Full wwPDB X-ray Structure Validation Report (i)

May 11, 2022 – 04:18 pm BST

PDB ID	:	7P4G
Title	:	Rabbit Muscle L-lactate dehydrogenase in complex with citrate
Authors	:	Iacovino, L.G.; Binda, C.; Hochkoeppler, A.
Deposited on	:	2021-07-11
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

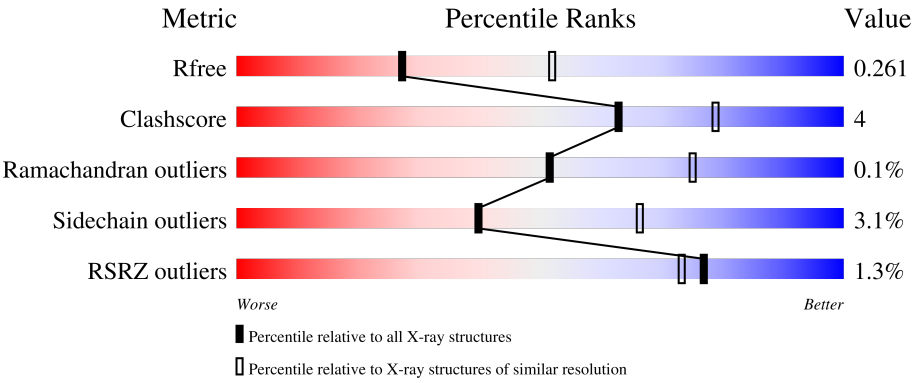
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	332	87% 9%
1	B	332	2% 86% 11%
1	C	332	87% 12%
1	D	332	84% 14%
1	E	332	3% 84% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	332	2% 84% 13%
1	G	332	% 91% 8%
1	H	332	% 83% 16%
1	I	332	% 86% 11%
1	J	332	% 85% 11%
1	K	332	% 85% 14%
1	L	332	86% 13%
1	M	332	% 87% 12%
1	N	332	2% 85% 14%
1	O	332	2% 86% 14%
1	P	332	3% 84% 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 41110 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.

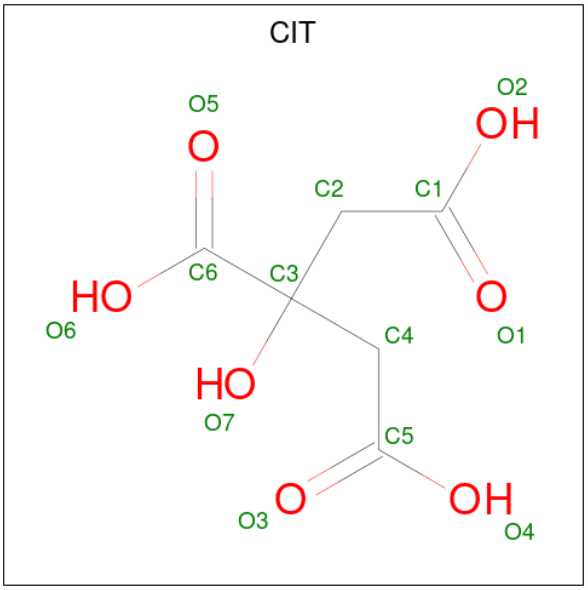
- Molecule 1 is a protein called L-lactate dehydrogenase A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	S	0	0	0
			2466	1579	421	452	14			
1	B	322	Total	C	N	O	S	0	0	0
			2482	1589	424	455	14			
1	C	327	Total	C	N	O	S	0	0	0
			2526	1613	436	463	14			
1	D	331	Total	C	N	O	S	0	0	0
			2558	1632	441	471	14			
1	E	320	Total	C	N	O	S	0	0	0
			2466	1579	421	452	14			
1	F	322	Total	C	N	O	S	0	0	0
			2482	1589	424	455	14			
1	G	331	Total	C	N	O	S	0	0	0
			2558	1632	441	471	14			
1	H	330	Total	C	N	O	S	0	0	0
			2553	1629	440	470	14			
1	I	320	Total	C	N	O	S	0	0	0
			2466	1579	421	452	14			
1	J	319	Total	C	N	O	S	0	0	0
			2454	1573	419	448	14			
1	K	330	Total	C	N	O	S	0	0	0
			2553	1629	440	470	14			
1	L	331	Total	C	N	O	S	0	0	0
			2558	1632	441	471	14			
1	M	331	Total	C	N	O	S	0	0	0
			2558	1632	441	471	14			
1	N	331	Total	C	N	O	S	0	0	0
			2558	1632	441	471	14			
1	O	331	Total	C	N	O	S	0	0	0
			2558	1632	441	471	14			
1	P	325	Total	C	N	O	S	0	0	0
			2507	1604	430	459	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	SER	THR	engineered mutation	UNP P13491
B	248	SER	THR	engineered mutation	UNP P13491
C	248	SER	THR	engineered mutation	UNP P13491
D	248	SER	THR	engineered mutation	UNP P13491
E	248	SER	THR	engineered mutation	UNP P13491
F	248	SER	THR	engineered mutation	UNP P13491
G	248	SER	THR	engineered mutation	UNP P13491
H	248	SER	THR	engineered mutation	UNP P13491
I	248	SER	THR	engineered mutation	UNP P13491
J	248	SER	THR	engineered mutation	UNP P13491
K	248	SER	THR	engineered mutation	UNP P13491
L	248	SER	THR	engineered mutation	UNP P13491
M	248	SER	THR	engineered mutation	UNP P13491
N	248	SER	THR	engineered mutation	UNP P13491
O	248	SER	THR	engineered mutation	UNP P13491
P	248	SER	THR	engineered mutation	UNP P13491

- Molecule 2 is CITRIC ACID (three-letter code: 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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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
2	G	1	Total C O 13 6 7	0	0
2	H	1	Total C O 13 6 7	0	0
2	I	1	Total C O 13 6 7	0	0
2	J	1	Total C O 13 6 7	0	0
2	K	1	Total C O 13 6 7	0	0
2	L	1	Total C O 13 6 7	0	0
2	M	1	Total C O 13 6 7	0	0
2	N	1	Total C O 13 6 7	0	0
2	O	1	Total C O 13 6 7	0	0
2	P	1	Total C O 13 6 7	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	41	Total O 41 41	0	0
3	B	47	Total O 47 47	0	0
3	C	49	Total O 49 49	0	0
3	D	38	Total O 38 38	0	0
3	E	38	Total O 38 38	0	0

Continued on next page...

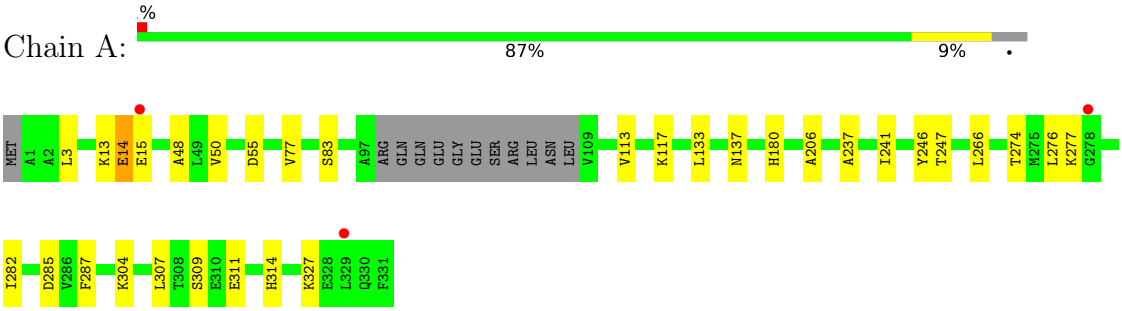
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	28	Total O 28 28	0	0
3	G	28	Total O 28 28	0	0
3	H	32	Total O 32 32	0	0
3	I	29	Total O 29 29	0	0
3	J	33	Total O 33 33	0	0
3	K	33	Total O 33 33	0	0
3	L	37	Total O 37 37	0	0
3	M	42	Total O 42 42	0	0
3	N	40	Total O 40 40	0	0
3	O	44	Total O 44 44	0	0
3	P	40	Total O 40 40	0	0

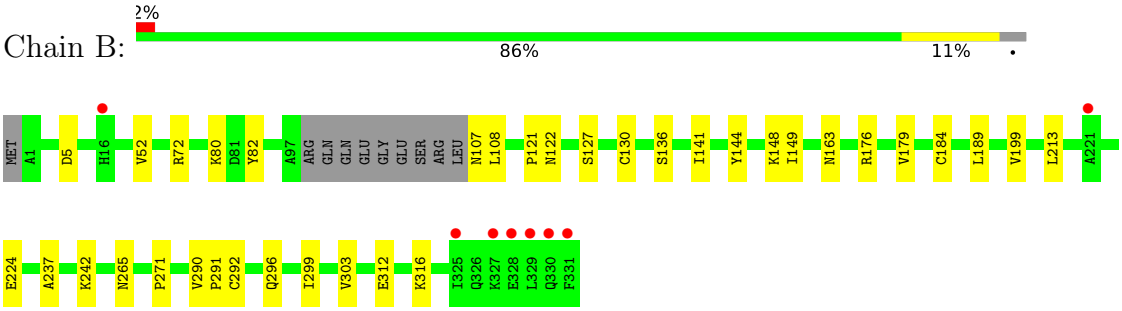
3 Residue-property plots (i)

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.

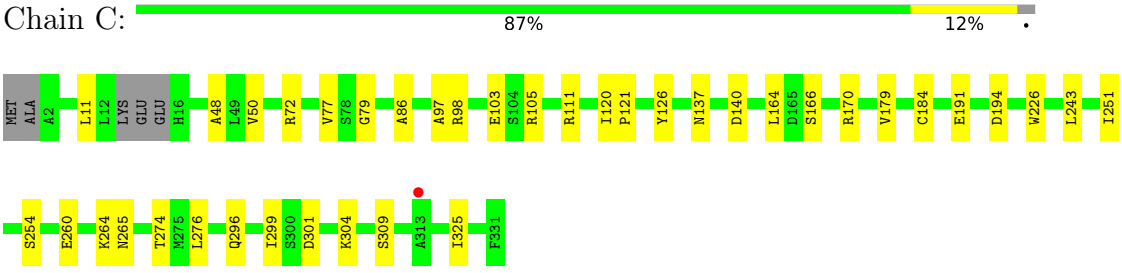
• Molecule 1: L-lactate dehydrogenase A chain



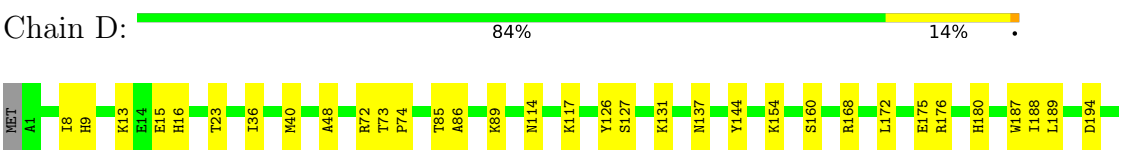
• Molecule 1: L-lactate dehydrogenase A chain



• Molecule 1: L-lactate dehydrogenase A chain

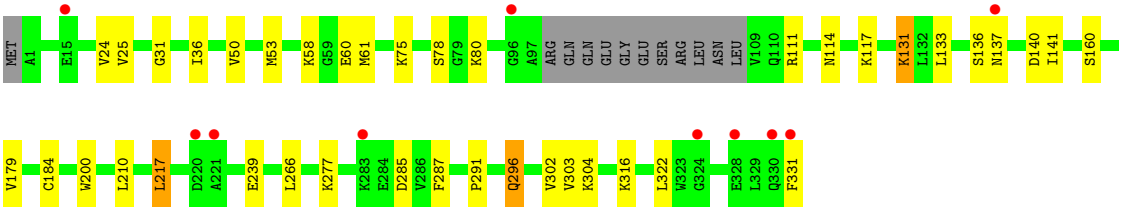


• Molecule 1: L-lactate dehydrogenase A chain



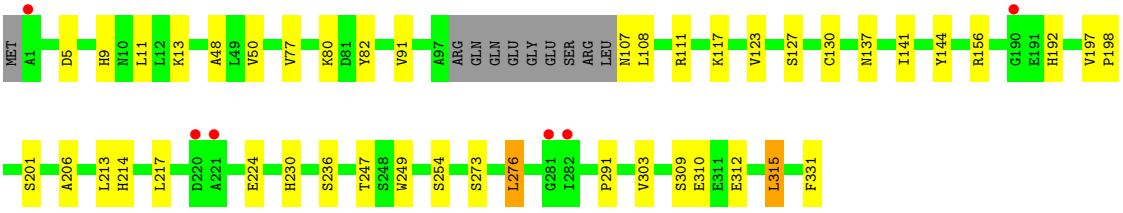
• Molecule 1: L-lactate dehydrogenase A chain

Chain E:



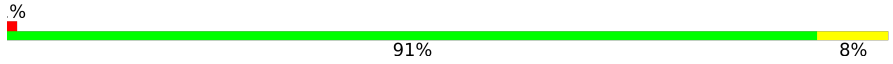
• Molecule 1: L-lactate dehydrogenase A chain

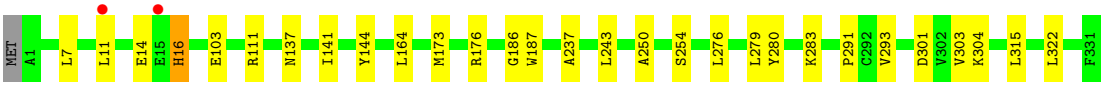
Chain F:



• Molecule 1: L-lactate dehydrogenase A chain

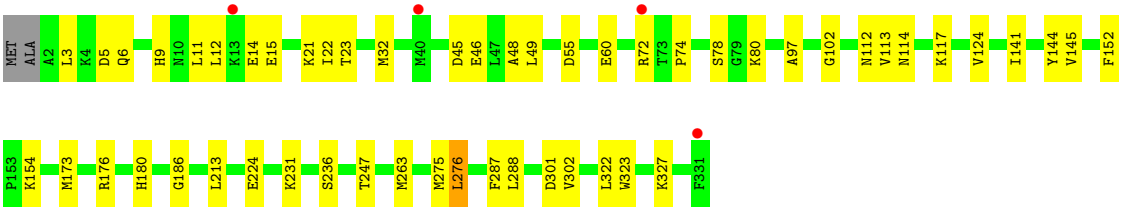
Chain G:





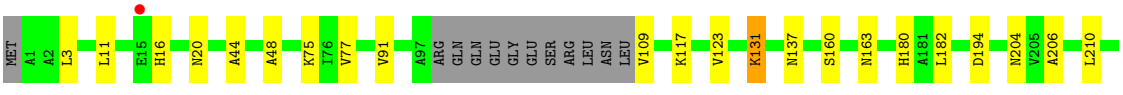
• Molecule 1: L-lactate dehydrogenase A chain

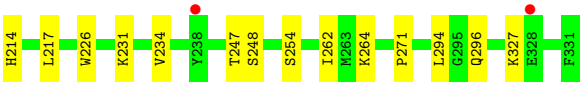
Chain H:



• Molecule 1: L-lactate dehydrogenase A chain

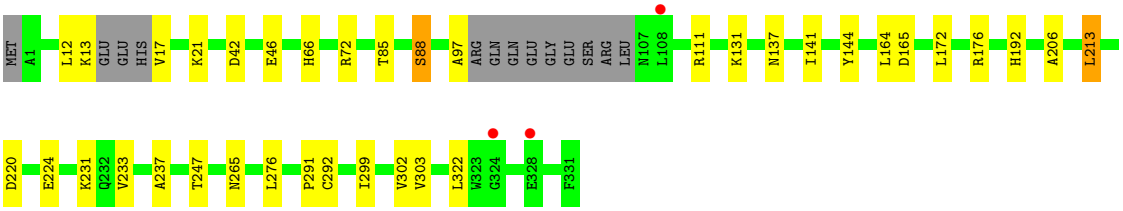
Chain I:





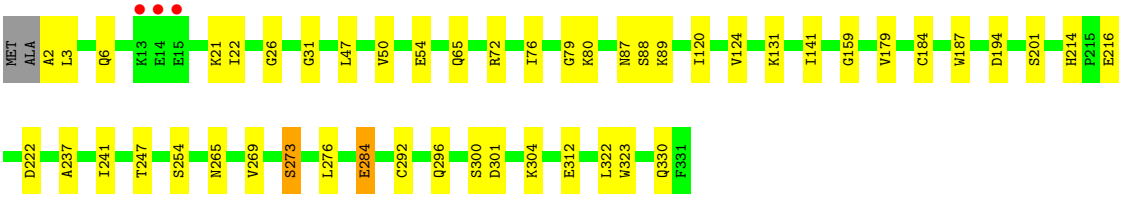
• Molecule 1: L-lactate dehydrogenase A chain

Chain J:



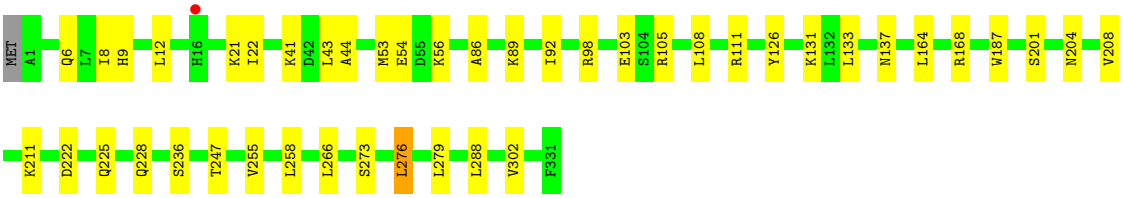
• Molecule 1: L-lactate dehydrogenase A chain

Chain K:



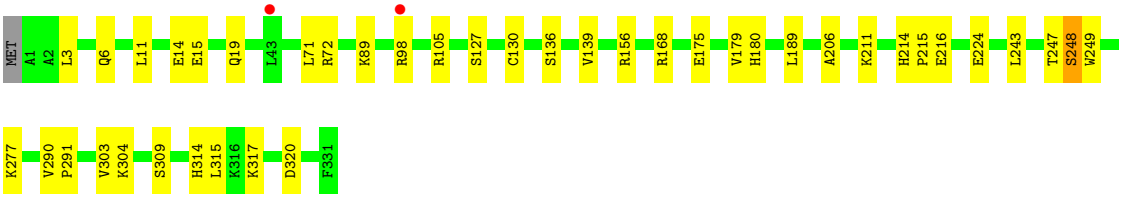
• Molecule 1: L-lactate dehydrogenase A chain

Chain L:



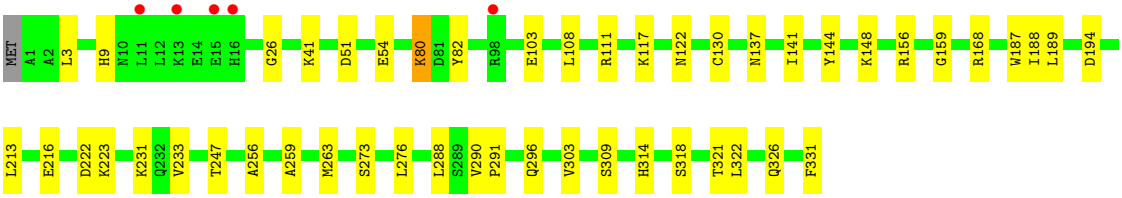
• Molecule 1: L-lactate dehydrogenase A chain

Chain M:

