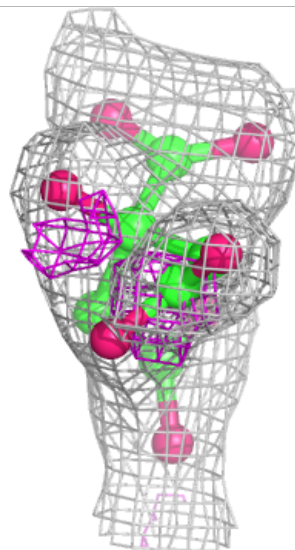
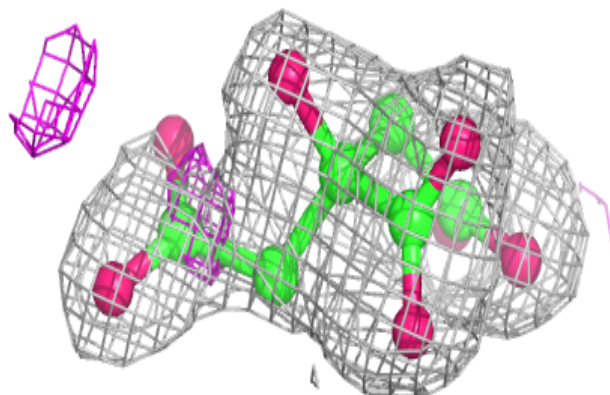
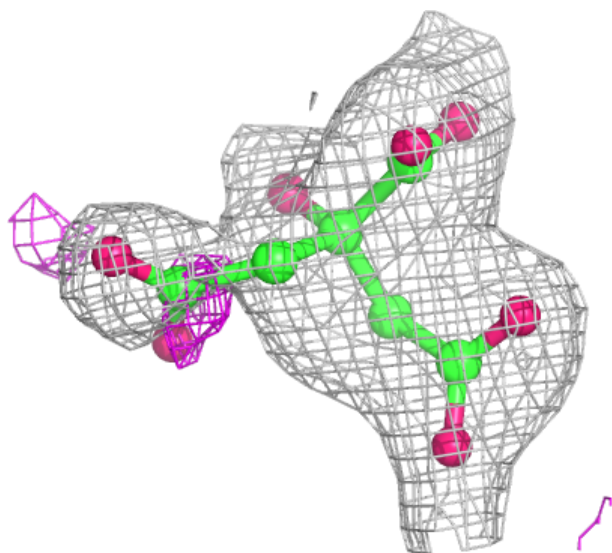
Electron density around CIT E 201:

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



Electron density around CIT A 201:

$2mF_o-DF_c$ (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.