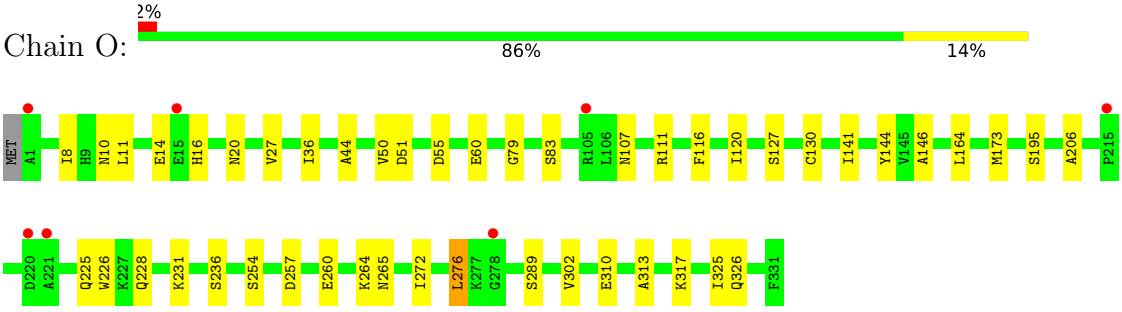


• Molecule 1: L-lactate dehydrogenase A chain

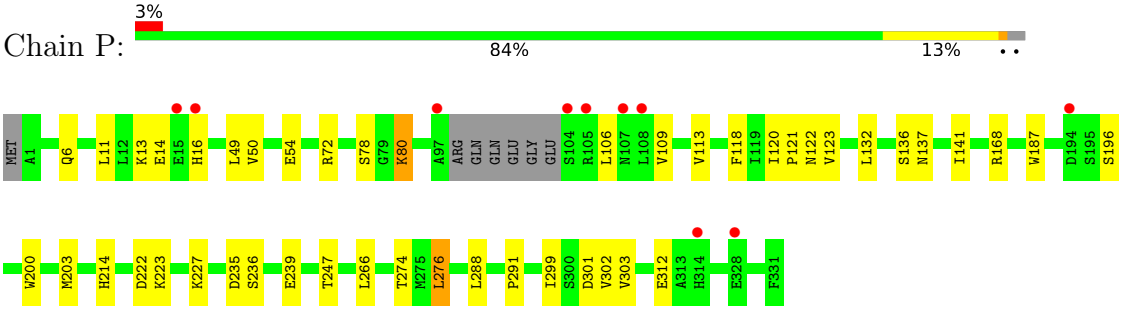
Chain N:



• Molecule 1: L-lactate dehydrogenase A chain



• Molecule 1: L-lactate dehydrogenase A chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	83.70Å 141.57Å 148.14Å 114.55° 94.69° 102.20°	Depositor
Resolution (Å)	49.02 – 2.60 48.97 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.4 (49.02-2.60) 93.4 (48.97-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.199 , 0.260 0.205 , 0.261	Depositor DCC
R_{free} test set	8434 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	41110	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.69	0/2511	0.79	0/3396
1	B	0.69	0/2527	0.79	0/3418
1	C	0.69	0/2571	0.80	0/3476
1	D	0.69	0/2604	0.81	0/3521
1	E	0.69	0/2511	0.79	0/3396
1	F	0.71	0/2527	0.81	0/3418
1	G	0.68	0/2604	0.79	0/3521
1	H	0.69	0/2599	0.80	0/3514
1	I	0.69	0/2511	0.79	0/3396
1	J	0.69	0/2497	0.80	0/3376
1	K	0.69	0/2599	0.80	0/3514
1	L	0.70	0/2604	0.81	0/3521
1	M	0.71	0/2604	0.81	1/3521 (0.0%)
1	N	0.70	0/2604	0.81	0/3521
1	O	0.69	0/2604	0.80	0/3521
1	P	0.68	0/2552	0.80	0/3451
All	All	0.69	0/41029	0.80	1/55481 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	156	ARG	NE-CZ-NH2	-5.24	117.68	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2466	0	2546	17	0
1	B	2482	0	2563	23	0
1	C	2526	0	2603	25	0
1	D	2558	0	2637	33	0
1	E	2466	0	2546	27	0
1	F	2482	0	2563	26	0
1	G	2558	0	2637	24	0
1	H	2553	0	2629	29	0
1	I	2466	0	2546	25	0
1	J	2454	0	2543	23	0
1	K	2553	0	2629	29	0
1	L	2558	0	2637	24	0
1	M	2558	0	2637	19	0
1	N	2558	0	2637	28	0
1	O	2558	0	2637	32	0
1	P	2507	0	2592	26	0
2	A	13	0	5	2	0
2	B	13	0	5	2	0
2	C	13	0	5	3	0
2	D	13	0	5	3	0
2	E	13	0	5	3	0
2	F	13	0	5	3	0
2	G	13	0	5	3	0
2	H	13	0	5	2	0
2	I	13	0	5	2	0
2	J	13	0	5	3	0
2	K	13	0	5	0	0
2	L	13	0	5	4	0
2	M	13	0	5	3	0
2	N	13	0	5	3	0
2	O	13	0	5	1	0
2	P	13	0	5	2	0
3	A	41	0	0	0	0
3	B	47	0	0	1	0
3	C	49	0	0	1	0
3	D	38	0	0	2	0
3	E	38	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	28	0	0	0	0
3	G	28	0	0	0	0
3	H	32	0	0	1	0
3	I	29	0	0	1	0
3	J	33	0	0	0	0
3	K	33	0	0	2	0
3	L	37	0	0	1	0
3	M	42	0	0	0	0
3	N	40	0	0	0	0
3	O	44	0	0	0	0
3	P	40	0	0	0	0
All	All	41110	0	41662	353	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 4.

All (353) 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:H:247:THR:OG1	2:H:401:CIT:H22	1.71	0.91
1:B:237:ALA:HB2	2:B:401:CIT:O2	1.73	0.88
1:L:137:ASN:HD21	2:L:401:CIT:C6	1.97	0.77
1:D:247:THR:OG1	2:D:401:CIT:H22	1.85	0.76
1:O:120:ILE:HD13	1:O:146:ALA:HA	1.70	0.74
1:D:168:ARG:NH2	2:D:401:CIT:O1	2.19	0.74
1:O:276:LEU:HG	1:O:276:LEU:O	1.89	0.72
1:D:300:SER:OG	1:D:301:ASP:OD1	2.08	0.70
1:E:302:VAL:HG23	1:F:11:LEU:HD11	1.75	0.69
1:F:247:THR:OG1	2:F:401:CIT:H22	1.93	0.68
1:B:265:ASN:HD22	1:B:296:GLN:H	1.39	0.67
1:G:304:LYS:NZ	1:H:5:ASP:O	2.26	0.67
1:A:206:ALA:HA	1:D:187:TRP:CZ2	2.30	0.67
1:F:137:ASN:HD21	2:F:401:CIT:C6	2.08	0.67
1:N:117:LYS:HE3	1:N:331:PHE:OXT	1.94	0.66
1:P:291:PRO:HB2	1:P:303:VAL:HB	1.77	0.66
1:D:216:GLU:O	1:D:219:THR:HG22	1.96	0.65
1:N:247:THR:OG1	2:N:401:CIT:H22	1.96	0.65
1:B:52:VAL:HA	1:B:80:LYS:HD3	1.79	0.65
1:B:176:ARG:NH2	1:B:224:GLU:O	2.30	0.64
1:D:137:ASN:HD21	2:D:401:CIT:C6	2.11	0.64
1:M:168:ARG:NH2	2:M:401:CIT:O1	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:137:ASN:HD21	2:E:401:CIT:C6	2.11	0.63
1:J:137:ASN:HD21	2:J:401:CIT:C6	2.11	0.63
1:O:302:VAL:HG23	1:P:11:LEU:HD11	1.80	0.63
1:H:141:ILE:HG13	1:H:322:LEU:HD22	1.80	0.63
1:I:11:LEU:HD11	1:J:302:VAL:HG23	1.80	0.63
1:E:141:ILE:HG23	1:E:322:LEU:HD22	1.81	0.62
1:A:277:LYS:HD3	1:A:285:ASP:OD2	1.99	0.62
1:F:117:LYS:NZ	1:F:331:PHE:O	2.32	0.62
1:D:276:LEU:HD21	1:D:288:LEU:HB2	1.82	0.62
1:C:98:ARG:NH2	3:C:502:HOH:O	2.28	0.62
1:C:304:LYS:HD2	1:D:9:HIS:HB2	1.80	0.62
1:I:131:LYS:HE3	1:I:296:GLN:O	2.01	0.61
1:C:137:ASN:HD21	2:C:401:CIT:C6	2.13	0.61
1:F:197:VAL:HG21	1:F:315:LEU:HD13	1.83	0.61
1:J:206:ALA:HA	1:K:187:TRP:CZ2	2.35	0.60
1:B:149:ILE:O	1:J:13:LYS:HE3	2.01	0.60
1:J:292:CYS:HB3	1:J:299:ILE:HG23	1.84	0.60
1:B:291:PRO:HB2	1:B:303:VAL:HB	1.84	0.59
1:I:214:HIS:HB2	1:K:3:LEU:HD13	1.84	0.59
1:A:237:ALA:HB2	2:A:401:CIT:O1	2.02	0.59
1:J:237:ALA:HB2	2:J:401:CIT:O1	2.03	0.59
1:D:172:LEU:O	1:D:175:GLU:HG3	2.02	0.59
1:M:291:PRO:HB2	1:M:303:VAL:HB	1.85	0.59
1:A:241:ILE:HG12	1:A:246:TYR:HA	1.85	0.58
1:I:247:THR:HG23	3:K:507:HOH:O	2.03	0.58
1:O:225:GLN:HB3	1:O:228:GLN:HG2	1.85	0.58
1:M:14:GLU:OE1	1:M:14:GLU:HA	2.02	0.58
1:H:154:LYS:NZ	3:H:501:HOH:O	2.33	0.58
1:K:141:ILE:HG13	1:K:322:LEU:HD22	1.86	0.58
1:J:206:ALA:HA	1:K:187:TRP:CE2	2.38	0.58
1:E:291:PRO:HB2	1:E:303:VAL:HB	1.85	0.57
1:F:213:LEU:HD21	1:H:6:GLN:HB3	1.87	0.57
1:K:2:ALA:O	1:K:6:GLN:HG3	2.04	0.57
1:P:106:LEU:HA	1:P:109:VAL:HG12	1.86	0.57
1:G:137:ASN:HD21	2:G:401:CIT:C6	2.17	0.57
1:A:137:ASN:HD21	2:A:401:CIT:C6	2.18	0.57
1:B:189:LEU:HD12	1:B:199:VAL:HG21	1.87	0.57
1:F:127:SER:HB3	1:F:130:CYS:HB3	1.86	0.57
1:K:50:VAL:HG12	1:K:79:GLY:O	2.05	0.56
1:K:179:VAL:CG2	1:K:184:CYS:SG	2.93	0.56
1:F:309:SER:HA	1:F:312:GLU:OE1	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:200:TRP:CE3	1:P:203:MET:SD	2.98	0.56
1:F:130:CYS:O	1:F:156:ARG:NH1	2.39	0.56
1:C:103:GLU:OE2	1:C:111:ARG:HD3	2.06	0.56
1:J:291:PRO:HB2	1:J:303:VAL:HB	1.88	0.55
1:N:80:LYS:HD3	1:N:80:LYS:N	2.21	0.55
1:P:235:ASP:O	1:P:239:GLU:HG2	2.04	0.55
1:C:140:ASP:OD2	1:C:191:GLU:HA	2.07	0.55
1:M:206:ALA:HA	1:P:187:TRP:CZ2	2.41	0.55
1:I:214:HIS:CB	1:K:3:LEU:HD13	2.37	0.55
2:F:401:CIT:C6	2:F:401:CIT:O2	2.55	0.54
1:O:60:GLU:OE1	1:O:60:GLU:HA	2.06	0.54
1:I:3:LEU:HD13	1:K:214:HIS:CB	2.37	0.54
1:M:214:HIS:CE1	1:M:224:GLU:HG3	2.42	0.54
1:O:141:ILE:O	1:O:144:TYR:HB3	2.06	0.54
1:O:141:ILE:HG21	1:O:325:ILE:HD11	1.89	0.54
1:K:300:SER:OG	1:K:301:ASP:OD1	2.14	0.54
1:B:82:TYR:CG	1:B:122:ASN:HB3	2.42	0.54
1:B:237:ALA:CB	2:B:401:CIT:O2	2.51	0.54
1:B:265:ASN:ND2	1:B:296:GLN:H	2.06	0.54
1:D:16:HIS:CD2	1:N:223:LYS:HD3	2.42	0.54
1:M:211:LYS:O	1:M:215:PRO:HA	2.07	0.54
1:N:189:LEU:HD22	1:N:290:VAL:HA	1.90	0.54
1:E:111:ARG:HA	1:E:114:ASN:HD22	1.71	0.54
1:I:210:LEU:HG	1:K:3:LEU:HD21	1.90	0.54
1:K:304:LYS:HD2	1:L:9:HIS:HB2	1.89	0.54
1:L:21:LYS:NZ	3:L:502:HOH:O	2.40	0.54
1:I:91:VAL:HG21	1:I:123:VAL:HG13	1.90	0.54
1:A:206:ALA:HA	1:D:187:TRP:CE2	2.43	0.53
1:L:53:MET:HB3	1:L:56:LYS:HB3	1.90	0.53
1:C:103:GLU:OE1	1:C:111:ARG:NH2	2.41	0.53
1:E:60:GLU:OE1	1:E:60:GLU:HA	2.10	0.52
1:E:61:MET:SD	1:E:78:SER:OG	2.66	0.52
1:L:22:ILE:HD12	1:L:44:ALA:HB2	1.89	0.52
1:G:164:LEU:HD23	2:G:401:CIT:O1	2.09	0.52
1:K:179:VAL:HG23	1:K:184:CYS:SG	2.50	0.52
1:K:65:GLN:NE2	1:K:76:ILE:O	2.39	0.52
1:L:247:THR:OG1	2:L:401:CIT:H22	2.09	0.52
1:E:131:LYS:HE3	1:E:296:GLN:O	2.10	0.52
1:G:237:ALA:HB2	2:G:401:CIT:O2	2.10	0.52
1:D:175:GLU:HB2	3:D:502:HOH:O	2.10	0.52
1:F:141:ILE:O	1:F:144:TYR:HB3	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:50:VAL:HG12	1:O:79:GLY:O	2.09	0.51
1:G:14:GLU:HG2	1:G:16:HIS:CD2	2.45	0.51
1:I:3:LEU:HD13	1:K:214:HIS:HB2	1.92	0.51
1:G:279:LEU:HG	1:G:280:TYR:CD1	2.46	0.51
1:I:182:LEU:HD11	1:K:72:ARG:NH1	2.26	0.51
1:N:3:LEU:HD13	1:P:214:HIS:HB2	1.91	0.51
1:O:276:LEU:O	1:O:276:LEU:CG	2.58	0.51
1:F:108:LEU:HD22	1:F:111:ARG:NH2	2.26	0.51
1:D:72:ARG:NH2	3:D:504:HOH:O	2.41	0.51
1:E:277:LYS:NZ	3:E:501:HOH:O	2.32	0.51
1:M:19:GLN:O	1:M:89:LYS:HE3	2.10	0.51
1:E:266:LEU:O	1:H:180:HIS:HB2	2.11	0.51
1:O:11:LEU:CD2	1:P:302:VAL:HG23	2.41	0.51
1:H:275:MET:HB2	1:H:287:PHE:CZ	2.47	0.50
1:I:163:ASN:HA	1:I:271:PRO:HG2	1.92	0.50
1:K:21:LYS:HB3	1:K:88:SER:HA	1.92	0.50
1:K:54:GLU:OE1	1:K:80:LYS:HE3	2.11	0.50
1:O:116:PHE:CD2	1:O:120:ILE:HD11	2.47	0.50
1:A:3:LEU:HD23	1:C:226:TRP:CZ2	2.47	0.50
1:O:164:LEU:HD23	2:O:401:CIT:O1	2.11	0.50
1:A:180:HIS:HB2	1:D:266:LEU:O	2.12	0.50
1:H:21:LYS:HA	1:H:46:GLU:O	2.12	0.50
1:I:262:ILE:HG12	1:I:294:LEU:HD11	1.94	0.50
1:N:141:ILE:HG12	1:N:322:LEU:HD22	1.93	0.50
1:P:200:TRP:HE3	1:P:203:MET:SD	2.34	0.49
1:D:86:ALA:HA	1:D:126:TYR:O	2.12	0.49
1:E:210:LEU:HD21	1:G:7:LEU:HD22	1.94	0.49
1:J:164:LEU:HD23	2:J:401:CIT:O2	2.12	0.49
1:C:97:ALA:HB1	1:C:111:ARG:NH1	2.28	0.49
1:E:58:LYS:HG2	1:G:243:LEU:HD13	1.94	0.49
1:H:176:ARG:NH2	1:H:224:GLU:O	2.46	0.49
1:J:141:ILE:O	1:J:144:TYR:HB3	2.12	0.49
1:N:26:GLY:HA2	1:N:51:ASP:OD2	2.13	0.49
1:N:41:LYS:HD3	1:N:256:ALA:HB1	1.94	0.49
1:P:54:GLU:HG2	1:P:80:LYS:HD3	1.94	0.49
1:H:45:ASP:O	1:H:74:PRO:HD2	2.13	0.49
1:I:217:LEU:HD12	1:I:226:TRP:CG	2.48	0.49
1:N:82:TYR:CG	1:N:122:ASN:HB3	2.47	0.49
1:G:11:LEU:HD11	1:H:302:VAL:HG13	1.94	0.49
1:P:276:LEU:HD12	1:P:288:LEU:HB2	1.95	0.49
1:C:11:LEU:CD1	1:D:302:VAL:HG13	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ARG:HD2	1:C:325:ILE:HD11	1.95	0.48
1:H:247:THR:HG1	2:H:401:CIT:H22	1.77	0.48
1:C:260:GLU:HG3	1:C:264:LYS:HD2	1.95	0.48
1:G:14:GLU:HG2	1:G:16:HIS:NE2	2.28	0.48
1:H:323:TRP:O	1:H:327:LYS:HG3	2.14	0.48
1:O:107:ASN:O	1:O:111:ARG:HG3	2.13	0.48
1:O:310:GLU:O	1:O:313:ALA:HB3	2.13	0.48
1:E:137:ASN:ND2	2:E:401:CIT:C6	2.75	0.48
1:E:140:ASP:HB3	1:E:287:PHE:O	2.13	0.48
1:F:206:ALA:HA	1:G:187:TRP:CE2	2.49	0.48
1:K:301:ASP:HB3	1:L:8:ILE:CG2	2.43	0.48
1:P:168:ARG:NH2	2:P:401:CIT:O2	2.44	0.48
1:A:266:LEU:O	1:D:180:HIS:HB2	2.14	0.48
1:B:127:SER:HB3	1:B:130:CYS:HB3	1.96	0.48
1:G:103:GLU:OE2	1:G:111:ARG:HD3	2.14	0.48
1:O:14:GLU:HB3	1:O:16:HIS:CE1	2.49	0.48
1:M:168:ARG:NH1	2:M:401:CIT:O1	2.47	0.47
1:E:302:VAL:HG23	1:F:11:LEU:CD1	2.43	0.47
1:H:141:ILE:O	1:H:144:TYR:HB3	2.14	0.47
1:M:3:LEU:HA	1:M:6:GLN:NE2	2.29	0.47
1:D:188:ILE:O	1:D:189:LEU:HD23	2.14	0.47
1:I:20:ASN:O	1:I:44:ALA:HA	2.15	0.47
1:K:265:ASN:HB2	1:K:296:GLN:HB3	1.96	0.47
1:O:10:ASN:HA	1:P:301:ASP:OD2	2.13	0.47
1:D:245:GLY:O	1:H:102:GLY:HA2	2.15	0.47
1:I:137:ASN:ND2	2:I:401:CIT:O4	2.48	0.47
1:D:13:LYS:O	1:D:13:LYS:HG3	2.14	0.47
1:N:141:ILE:CG1	1:N:322:LEU:HD22	2.45	0.47
1:D:36:ILE:O	1:D:40:MET:HG3	2.15	0.47
1:E:302:VAL:CG2	1:F:11:LEU:HD11	2.44	0.47
1:I:180:HIS:HB2	1:L:266:LEU:O	2.15	0.47
1:L:89:LYS:O	1:L:131:LYS:HE2	2.15	0.47
1:L:279:LEU:HD13	1:L:302:VAL:HG21	1.96	0.47
1:L:276:LEU:HD21	1:L:288:LEU:HB2	1.97	0.47
1:C:164:LEU:HD22	1:C:251:ILE:HA	1.96	0.47
1:N:54:GLU:HA	1:N:80:LYS:HD2	1.97	0.47
1:A:55:ASP:O	1:C:243:LEU:HB3	2.15	0.47
1:E:179:VAL:HG22	1:E:184:CYS:SG	2.54	0.47
1:F:198:PRO:HD3	1:F:230:HIS:CE1	2.50	0.47
1:H:60:GLU:OE1	1:H:60:GLU:HA	2.14	0.47
1:I:206:ALA:HA	1:L:187:TRP:CZ2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:216:GLU:O	1:N:222:ASP:HB2	2.13	0.46
1:J:176:ARG:NH1	1:J:224:GLU:O	2.38	0.46
1:C:137:ASN:ND2	2:C:401:CIT:C6	2.77	0.46
1:F:276:LEU:HD13	1:F:276:LEU:O	2.16	0.46
1:M:304:LYS:HD2	1:N:9:HIS:HB2	1.96	0.46
1:N:291:PRO:HB2	1:N:303:VAL:HB	1.97	0.46
1:I:16:HIS:NE2	1:J:265:ASN:ND2	2.63	0.46
1:I:194:ASP:HA	1:I:234:VAL:HG11	1.98	0.46
1:H:23:THR:HA	1:H:48:ALA:O	2.15	0.46
1:N:168:ARG:HH22	2:N:401:CIT:C1	2.28	0.46
1:A:276:LEU:HD23	1:A:282:ILE:HD12	1.97	0.46
1:J:66:HIS:CE1	1:L:236:SER:HB2	2.51	0.46
1:B:179:VAL:CG2	1:B:184:CYS:SG	3.04	0.46
1:D:144:TYR:HA	1:D:287:PHE:CE2	2.51	0.46
1:O:20:ASN:O	1:O:44:ALA:HA	2.16	0.46
1:B:292:CYS:HB3	1:B:299:ILE:HG23	1.98	0.46
1:E:25:VAL:HG22	1:E:50:VAL:CG1	2.46	0.46
1:G:173:MET:HE1	1:G:186:GLY:HA3	1.98	0.46
1:A:113:VAL:O	1:A:117:LYS:HG3	2.17	0.45
1:C:48:ALA:HA	1:C:77:VAL:O	2.16	0.45
1:D:89:LYS:O	1:D:131:LYS:HE2	2.16	0.45
1:P:120:ILE:HB	1:P:121:PRO:HD3	1.98	0.45
1:B:265:ASN:HD22	1:B:296:GLN:N	2.11	0.45
1:B:141:ILE:O	1:B:144:TYR:HB3	2.16	0.45
1:O:27:VAL:HG22	1:O:51:ASP:CB	2.46	0.45
1:O:141:ILE:CG2	1:O:325:ILE:HD11	2.45	0.45
1:P:123:VAL:HG11	1:P:132:LEU:HD21	1.99	0.45
1:D:23:THR:HA	1:D:48:ALA:O	2.17	0.45
1:I:48:ALA:HA	1:I:77:VAL:O	2.17	0.45
1:J:21:LYS:HA	1:J:46:GLU:O	2.16	0.45
1:K:141:ILE:CG1	1:K:322:LEU:HD22	2.46	0.45
1:E:179:VAL:CG2	1:E:184:CYS:SG	3.05	0.45
1:E:304:LYS:NZ	1:F:5:ASP:O	2.49	0.45
1:N:187:TRP:CE2	1:O:206:ALA:HA	2.52	0.45
1:E:304:LYS:HD2	1:F:9:HIS:HB2	1.99	0.45
1:N:137:ASN:HD21	2:N:401:CIT:C6	2.29	0.45
1:F:50:VAL:HG11	1:F:82:TYR:CZ	2.51	0.45
1:P:137:ASN:HD21	2:P:401:CIT:C6	2.30	0.45
1:G:14:GLU:HB3	1:G:16:HIS:CD2	2.51	0.45
1:H:113:VAL:HG22	1:H:145:VAL:HG21	1.99	0.45
1:I:264:LYS:HE2	1:J:42:ASP:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:204:ASN:HB2	1:L:208:VAL:O	2.17	0.45
2:I:401:CIT:O2	2:I:401:CIT:C6	2.64	0.44
1:L:255:VAL:O	1:L:258:LEU:HB2	2.17	0.44
1:N:141:ILE:O	1:N:144:TYR:HB3	2.18	0.44
1:N:144:TYR:CD2	1:N:326:GLN:HG2	2.53	0.44
1:P:49:LEU:O	1:P:78:SER:HA	2.17	0.44
1:P:109:VAL:O	1:P:113:VAL:HG23	2.17	0.44
1:O:265:ASN:HD21	1:P:16:HIS:CD2	2.36	0.44
1:A:274:THR:O	1:A:287:PHE:HA	2.18	0.44
1:M:180:HIS:HB2	1:P:266:LEU:O	2.17	0.44
1:O:120:ILE:CD1	1:O:146:ALA:HA	2.44	0.44
1:I:204:ASN:HA	1:I:210:LEU:HD13	1.98	0.44
1:I:247:THR:CG2	3:K:507:HOH:O	2.63	0.44
1:J:85:THR:O	1:J:88:SER:OG	2.34	0.44
1:O:8:ILE:CG2	1:P:301:ASP:HB3	2.48	0.44
1:K:284:GLU:HG3	1:K:323:TRP:CD2	2.53	0.44
1:P:118:PHE:O	1:P:122:ASN:ND2	2.42	0.44
1:C:11:LEU:HD22	1:D:154:LYS:HE3	1.98	0.44
1:C:50:VAL:HG12	1:C:79:GLY:O	2.18	0.44
1:C:301:ASP:HB3	1:D:8:ILE:CG2	2.48	0.44
1:G:141:ILE:HG13	1:G:322:LEU:HD22	2.00	0.43
1:L:225:GLN:HB3	1:L:228:GLN:HG2	1.99	0.43
1:G:304:LYS:HD2	1:H:9:HIS:HB2	2.00	0.43
1:K:22:ILE:O	1:K:47:LEU:HA	2.18	0.43
1:F:291:PRO:HB2	1:F:303:VAL:HB	1.99	0.43
1:K:26:GLY:O	1:K:31:GLY:HA3	2.17	0.43
1:N:103:GLU:OE2	1:N:111:ARG:HD3	2.18	0.43
1:G:291:PRO:HB2	1:G:303:VAL:HB	2.00	0.43
1:K:89:LYS:O	1:K:131:LYS:HE2	2.18	0.43
1:O:116:PHE:CD2	1:O:120:ILE:CD1	3.01	0.43
1:A:13:LYS:O	1:A:15:GLU:N	2.51	0.43
1:E:24:VAL:HG11	1:E:31:GLY:O	2.18	0.43
1:L:86:ALA:HA	1:L:126:TYR:O	2.18	0.43
1:B:121:PRO:HB3	1:J:13:LYS:HB3	2.00	0.43
1:B:163:ASN:HA	1:B:271:PRO:HG2	2.00	0.43
1:D:280:TYR:CE1	1:D:290:VAL:HG11	2.54	0.43
1:H:231:LYS:HA	1:H:231:LYS:HE2	2.00	0.43
1:M:136:SER:O	1:M:139:VAL:HA	2.19	0.43
1:G:293:VAL:HB	1:G:301:ASP:HB2	2.00	0.43
1:O:173:MET:HG3	1:O:226:TRP:HZ3	1.84	0.43
1:K:159:GLY:HA3	1:K:273:SER:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:19:GLN:HG2	1:N:296:GLN:OE1	2.19	0.42
1:M:127:SER:HB3	1:M:130:CYS:HB3	2.01	0.42
1:P:109:VAL:CG2	1:P:141:ILE:HG21	2.48	0.42
1:A:307:LEU:HD22	1:A:311:GLU:HB3	2.01	0.42
1:M:248:SER:HB3	1:M:249:TRP:H	1.64	0.42
1:C:179:VAL:HG23	1:C:184:CYS:SG	2.59	0.42
1:J:213:LEU:HD21	1:L:6:GLN:CB	2.49	0.42
1:L:164:LEU:HD23	2:L:401:CIT:O2	2.19	0.42
1:O:254:SER:O	1:O:257:ASP:HB3	2.19	0.42
1:O:272:ILE:O	1:O:289:SER:HA	2.18	0.42
1:C:120:ILE:HB	1:C:121:PRO:HD3	2.02	0.42
1:F:91:VAL:HG21	1:F:123:VAL:HG13	2.01	0.42
1:F:206:ALA:HA	1:G:187:TRP:CZ2	2.54	0.42
1:G:141:ILE:CG1	1:G:322:LEU:HD22	2.48	0.42
1:H:124:VAL:HG22	1:H:152:PHE:CZ	2.54	0.42
1:L:168:ARG:NH2	2:L:401:CIT:O2	2.51	0.42
1:C:166:SER:O	1:C:170:ARG:HG3	2.20	0.42
1:F:214:HIS:HB2	1:H:3:LEU:HD13	2.01	0.42
1:L:103:GLU:OE2	1:L:111:ARG:HD3	2.18	0.42
1:N:213:LEU:HD21	1:P:6:GLN:O	2.20	0.42
1:B:108:LEU:C	1:B:108:LEU:HD13	2.40	0.42
1:D:216:GLU:HG3	1:D:222:ASP:HA	2.01	0.42
1:E:200:TRP:HB3	1:E:217:LEU:HD23	2.00	0.42
1:I:109:VAL:N	3:I:505:HOH:O	2.52	0.42
1:J:141:ILE:HG13	1:J:322:LEU:HD22	2.00	0.42
1:J:165:ASP:OD1	1:J:192:HIS:ND1	2.51	0.42
1:K:120:ILE:O	1:K:124:VAL:HG23	2.20	0.42
1:P:274:THR:HB	1:P:299:ILE:HD13	2.02	0.42
1:D:114:ASN:HA	1:D:117:LYS:HE3	2.02	0.42
1:F:48:ALA:HA	1:F:77:VAL:O	2.19	0.42
1:G:164:LEU:HD11	1:G:250:ALA:HB1	2.02	0.42
1:G:276:LEU:O	1:G:276:LEU:HG	2.19	0.42
1:G:276:LEU:HD23	1:G:276:LEU:H	1.84	0.42
1:J:131:LYS:N	1:J:131:LYS:HD3	2.35	0.42
1:M:189:LEU:HD22	1:M:290:VAL:HA	2.02	0.42
1:L:41:LYS:HE3	1:L:43:LEU:HD11	2.02	0.41
1:N:159:GLY:HA3	1:N:273:SER:HB3	2.01	0.41
1:O:260:GLU:HG2	1:O:264:LYS:HD2	2.02	0.41
1:E:117:LYS:HD2	1:E:331:PHE:OXT	2.21	0.41
1:M:71:LEU:O	1:M:72:ARG:HD2	2.20	0.41
1:O:144:TYR:CD2	1:O:326:GLN:HG2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:THR:O	1:D:127:SER:OG	2.37	0.41
1:F:13:LYS:HA	1:F:13:LYS:HD3	1.76	0.41
1:H:22:ILE:HD11	1:H:263:MET:HG3	2.02	0.41
1:H:173:MET:HE1	1:H:186:GLY:HA3	2.01	0.41
1:N:130:CYS:O	1:N:156:ARG:NH1	2.47	0.41
1:D:176:ARG:NH2	1:D:224:GLU:O	2.48	0.41
1:H:97:ALA:N	1:H:112:ASN:OD1	2.49	0.41
1:I:75:LYS:HD2	1:I:75:LYS:HA	1.92	0.41
1:K:269:VAL:HA	1:K:292:CYS:O	2.20	0.41
1:M:247:THR:OG1	2:M:401:CIT:H22	2.20	0.41
1:C:86:ALA:HA	1:C:126:TYR:O	2.21	0.41
1:J:97:ALA:HB1	1:J:111:ARG:NH1	2.35	0.41
1:N:259:ALA:O	1:N:263:MET:HG2	2.20	0.41
1:L:201:SER:HA	1:L:211:LYS:HD3	2.02	0.41
2:C:401:CIT:C6	2:C:401:CIT:O2	2.69	0.41
1:H:49:LEU:O	1:H:78:SER:HA	2.20	0.41
1:H:114:ASN:HA	1:H:117:LYS:HG2	2.03	0.41
1:H:276:LEU:CD2	1:H:288:LEU:HB2	2.51	0.41
1:P:106:LEU:O	1:P:109:VAL:HG12	2.21	0.41
1:B:189:LEU:HD22	1:B:290:VAL:HA	2.02	0.41
1:D:172:LEU:O	1:D:175:GLU:CG	2.67	0.41
1:E:111:ARG:HA	1:E:114:ASN:ND2	2.35	0.41
1:F:249:TRP:HZ2	1:H:32:MET:HB3	1.86	0.41
1:N:188:ILE:CD1	1:N:233:VAL:HG11	2.51	0.41
1:B:52:VAL:HG12	1:B:80:LYS:HE2	2.04	0.41
1:D:73:THR:HA	1:D:74:PRO:HD2	1.99	0.41
1:K:237:ALA:O	1:K:241:ILE:HG13	2.21	0.41
1:C:265:ASN:HB2	1:C:296:GLN:HB3	2.02	0.40
1:E:25:VAL:HG22	1:E:50:VAL:HG13	2.03	0.40
1:M:243:LEU:HB3	1:O:55:ASP:O	2.21	0.40
1:A:304:LYS:NZ	1:B:5:ASP:O	2.54	0.40
1:N:276:LEU:HD22	1:N:288:LEU:HB2	2.03	0.40
1:B:72:ARG:NH2	3:B:505:HOH:O	2.50	0.40
1:B:312:GLU:O	1:B:316:LYS:HG3	2.22	0.40
1:C:179:VAL:CG2	1:C:184:CYS:SG	3.10	0.40
1:C:274:THR:HB	1:C:299:ILE:HD13	2.04	0.40
1:O:127:SER:HB3	1:O:130:CYS:HB3	2.02	0.40
1:L:92:ILE:HA	1:L:133:LEU:O	2.22	0.40
1:O:36:ILE:HD12	1:O:36:ILE:HA	1.96	0.40
1:A:48:ALA:HA	1:A:77:VAL:O	2.21	0.40
1:E:36:ILE:HD12	1:E:36:ILE:HA	1.98	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:401:CIT:O2	2:E:401:CIT:O5	2.39	0.40
1:G:141:ILE:O	1:G:144:TYR:HB3	2.21	0.40
1:J:172:LEU:HD12	1:J:233:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	316/332 (95%)	304 (96%)	11 (4%)	1 (0%)	41	64
1	B	318/332 (96%)	307 (96%)	11 (4%)	0	100	100
1	C	323/332 (97%)	308 (95%)	15 (5%)	0	100	100
1	D	329/332 (99%)	311 (94%)	17 (5%)	1 (0%)	41	64
1	E	316/332 (95%)	303 (96%)	12 (4%)	1 (0%)	41	64
1	F	318/332 (96%)	302 (95%)	16 (5%)	0	100	100
1	G	329/332 (99%)	320 (97%)	9 (3%)	0	100	100
1	H	328/332 (99%)	310 (94%)	18 (6%)	0	100	100
1	I	316/332 (95%)	303 (96%)	13 (4%)	0	100	100
1	J	313/332 (94%)	305 (97%)	8 (3%)	0	100	100
1	K	328/332 (99%)	311 (95%)	16 (5%)	1 (0%)	41	64
1	L	329/332 (99%)	313 (95%)	15 (5%)	1 (0%)	41	64
1	M	329/332 (99%)	315 (96%)	13 (4%)	1 (0%)	41	64
1	N	329/332 (99%)	318 (97%)	11 (3%)	0	100	100
1	O	329/332 (99%)	317 (96%)	12 (4%)	0	100	100
1	P	321/332 (97%)	305 (95%)	15 (5%)	1 (0%)	41	64
All	All	5171/5312 (97%)	4952 (96%)	212 (4%)	7 (0%)	51	75

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	E	285	ASP
1	D	222	ASP
1	M	15	GLU
1	K	222	ASP
1	P	222	ASP
1	L	222	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/285 (96%)	266 (97%)	8 (3%)	42	68
1	B	276/285 (97%)	271 (98%)	5 (2%)	59	80
1	C	281/285 (99%)	276 (98%)	5 (2%)	59	80
1	D	284/285 (100%)	275 (97%)	9 (3%)	39	65
1	E	274/285 (96%)	263 (96%)	11 (4%)	31	57
1	F	276/285 (97%)	264 (96%)	12 (4%)	29	54
1	G	284/285 (100%)	279 (98%)	5 (2%)	59	80
1	H	284/285 (100%)	273 (96%)	11 (4%)	32	58
1	I	274/285 (96%)	267 (97%)	7 (3%)	46	72
1	J	273/285 (96%)	264 (97%)	9 (3%)	38	64
1	K	284/285 (100%)	273 (96%)	11 (4%)	32	58
1	L	284/285 (100%)	277 (98%)	7 (2%)	47	73
1	M	284/285 (100%)	271 (95%)	13 (5%)	27	51
1	N	284/285 (100%)	275 (97%)	9 (3%)	39	65
1	O	284/285 (100%)	278 (98%)	6 (2%)	53	77
1	P	279/285 (98%)	266 (95%)	13 (5%)	26	50
All	All	4479/4560 (98%)	4338 (97%)	141 (3%)	40	66

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	50	VAL
1	A	83	SER
1	A	133	LEU
1	A	247	THR
1	A	309	SER
1	A	314	HIS
1	A	327	LYS
1	B	107	ASN
1	B	136	SER
1	B	148	LYS
1	B	213	LEU
1	B	242	LYS
1	C	72	ARG
1	C	194	ASP
1	C	254	SER
1	C	276	LEU
1	C	309	SER
1	D	15	GLU
1	D	160	SER
1	D	194	ASP
1	D	223	LYS
1	D	231	LYS
1	D	276	LEU
1	D	300	SER
1	D	301	ASP
1	D	317	LYS
1	E	53	MET
1	E	75	LYS
1	E	80	LYS
1	E	131	LYS
1	E	133	LEU
1	E	136	SER
1	E	160	SER
1	E	217	LEU
1	E	239	GLU
1	E	296	GLN
1	E	316	LYS
1	F	80	LYS
1	F	107	ASN
1	F	192	HIS
1	F	201	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	217	LEU
1	F	224	GLU
1	F	236	SER
1	F	254	SER
1	F	273	SER
1	F	276	LEU
1	F	310	GLU
1	F	315	LEU
1	G	16	HIS
1	G	176	ARG
1	G	254	SER
1	G	283	LYS
1	G	315	LEU
1	H	11	LEU
1	H	12	LEU
1	H	14	GLU
1	H	15	GLU
1	H	55	ASP
1	H	72	ARG
1	H	80	LYS
1	H	213	LEU
1	H	236	SER
1	H	276	LEU
1	H	301	ASP
1	I	117	LYS
1	I	131	LYS
1	I	160	SER
1	I	231	LYS
1	I	248	SER
1	I	254	SER
1	I	327	LYS
1	J	12	LEU
1	J	17	VAL
1	J	72	ARG
1	J	88	SER
1	J	213	LEU
1	J	220	ASP
1	J	231	LYS
1	J	247	THR
1	J	276	LEU
1	K	87	ASN
1	K	194	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	201	SER
1	K	216	GLU
1	K	247	THR
1	K	254	SER
1	K	273	SER
1	K	276	LEU
1	K	284	GLU
1	K	312	GLU
1	K	330	GLN
1	L	12	LEU
1	L	54	GLU
1	L	98	ARG
1	L	105	ARG
1	L	108	LEU
1	L	273	SER
1	L	276	LEU
1	M	11	LEU
1	M	98	ARG
1	M	105	ARG
1	M	175	GLU
1	M	179	VAL
1	M	216	GLU
1	M	248	SER
1	M	277	LYS
1	M	309	SER
1	M	314	HIS
1	M	315	LEU
1	M	317	LYS
1	M	320	ASP
1	N	80	LYS
1	N	108	LEU
1	N	148	LYS
1	N	194	ASP
1	N	231	LYS
1	N	309	SER
1	N	314	HIS
1	N	318	SER
1	N	321	THR
1	O	83	SER
1	O	195	SER
1	O	231	LYS
1	O	236	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	O	276	LEU
1	O	317	LYS
1	P	13	LYS
1	P	14	GLU
1	P	50	VAL
1	P	72	ARG
1	P	80	LYS
1	P	136	SER
1	P	196	SER
1	P	223	LYS
1	P	227	LYS
1	P	236	SER
1	P	247	THR
1	P	276	LEU
1	P	312	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	137	ASN
1	E	122	ASN
1	F	137	ASN
1	H	137	ASN
1	H	163	ASN
1	I	297	ASN
1	J	137	ASN
1	J	265	ASN
1	K	6	GLN
1	K	232	GLN
1	K	330	GLN
1	L	137	ASN
1	N	137	ASN
1	P	20	ASN
1	P	297	ASN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

16 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	N	401	-	3,12,12	0.64	0	3,17,17	0.77	0
2	CIT	F	401	-	3,12,12	0.64	0	3,17,17	0.87	0
2	CIT	C	401	-	3,12,12	0.65	0	3,17,17	1.05	0
2	CIT	K	401	-	3,12,12	0.63	0	3,17,17	0.63	0
2	CIT	E	401	-	3,12,12	0.56	0	3,17,17	0.32	0
2	CIT	I	401	-	3,12,12	0.75	0	3,17,17	0.31	0
2	CIT	L	401	-	3,12,12	0.77	0	3,17,17	0.47	0
2	CIT	G	401	-	3,12,12	0.70	0	3,17,17	1.05	0
2	CIT	B	401	-	3,12,12	0.57	0	3,17,17	0.63	0
2	CIT	P	401	-	3,12,12	0.60	0	3,17,17	0.46	0
2	CIT	H	401	-	3,12,12	0.76	0	3,17,17	1.15	0
2	CIT	D	401	-	3,12,12	0.85	0	3,17,17	0.65	0
2	CIT	J	401	-	3,12,12	0.47	0	3,17,17	0.78	0
2	CIT	O	401	-	3,12,12	0.55	0	3,17,17	0.65	0
2	CIT	A	401	-	3,12,12	0.63	0	3,17,17	0.56	0
2	CIT	M	401	-	3,12,12	0.78	0	3,17,17	0.59	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	N	401	-	-	1/6/16/16	-
2	CIT	F	401	-	-	2/6/16/16	-
2	CIT	C	401	-	-	1/6/16/16	-
2	CIT	K	401	-	-	2/6/16/16	-
2	CIT	E	401	-	-	3/6/16/16	-
2	CIT	I	401	-	-	3/6/16/16	-
2	CIT	L	401	-	-	3/6/16/16	-
2	CIT	G	401	-	-	3/6/16/16	-
2	CIT	B	401	-	-	1/6/16/16	-
2	CIT	P	401	-	-	1/6/16/16	-
2	CIT	H	401	-	-	0/6/16/16	-
2	CIT	D	401	-	-	0/6/16/16	-
2	CIT	J	401	-	-	3/6/16/16	-
2	CIT	O	401	-	-	3/6/16/16	-
2	CIT	A	401	-	-	4/6/16/16	-
2	CIT	M	401	-	-	3/6/16/16	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	CIT	C1-C2-C3-C6
2	E	401	CIT	C1-C2-C3-C6
2	F	401	CIT	C1-C2-C3-C6
2	G	401	CIT	C1-C2-C3-C6
2	I	401	CIT	C1-C2-C3-C6
2	J	401	CIT	C1-C2-C3-C6
2	L	401	CIT	C1-C2-C3-C6
2	M	401	CIT	C6-C3-C4-C5
2	O	401	CIT	C1-C2-C3-C6
2	E	401	CIT	C1-C2-C3-O7
2	I	401	CIT	C1-C2-C3-O7
2	L	401	CIT	C1-C2-C3-O7
2	O	401	CIT	C1-C2-C3-O7
2	A	401	CIT	C1-C2-C3-O7
2	I	401	CIT	C1-C2-C3-C4
2	J	401	CIT	C1-C2-C3-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	L	401	CIT	C1-C2-C3-C4
2	M	401	CIT	C2-C3-C4-C5
2	M	401	CIT	O7-C3-C4-C5
2	O	401	CIT	C1-C2-C3-C4
2	A	401	CIT	C1-C2-C3-C4
2	E	401	CIT	C1-C2-C3-C4
2	A	401	CIT	C6-C3-C4-C5
2	B	401	CIT	C1-C2-C3-C6
2	C	401	CIT	C6-C3-C4-C5
2	G	401	CIT	C6-C3-C4-C5
2	K	401	CIT	C1-C2-C3-C6
2	N	401	CIT	C1-C2-C3-C6
2	P	401	CIT	C1-C2-C3-C6
2	F	401	CIT	C1-C2-C3-O7
2	K	401	CIT	C1-C2-C3-O7
2	J	401	CIT	C1-C2-C3-C4
2	G	401	CIT	C1-C2-C3-O7

There are no ring outliers.

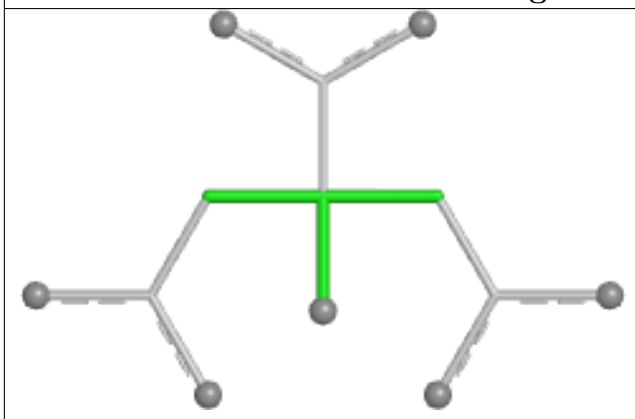
15 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	401	CIT	3	0
2	F	401	CIT	3	0
2	C	401	CIT	3	0
2	E	401	CIT	3	0
2	I	401	CIT	2	0
2	L	401	CIT	4	0
2	G	401	CIT	3	0
2	B	401	CIT	2	0
2	P	401	CIT	2	0
2	H	401	CIT	2	0
2	D	401	CIT	3	0
2	J	401	CIT	3	0
2	O	401	CIT	1	0
2	A	401	CIT	2	0
2	M	401	CIT	3	0

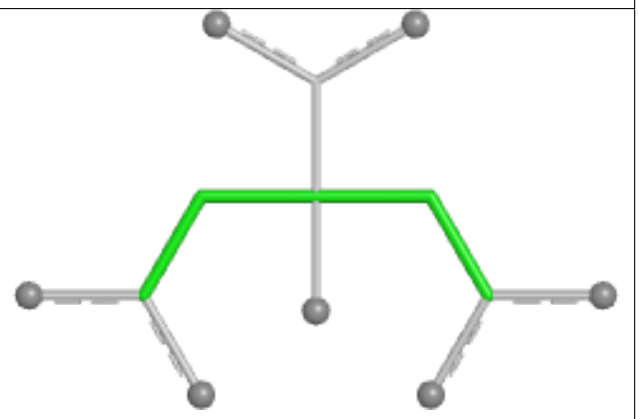
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

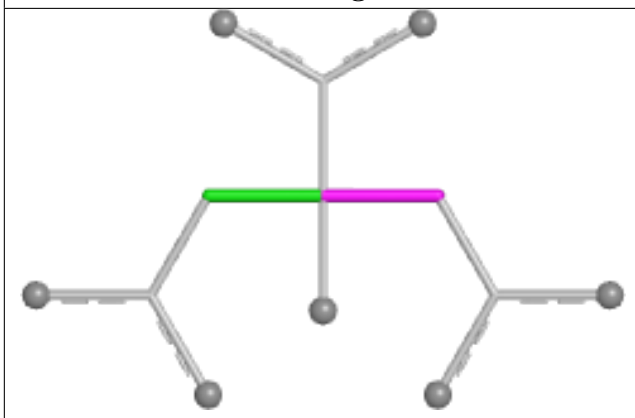
Ligand CIT N 401



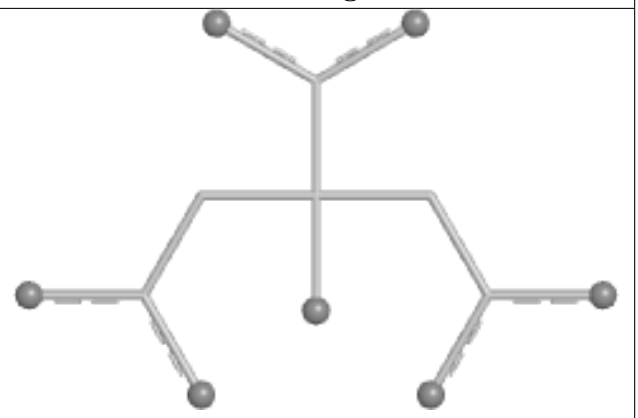
Bond lengths



Bond angles

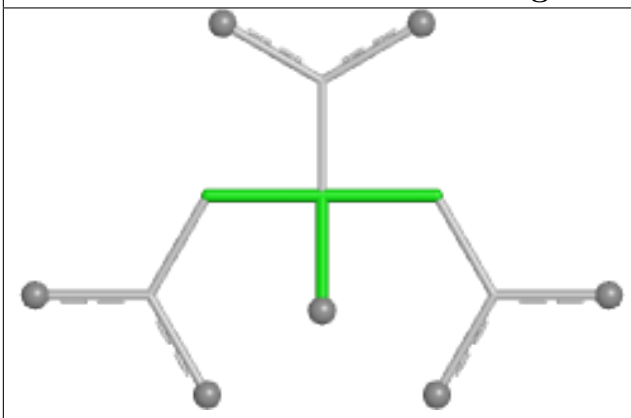


Torsions

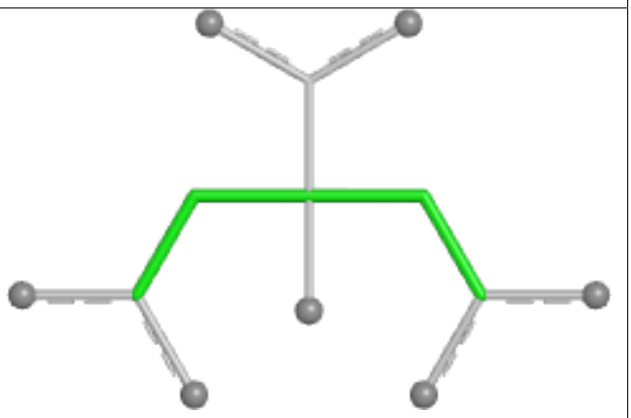


Rings

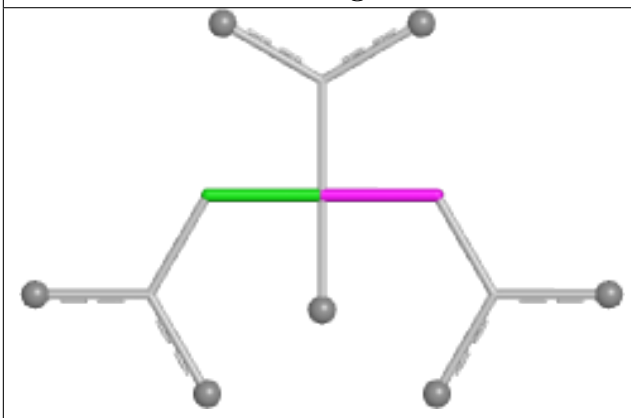
Ligand CIT F 401



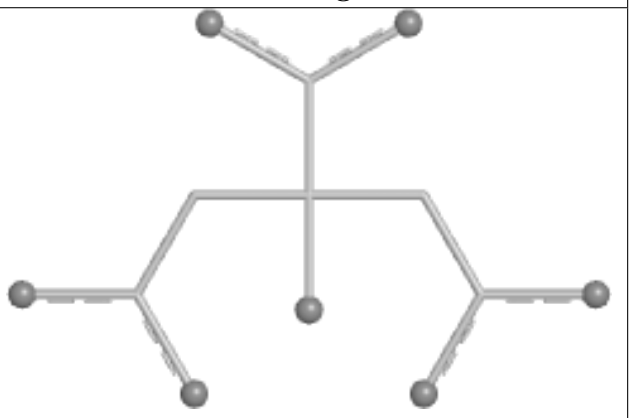
Bond lengths



Bond angles

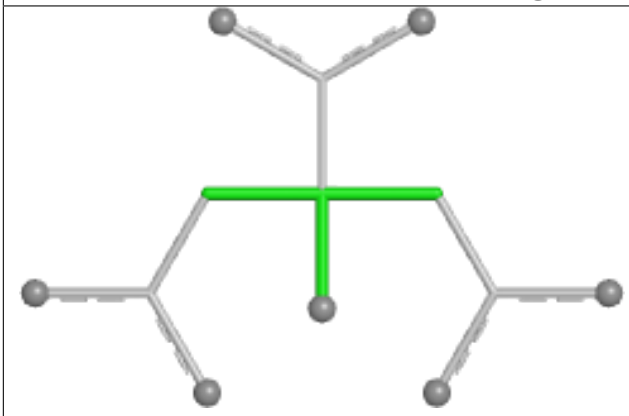


Torsions

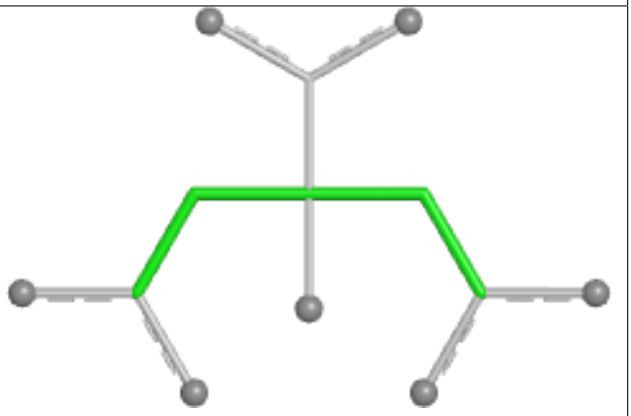


Rings

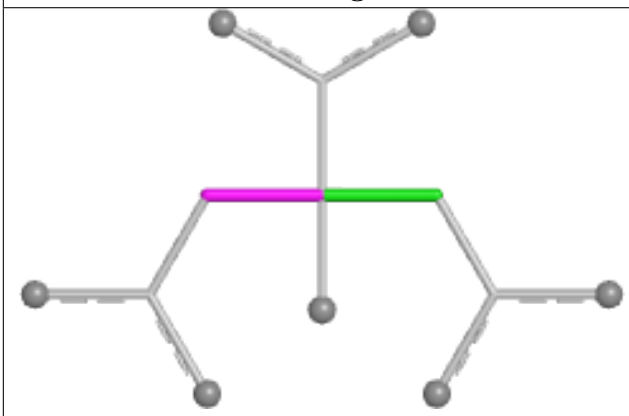
Ligand CIT C 401



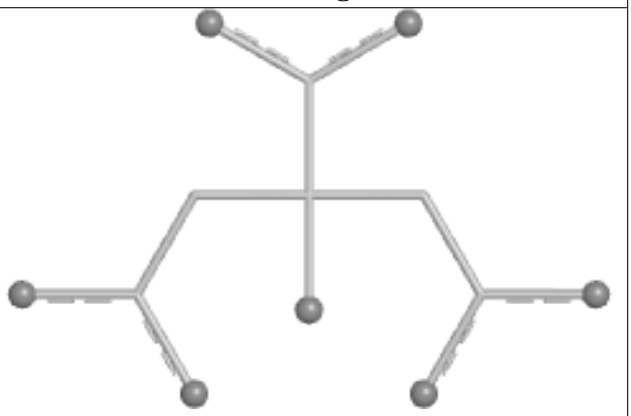
Bond lengths



Bond angles

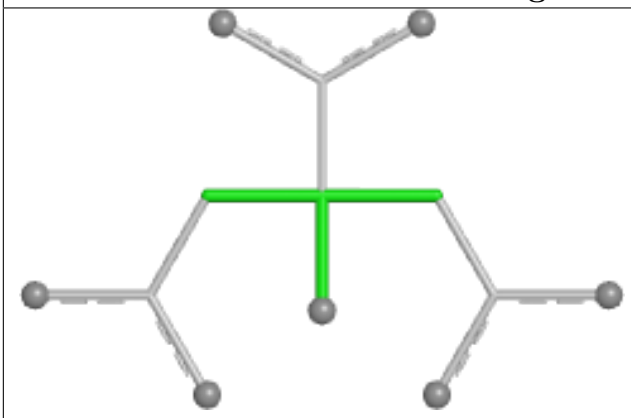


Torsions

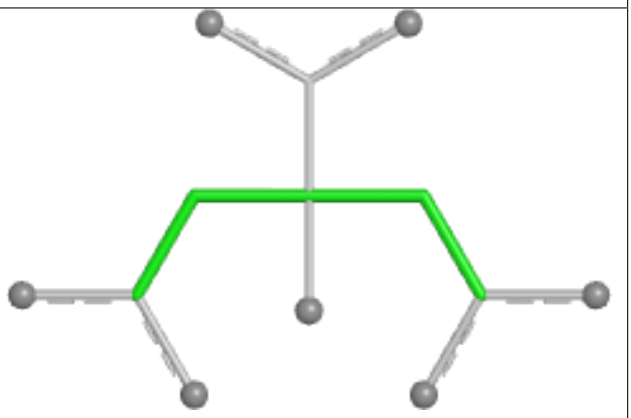


Rings

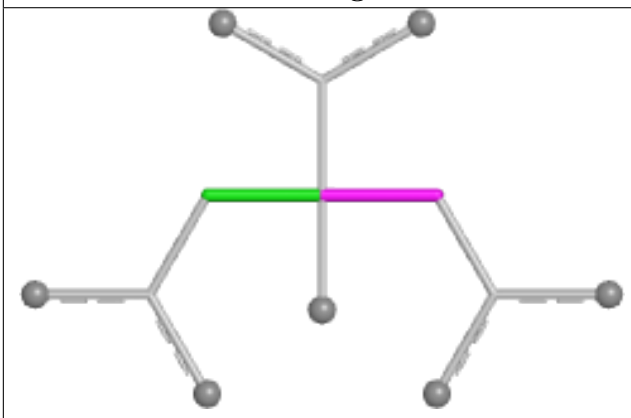
Ligand CIT K 401



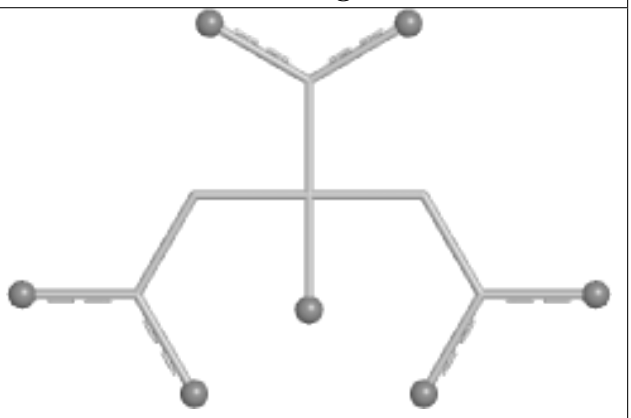
Bond lengths



Bond angles

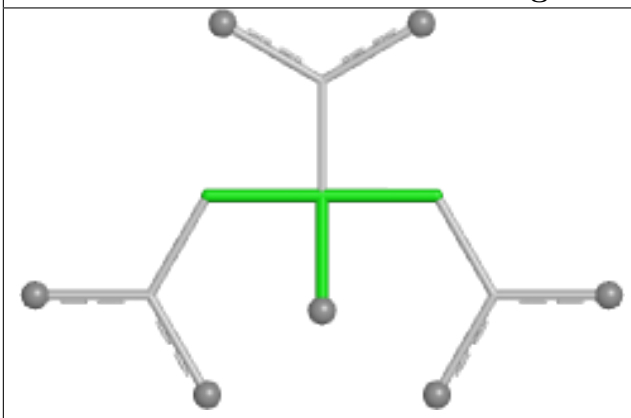


Torsions

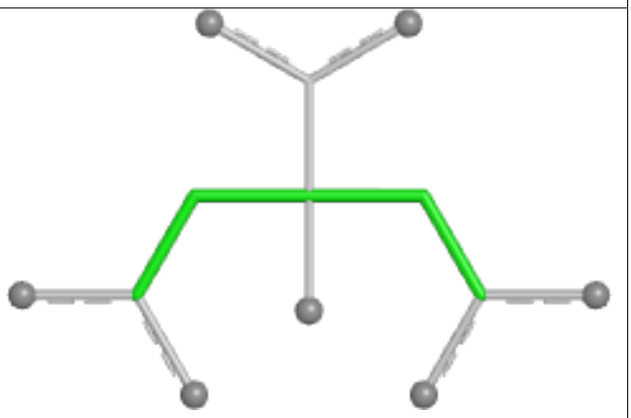


Rings

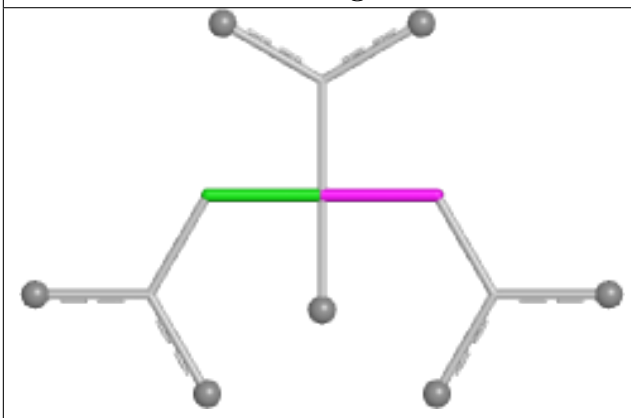
Ligand CIT E 401



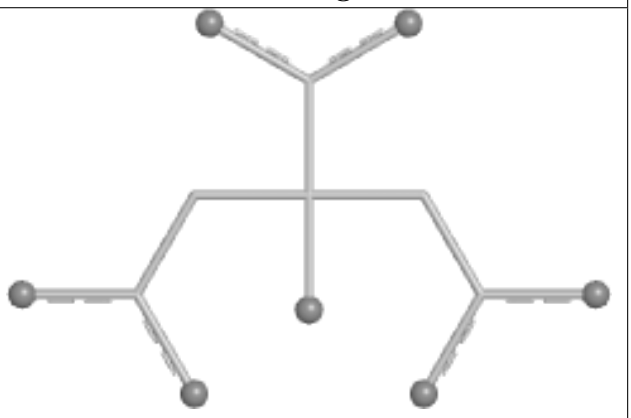
Bond lengths



Bond angles

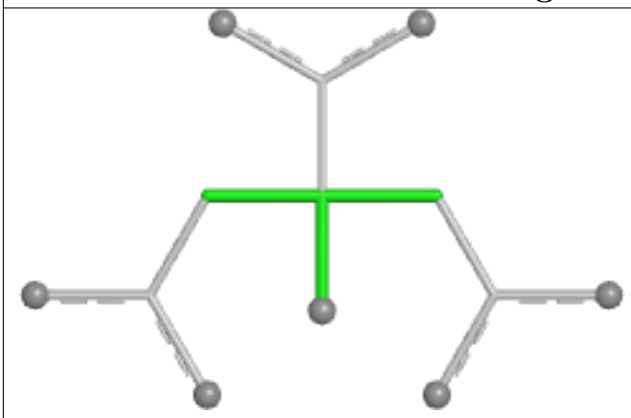


Torsions

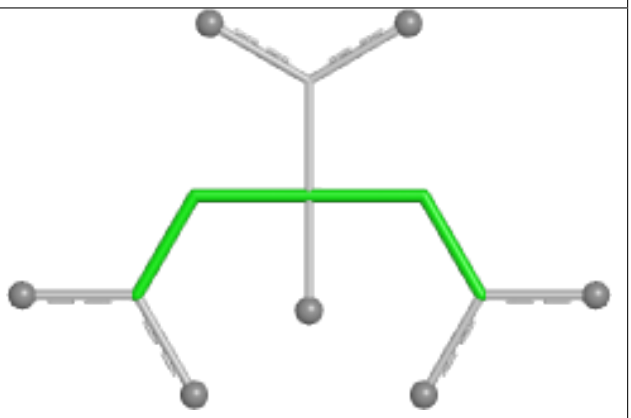


Rings

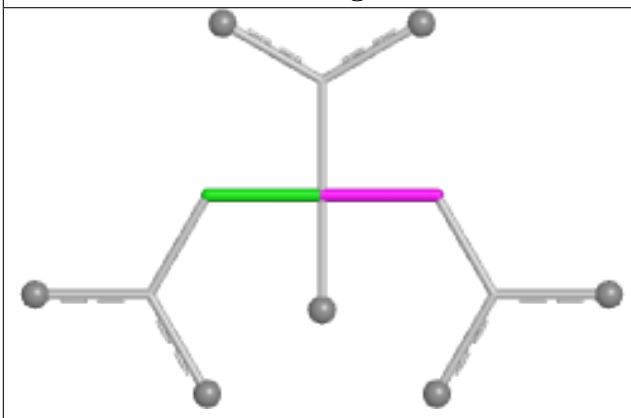
Ligand CIT I 401



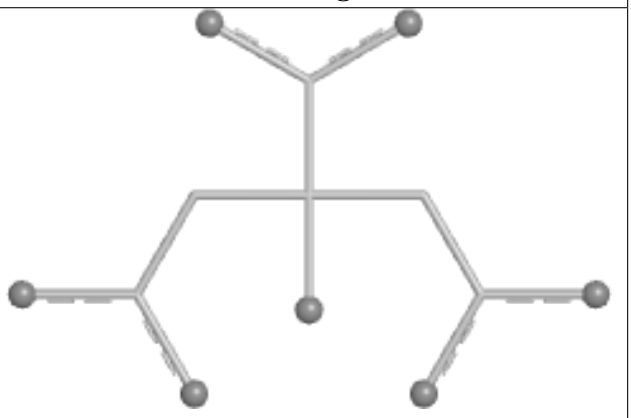
Bond lengths



Bond angles

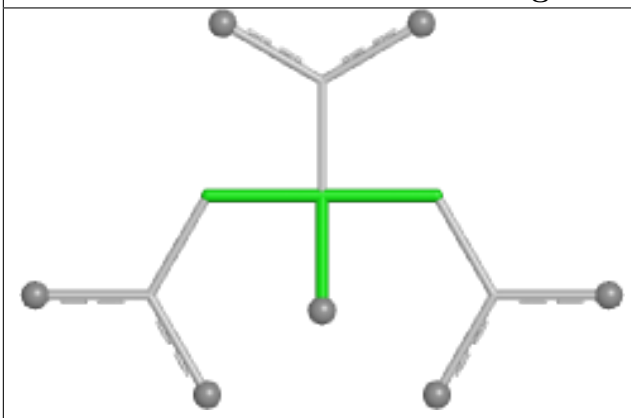


Torsions

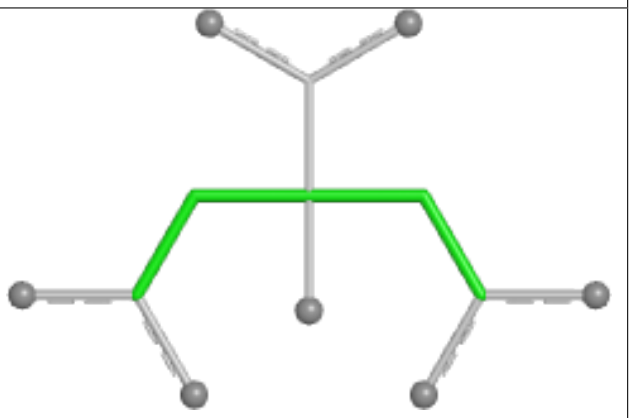


Rings

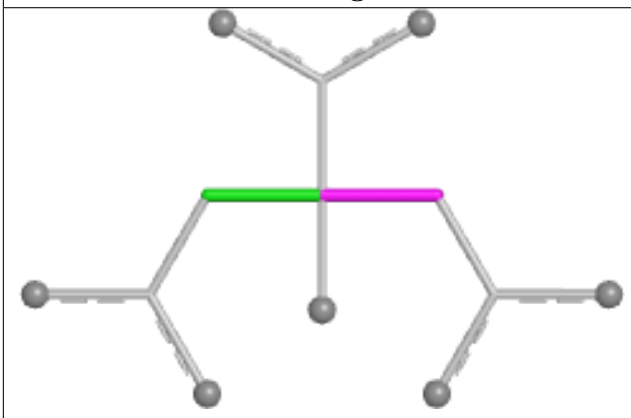
Ligand CIT L 401



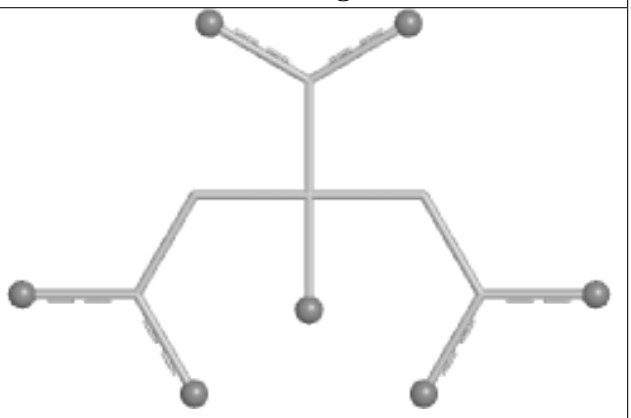
Bond lengths



Bond angles

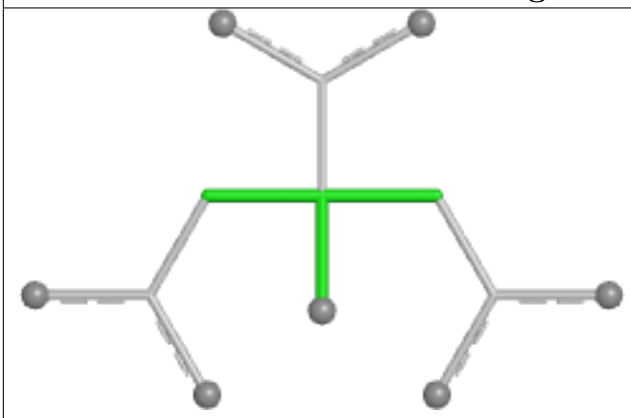


Torsions

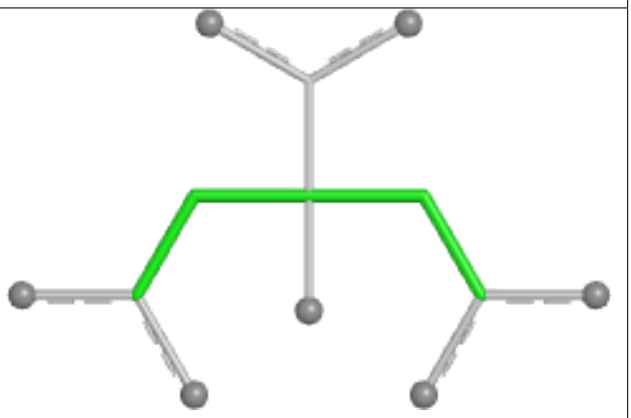


Rings

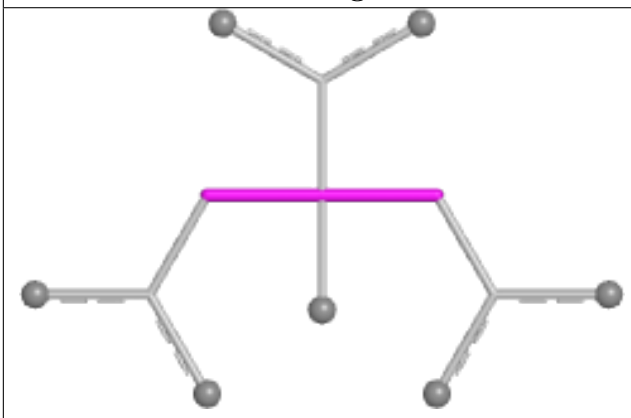
Ligand CIT G 401



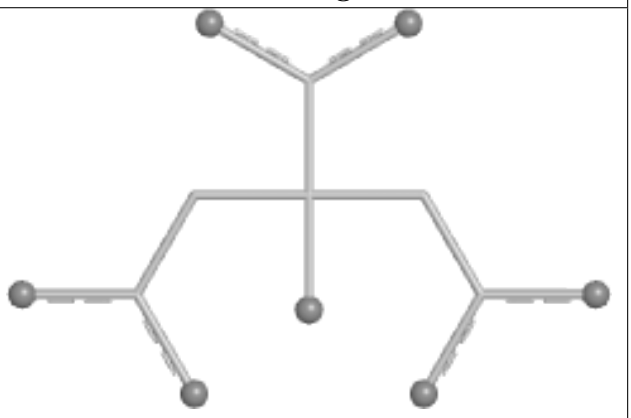
Bond lengths



Bond angles

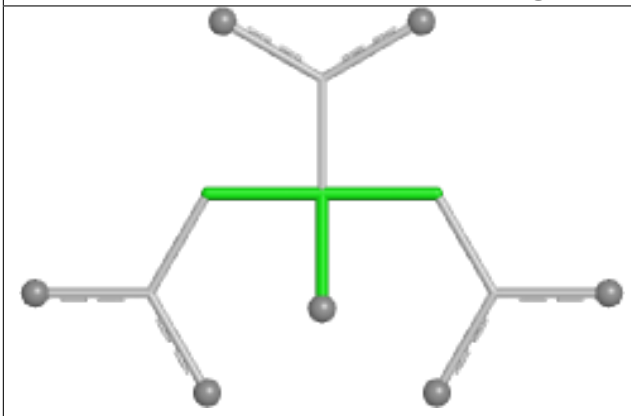


Torsions

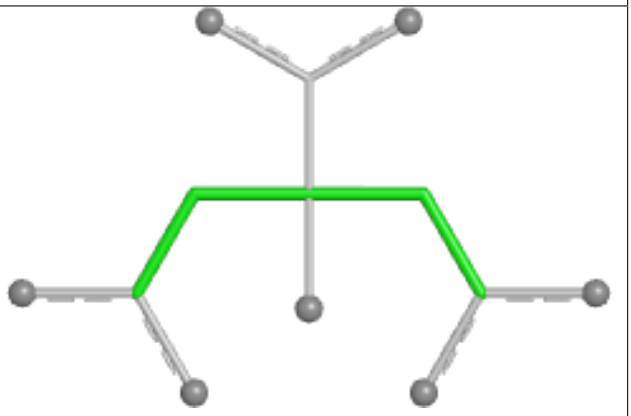


Rings

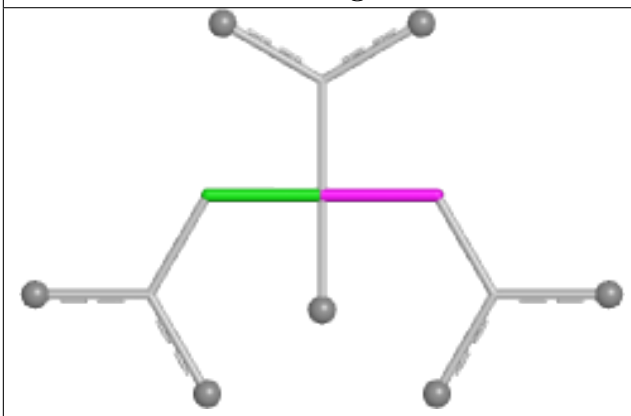
Ligand CIT B 401



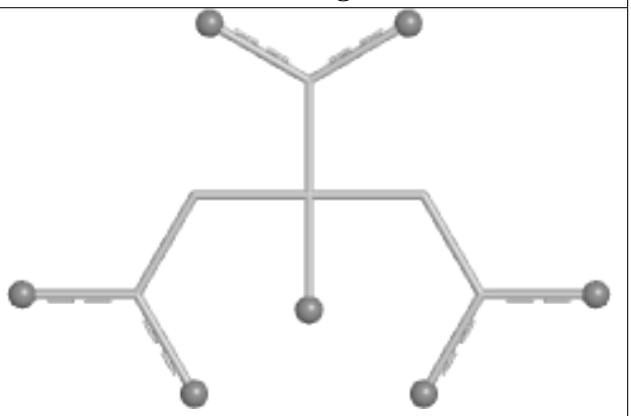
Bond lengths



Bond angles

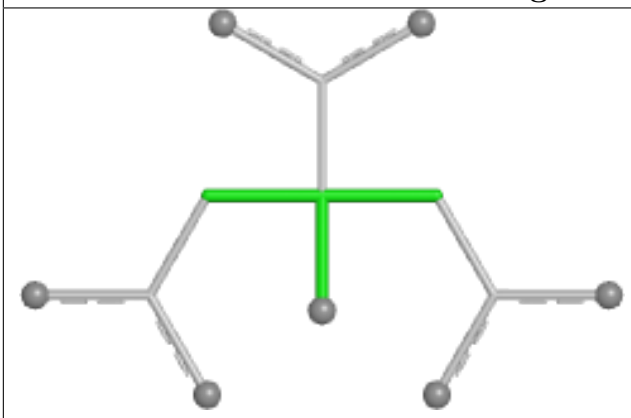


Torsions

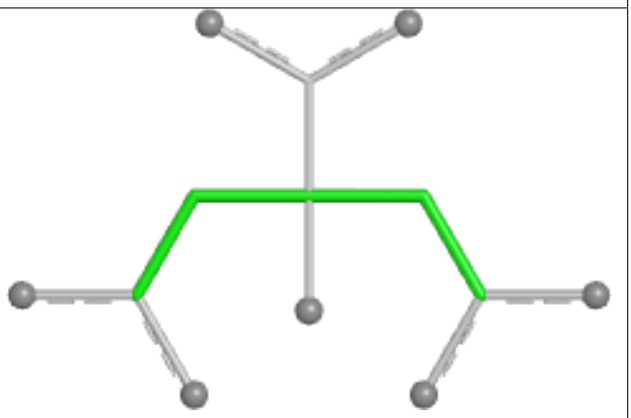


Rings

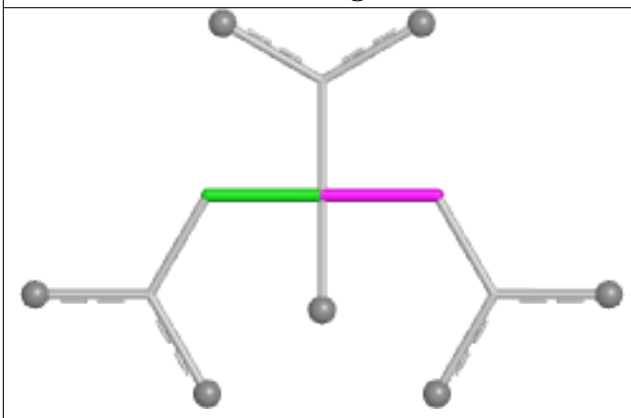
Ligand CIT P 401



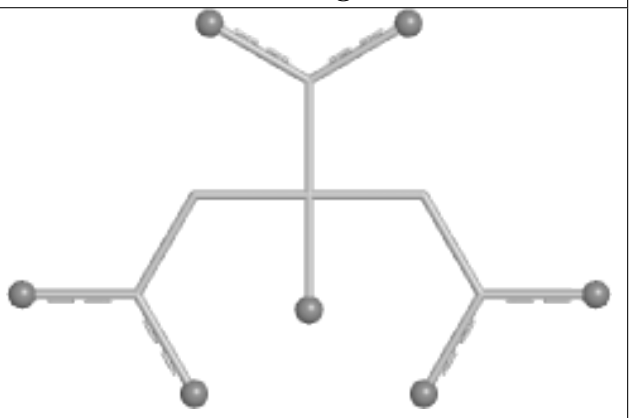
Bond lengths



Bond angles

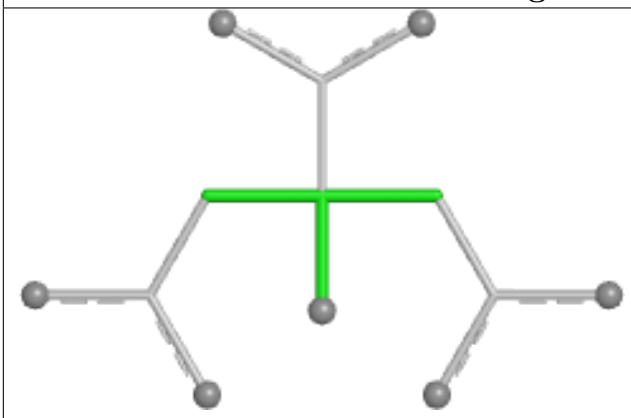


Torsions

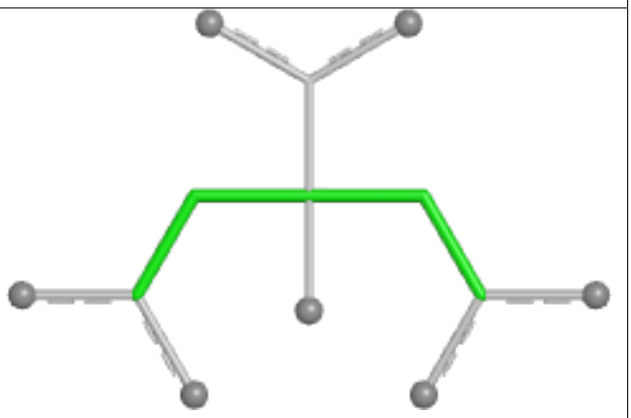


Rings

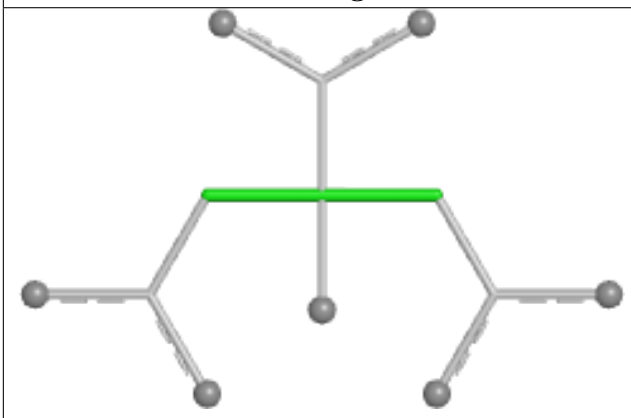
Ligand CIT H 401



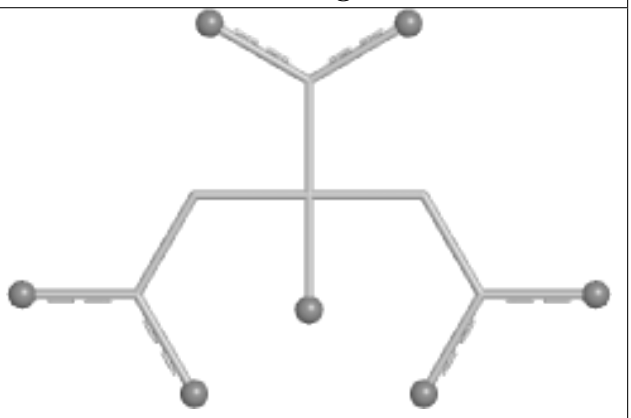
Bond lengths



Bond angles

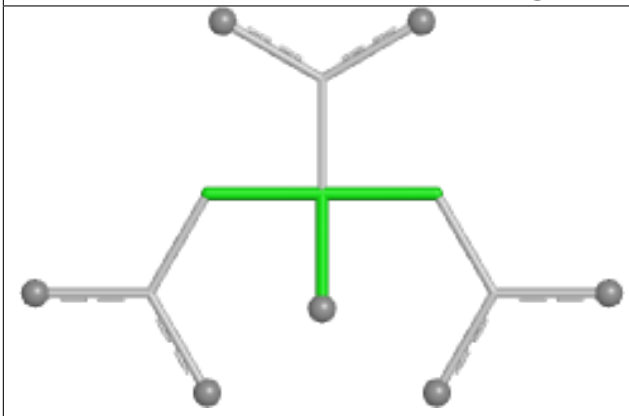


Torsions

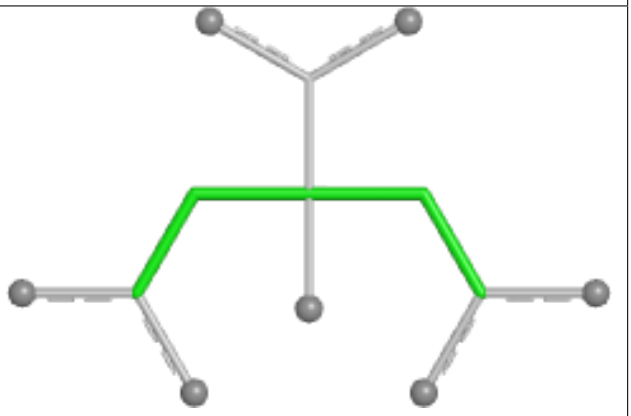


Rings

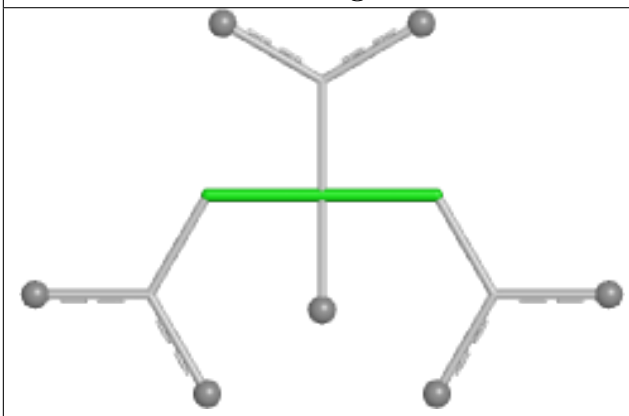
Ligand CIT D 401



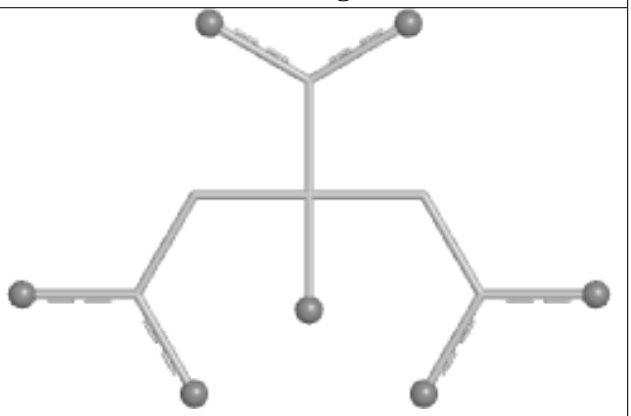
Bond lengths



Bond angles

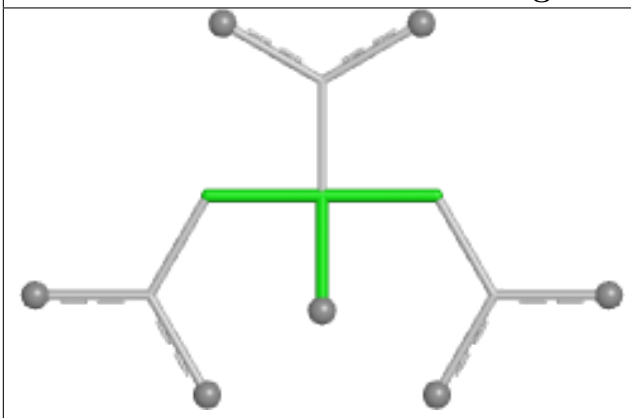


Torsions

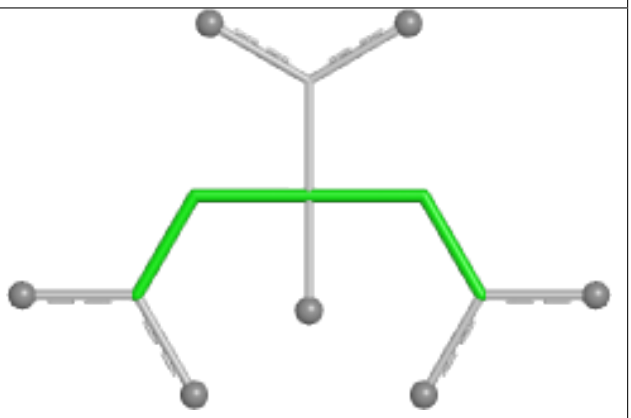


Rings

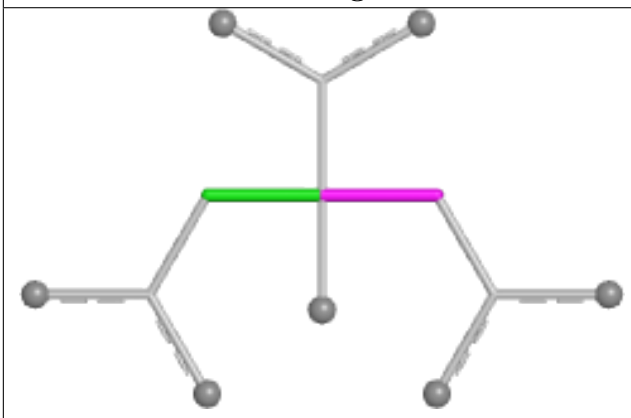
Ligand CIT J 401



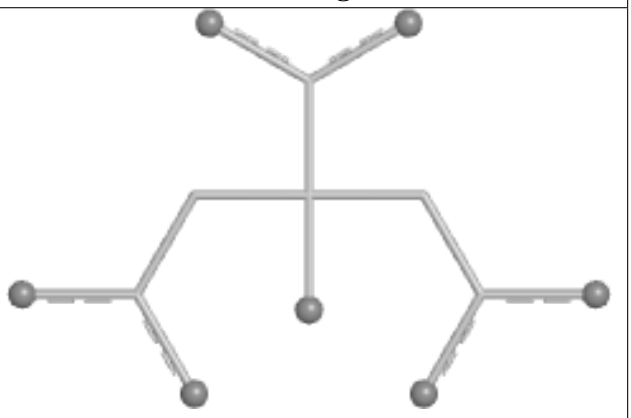
Bond lengths



Bond angles

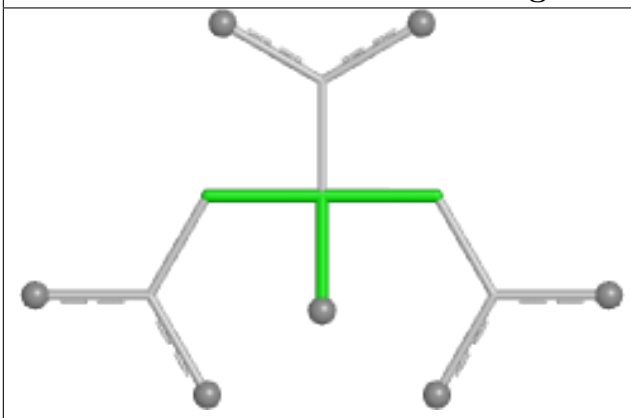


Torsions

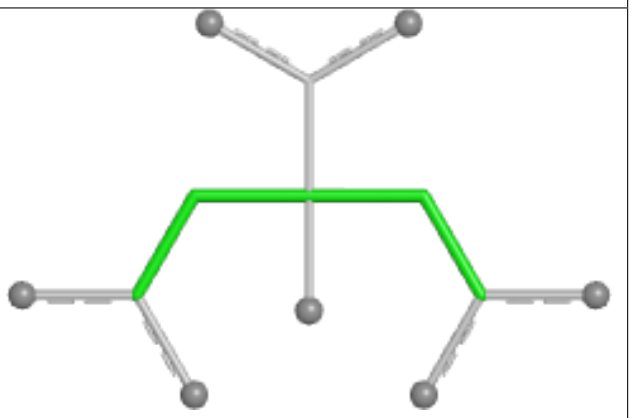


Rings

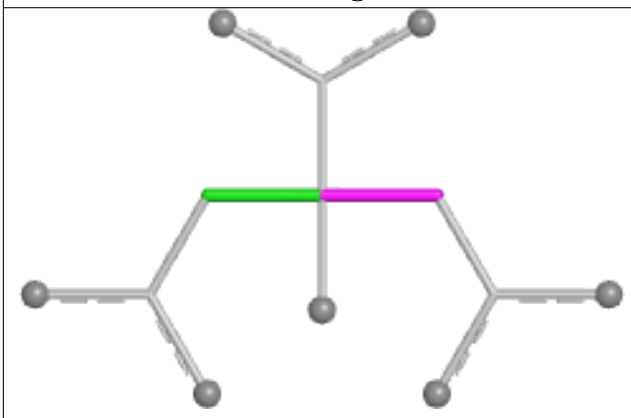
Ligand CIT O 401



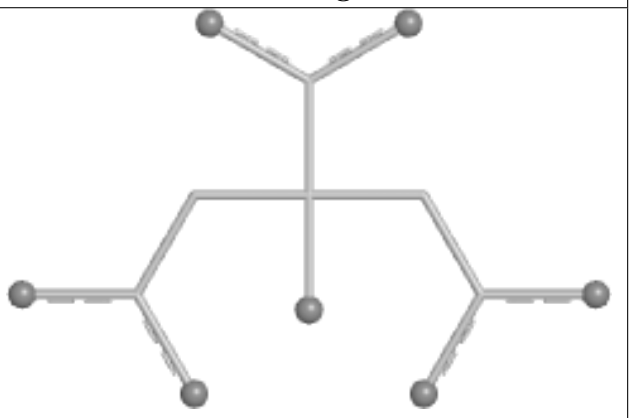
Bond lengths



Bond angles

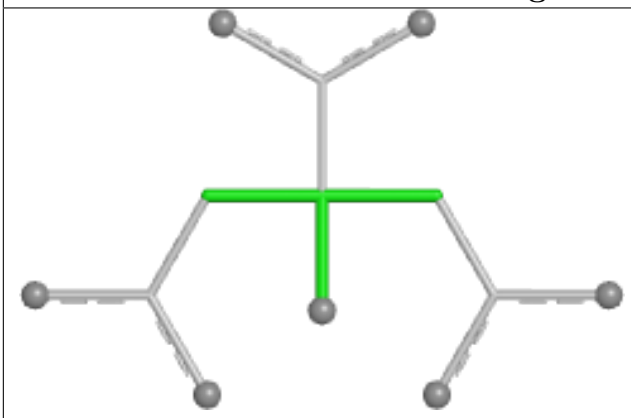


Torsions

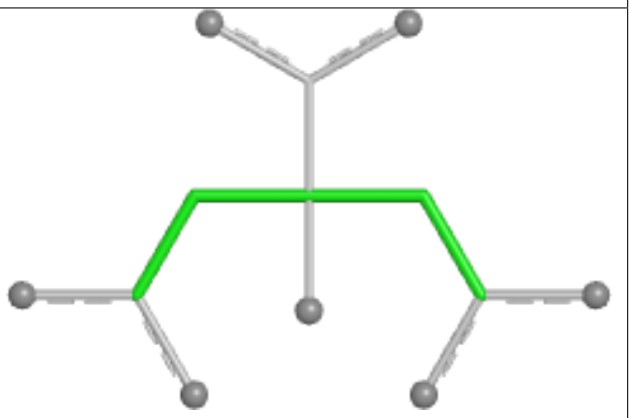


Rings

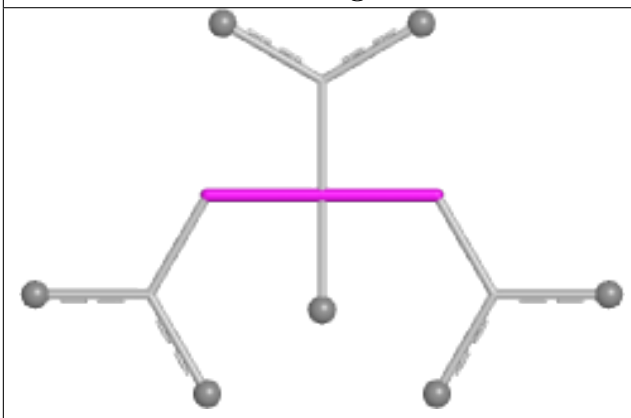
Ligand CIT A 401



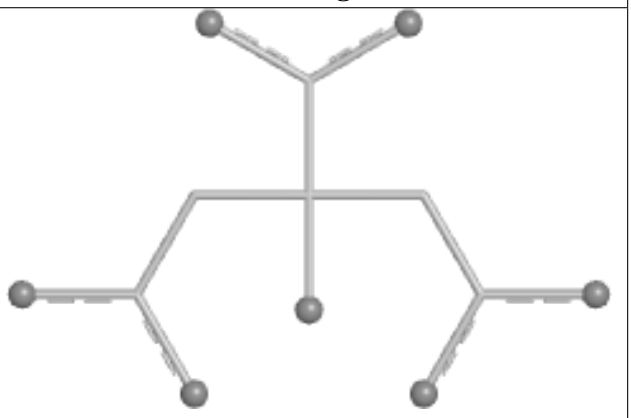
Bond lengths



Bond angles

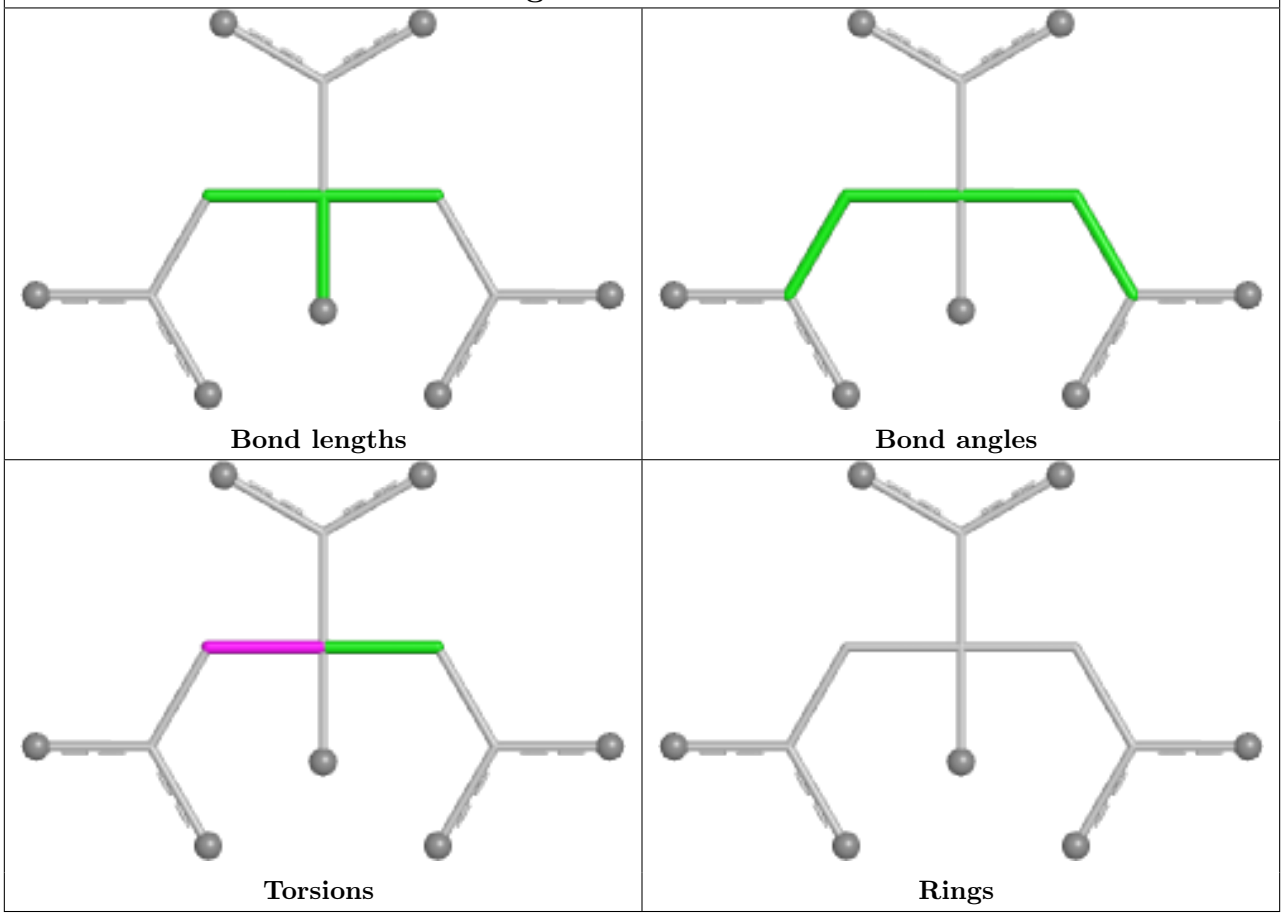


Torsions



Rings

Ligand CIT M 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	320/332 (96%)	-0.28	3 (0%)	84	82	19, 32, 53, 90	0
1	B	322/332 (96%)	-0.23	8 (2%)	57	51	17, 30, 55, 84	0
1	C	327/332 (98%)	-0.31	1 (0%)	94	93	16, 31, 50, 70	0
1	D	331/332 (99%)	-0.16	0	100	100	19, 32, 58, 100	0
1	E	320/332 (96%)	0.12	10 (3%)	49	42	19, 38, 69, 90	0
1	F	322/332 (96%)	0.05	6 (1%)	66	62	21, 35, 65, 88	0
1	G	331/332 (99%)	-0.10	2 (0%)	89	88	21, 34, 60, 93	0
1	H	330/332 (99%)	-0.04	4 (1%)	79	76	21, 39, 67, 89	0
1	I	320/332 (96%)	-0.18	3 (0%)	84	82	19, 34, 59, 87	0
1	J	319/332 (96%)	-0.15	3 (0%)	84	82	16, 31, 57, 82	0
1	K	330/332 (99%)	-0.19	3 (0%)	84	82	19, 35, 58, 84	0
1	L	331/332 (99%)	-0.12	1 (0%)	94	93	20, 36, 59, 109	0
1	M	331/332 (99%)	-0.13	2 (0%)	89	88	17, 31, 56, 95	0
1	N	331/332 (99%)	-0.19	5 (1%)	73	70	19, 31, 54, 96	0
1	O	331/332 (99%)	-0.10	7 (2%)	63	58	17, 32, 58, 94	0
1	P	325/332 (97%)	-0.02	10 (3%)	49	42	20, 33, 64, 91	0
All	All	5221/5312 (98%)	-0.13	68 (1%)	77	73	16, 33, 59, 109	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	221	ALA	5.1
1	E	328	GLU	4.2
1	O	15	GLU	4.1
1	E	221	ALA	3.9
1	E	96	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	P	104	SER	3.8
1	E	324	GLY	3.8
1	B	329	LEU	3.7
1	O	221	ALA	3.7
1	A	15	GLU	3.7
1	F	281	GLY	3.6
1	B	331	PHE	3.6
1	P	97	ALA	3.4
1	P	105	ARG	3.3
1	O	278	GLY	3.3
1	G	15	GLU	3.3
1	J	328	GLU	3.3
1	F	1	ALA	3.2
1	N	13	LYS	3.2
1	N	11	LEU	3.0
1	E	15	GLU	2.9
1	B	16	HIS	2.7
1	P	108	LEU	2.7
1	F	282	ILE	2.7
1	B	328	GLU	2.6
1	O	1	ALA	2.6
1	P	15	GLU	2.6
1	P	194	ASP	2.5
1	K	15	GLU	2.5
1	A	278	GLY	2.4
1	J	324	GLY	2.4
1	N	15	GLU	2.4
1	A	329	LEU	2.4
1	B	325	ILE	2.4
1	P	16	HIS	2.4
1	I	15	GLU	2.4
1	M	98	ARG	2.3
1	O	215	PRO	2.3
1	E	220	ASP	2.3
1	L	16	HIS	2.3
1	H	331	PHE	2.3
1	E	331	PHE	2.3
1	K	14	GLU	2.3
1	P	314	HIS	2.3
1	O	220	ASP	2.3
1	J	108	LEU	2.3
1	B	221	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	P	328	GLU	2.3
1	F	220	ASP	2.2
1	E	137	ASN	2.2
1	F	190	GLY	2.2
1	I	328	GLU	2.2
1	E	330	GLN	2.2
1	P	107	ASN	2.2
1	C	313	ALA	2.2
1	B	327	LYS	2.1
1	H	72	ARG	2.1
1	B	330	GLN	2.1
1	H	13	LYS	2.1
1	E	283	LYS	2.1
1	N	98	ARG	2.1
1	G	11	LEU	2.1
1	N	16	HIS	2.1
1	I	238	TYR	2.1
1	H	40	MET	2.1
1	K	13	LYS	2.0
1	M	43	LEU	2.0
1	O	105	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CIT	F	401	13/13	0.67	0.23	65,75,92,101	0
2	CIT	G	401	13/13	0.67	0.31	80,86,98,99	0

Continued on next page...

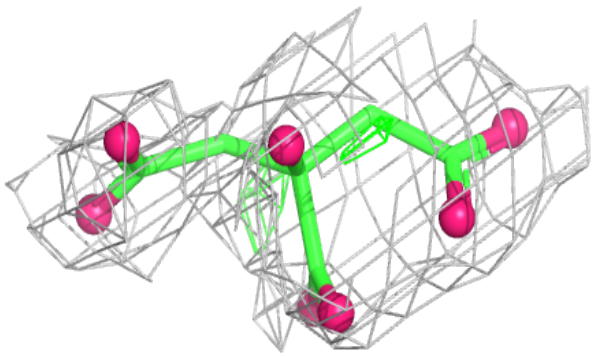
Continued from previous page...

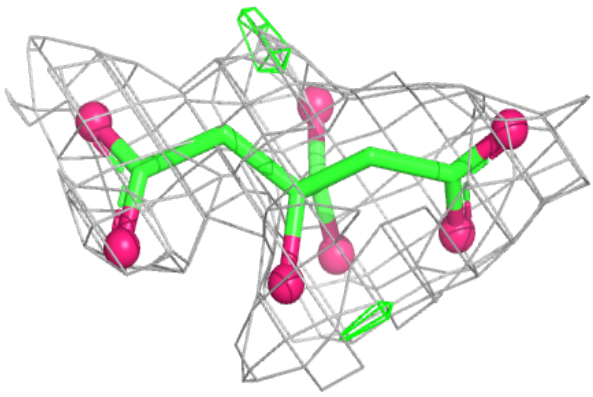
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CIT	L	401	13/13	0.69	0.28	77,80,90,93	0
2	CIT	B	401	13/13	0.72	0.35	71,77,90,99	0
2	CIT	K	401	13/13	0.73	0.28	79,87,101,111	0
2	CIT	O	401	13/13	0.73	0.34	78,84,93,100	0
2	CIT	A	401	13/13	0.77	0.27	69,74,80,80	0
2	CIT	J	401	13/13	0.78	0.31	65,73,76,81	0
2	CIT	M	401	13/13	0.78	0.26	49,66,74,82	0
2	CIT	N	401	13/13	0.78	0.25	69,78,102,102	0
2	CIT	D	401	13/13	0.78	0.25	59,77,85,88	0
2	CIT	P	401	13/13	0.78	0.37	69,74,79,86	0
2	CIT	E	401	13/13	0.79	0.37	63,67,83,84	0
2	CIT	I	401	13/13	0.81	0.22	65,81,88,92	0
2	CIT	H	401	13/13	0.81	0.37	73,82,93,93	0
2	CIT	C	401	13/13	0.86	0.18	56,70,74,74	0

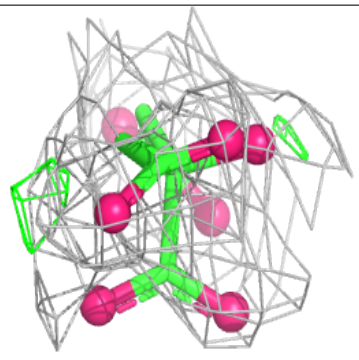
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CIT F 401:

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

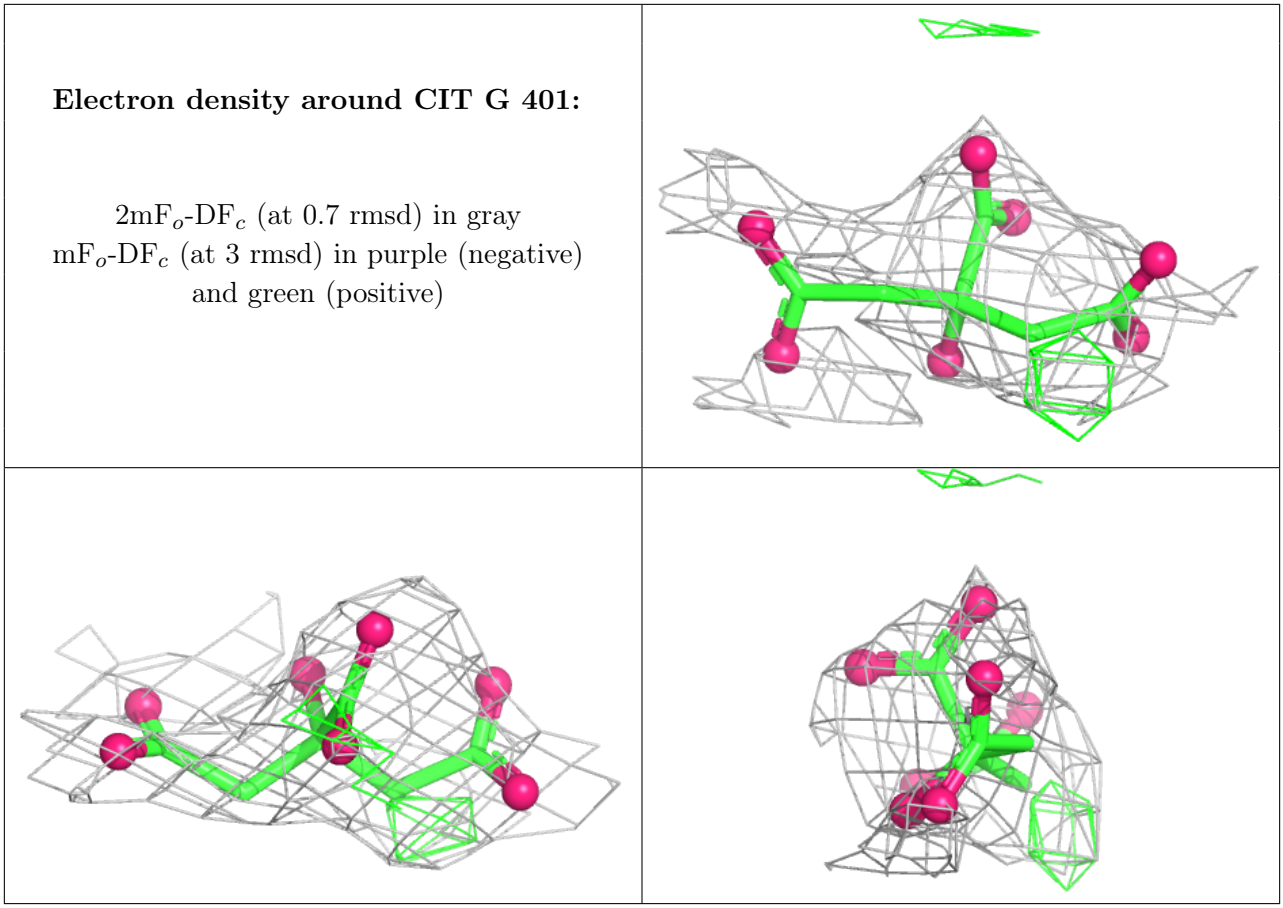






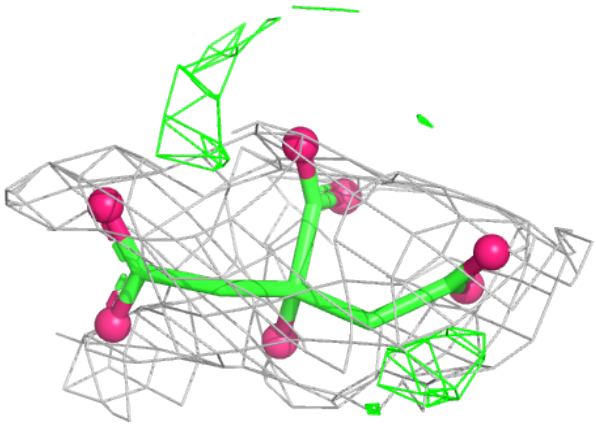
Electron density around CIT G 401:

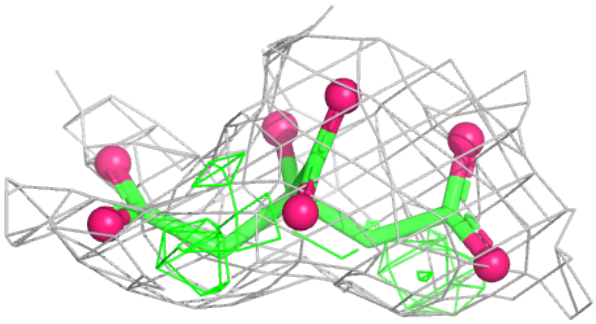
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

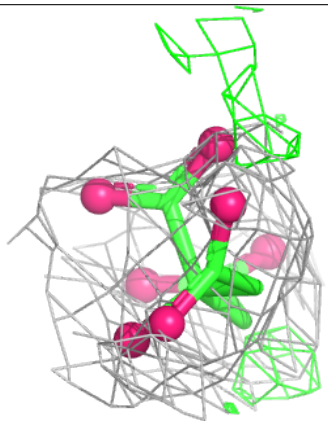


Electron density around CIT L 401:

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

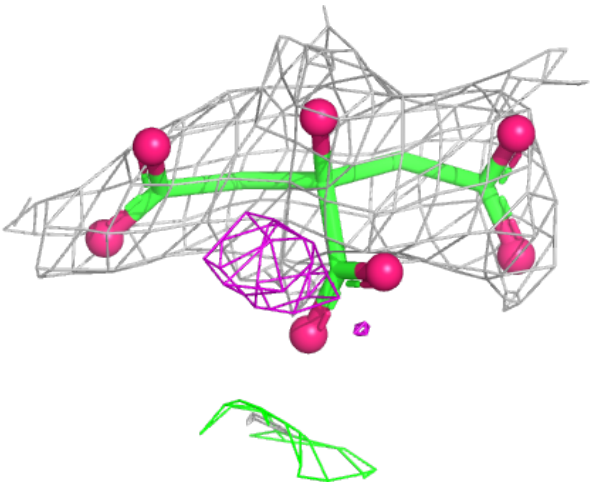


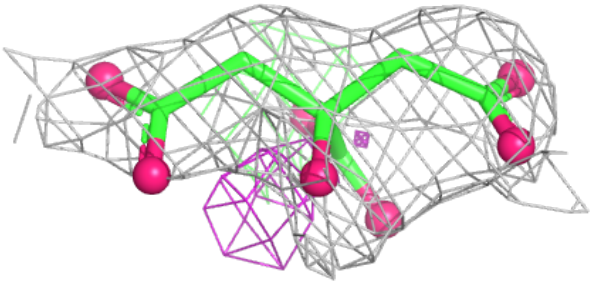


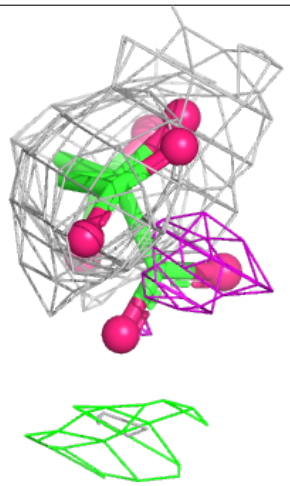


Electron density around CIT B 401:

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

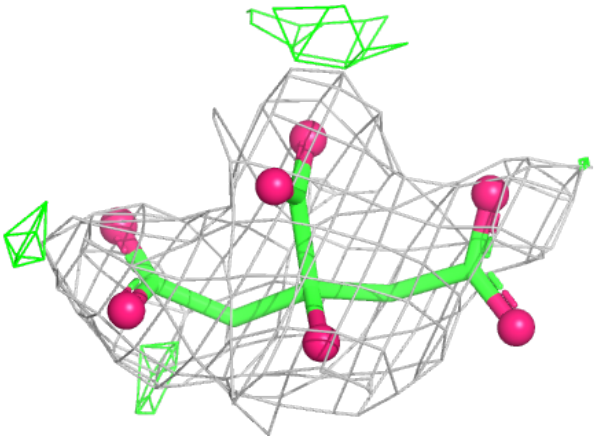


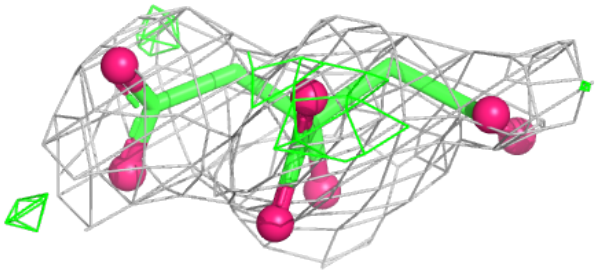


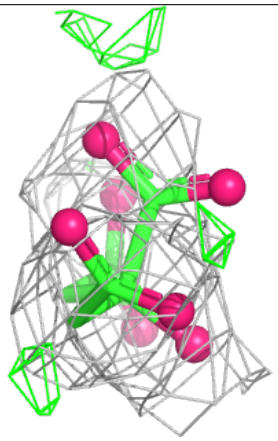


Electron density around CIT K 401:

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

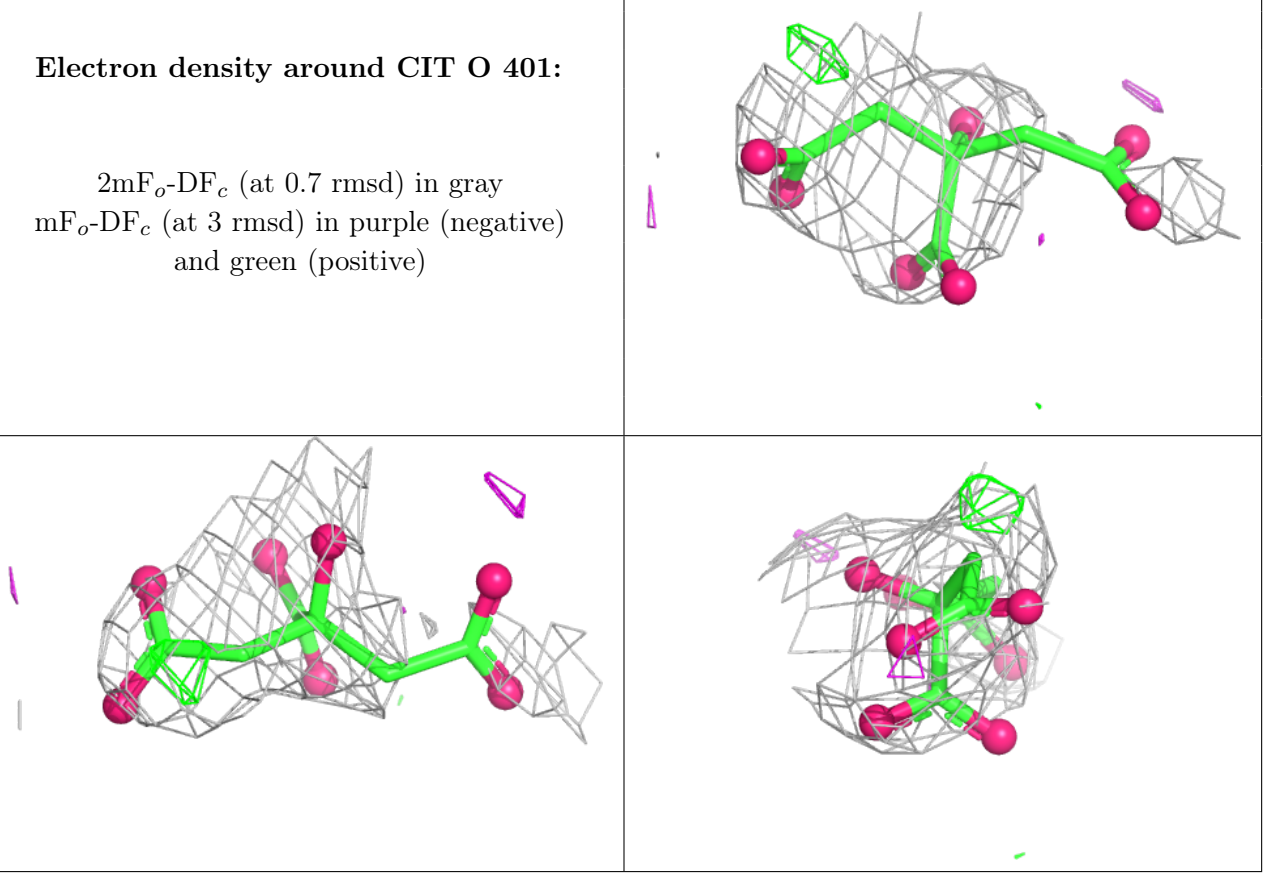






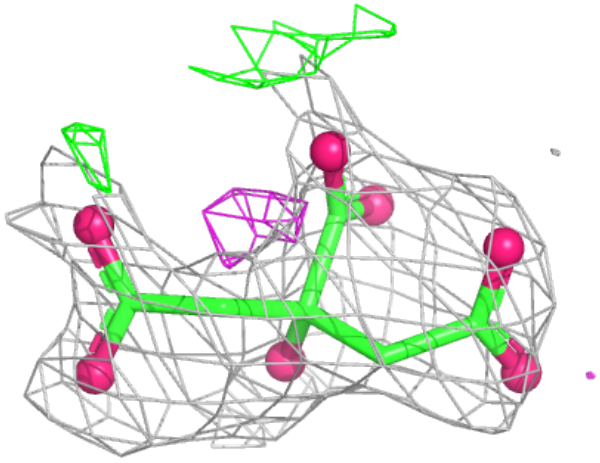
Electron density around CIT O 401:

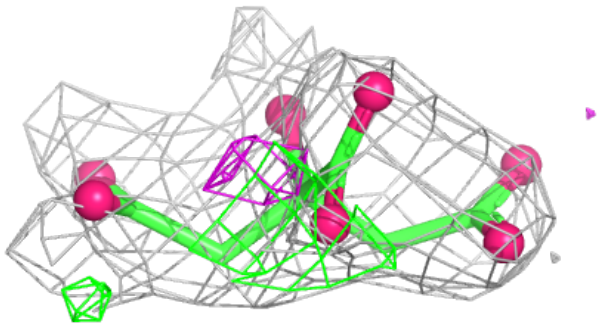
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

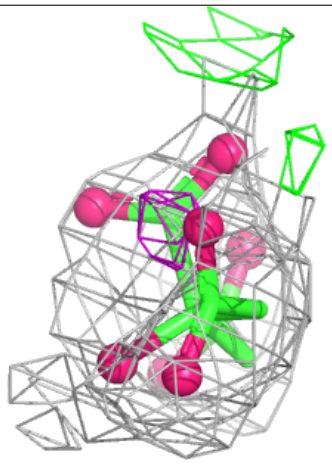


Electron density around CIT A 401:

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

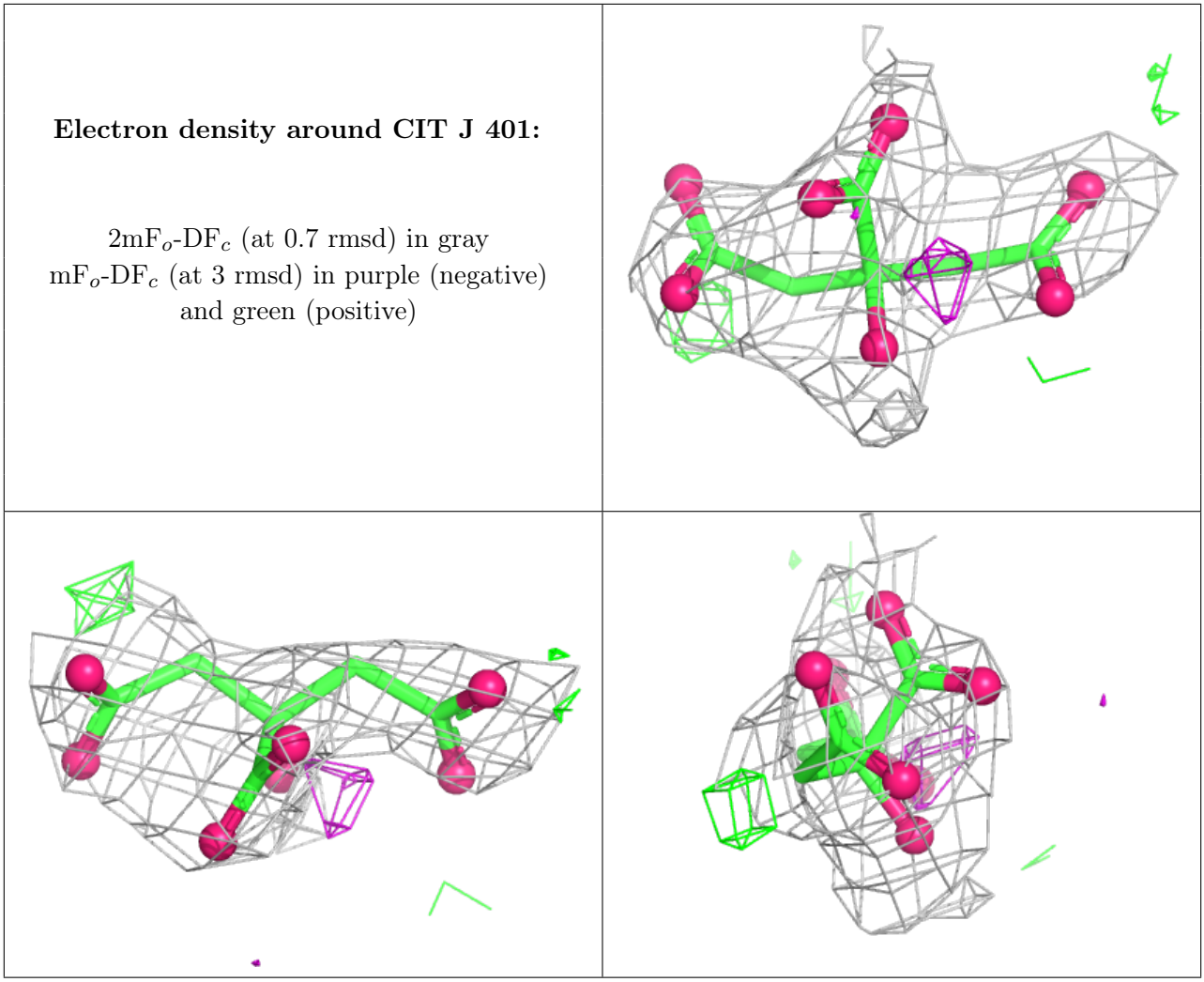






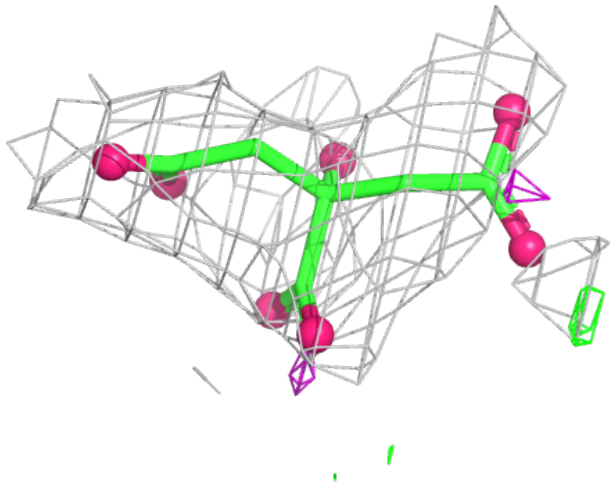
Electron density around CIT J 401:

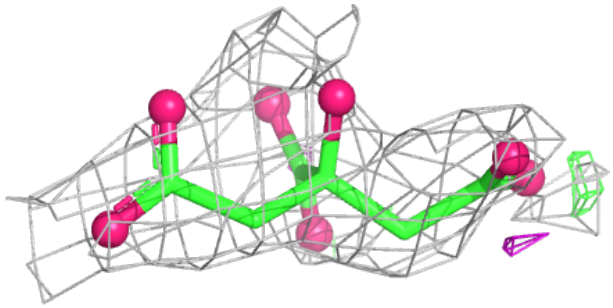
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

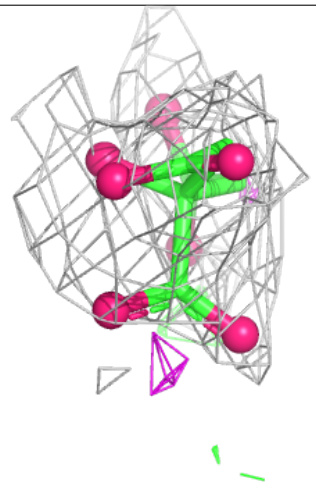


Electron density around CIT M 401:

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

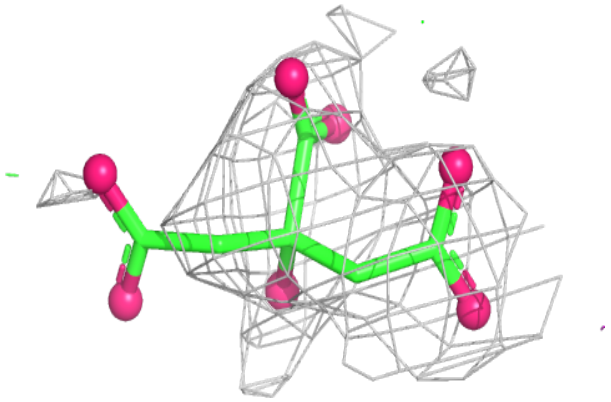


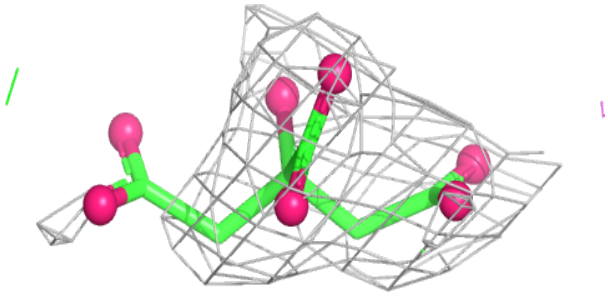


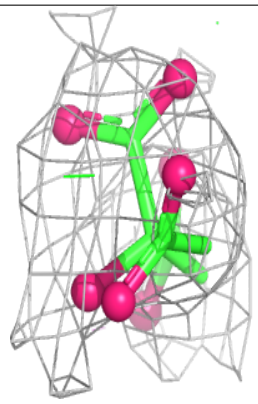


Electron density around CIT N 401:

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

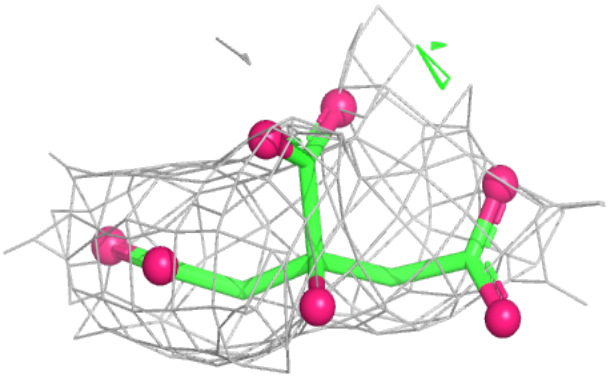


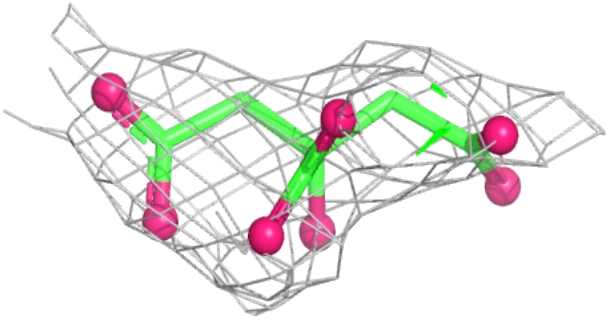


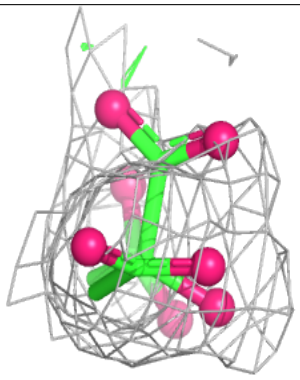


Electron density around CIT D 401:

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

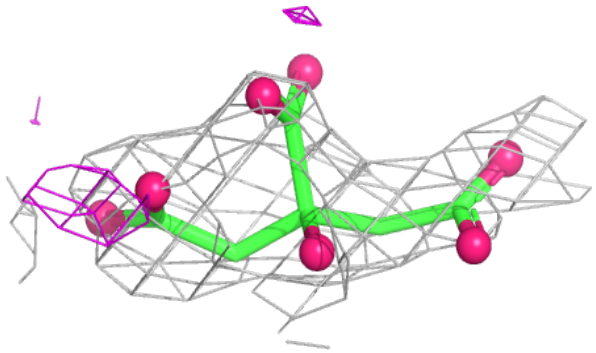


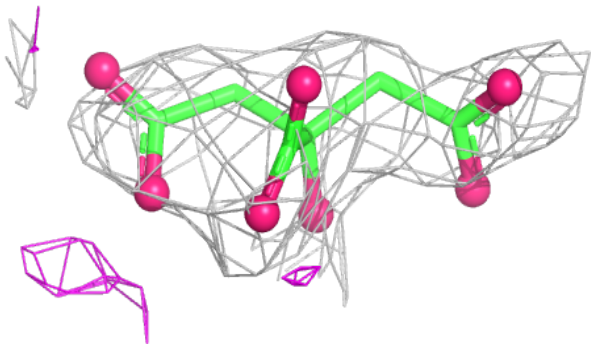


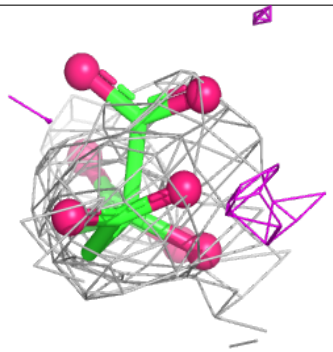


Electron density around CIT P 401:

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

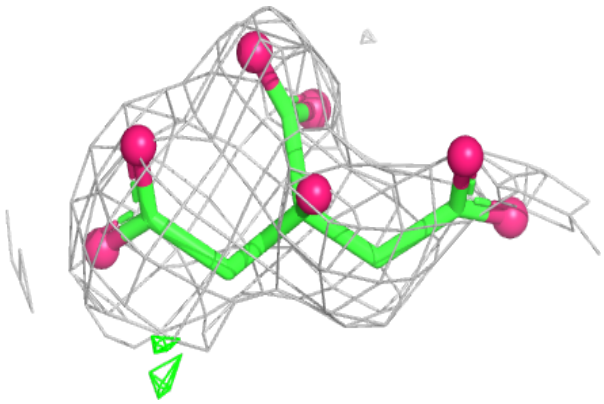


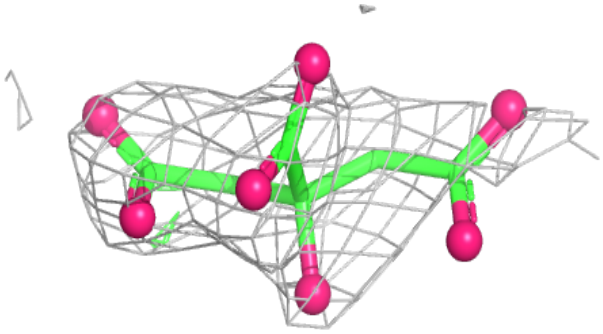


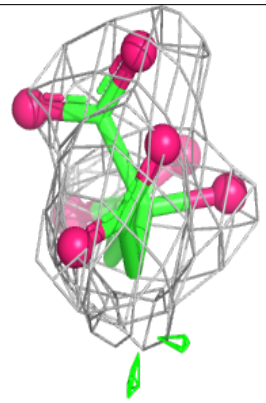


Electron density around CIT E 401:

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

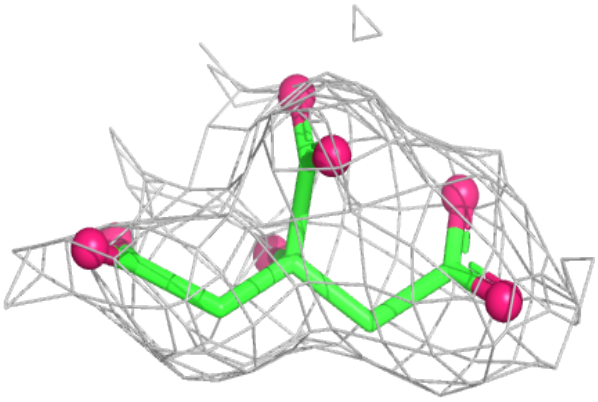


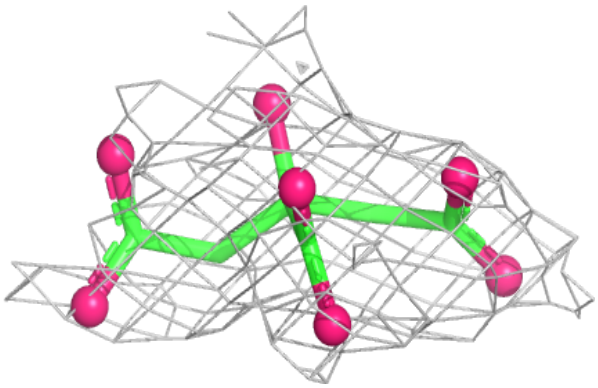


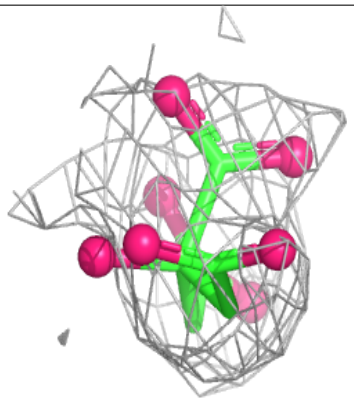


Electron density around CIT I 401:

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

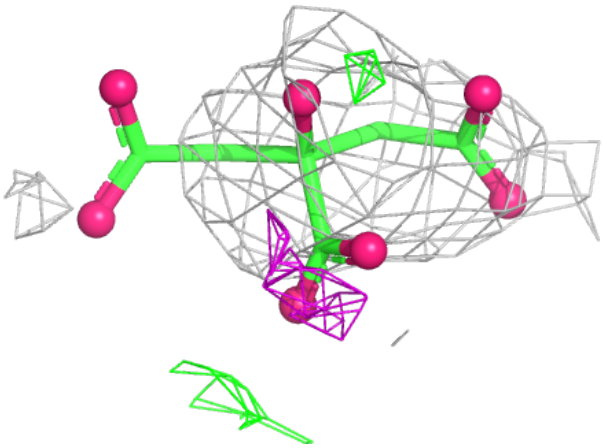


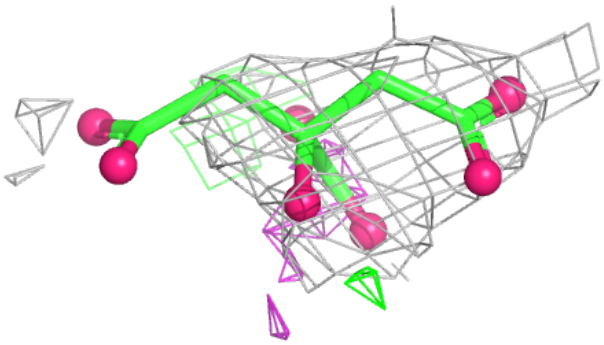


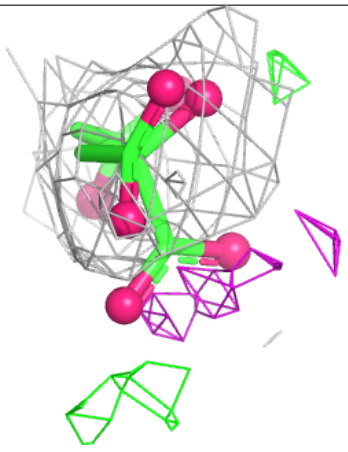


Electron density around CIT H 401:

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

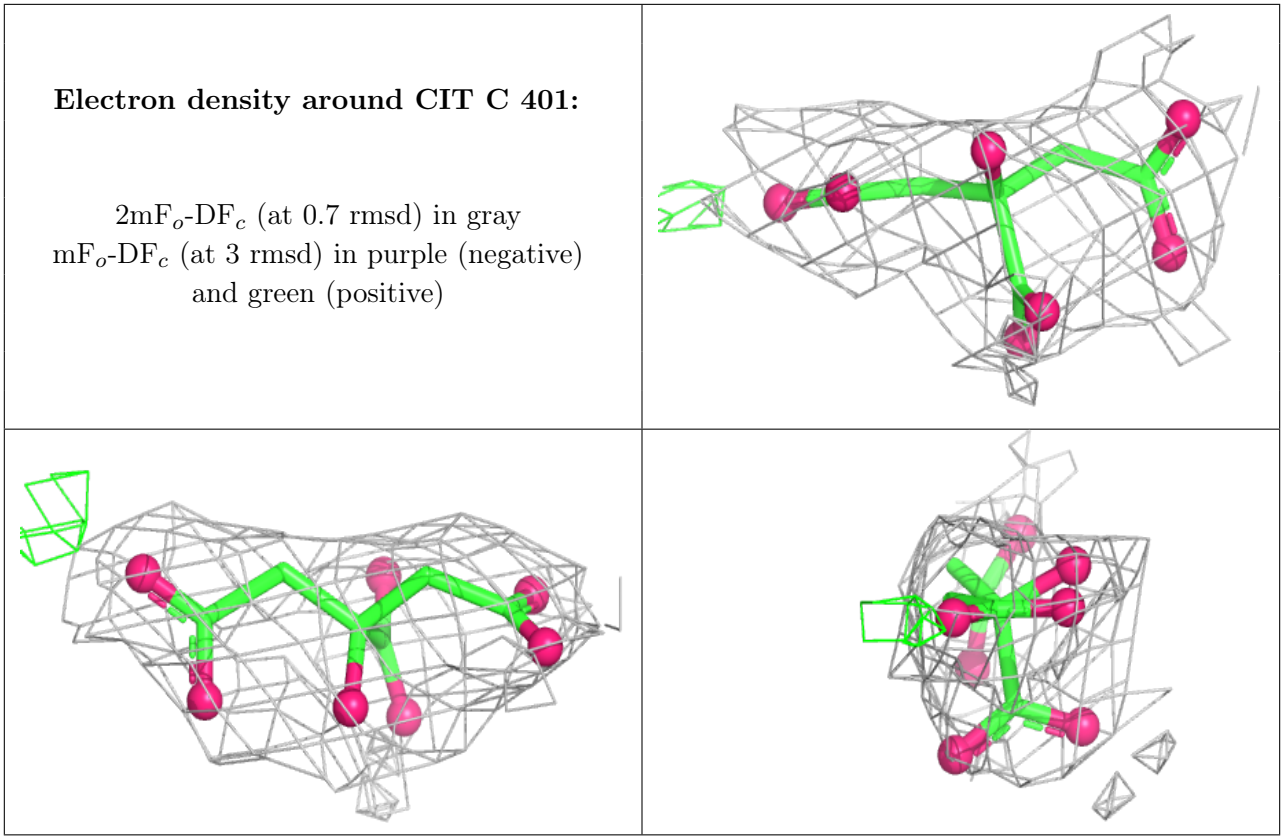






Electron density around CIT C 401:

$2mF_o$-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.