



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:56 PM UTC

PDB ID : 7WBR / pdb_00007wbr
Title : Citrate synthase/lyase from *Desulfurella acetivorans* Desace_08345
Authors : Yang, L.
Deposited on : 2021-12-17
Resolution : 2.19 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

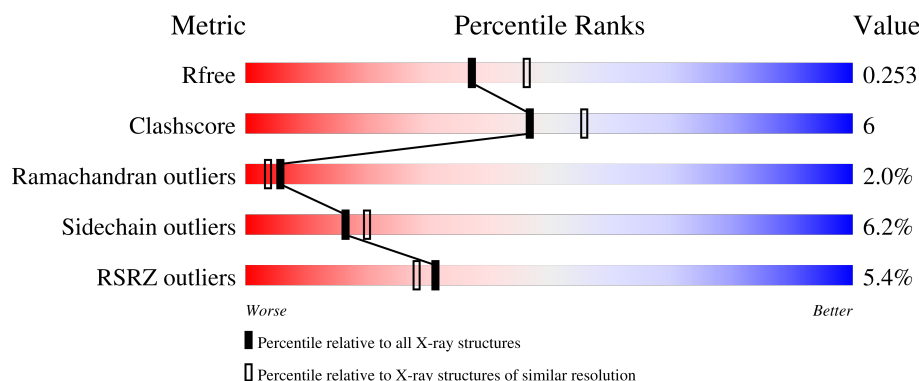
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	436	5% 76% 16% ...
1	B	436	3% 81% 12% ...
1	C	436	4% 82% 12% ...
1	D	436	3% 78% 16% ...
1	E	436	4% 78% 16% ...

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Mol	Chain	Length	Quality of chain
1	F	436	
1	G	436	
1	H	436	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CIT	F	501	-	X	-	-
2	CIT	H	501	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27573 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 Citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	423	Total	C	N	O	S	0	0	0
			3338	2150	559	611	18			
1	B	418	Total	C	N	O	S	0	0	0
			3290	2117	551	604	18			
1	C	423	Total	C	N	O	S	0	0	0
			3338	2150	559	611	18			
1	D	418	Total	C	N	O	S	0	0	0
			3286	2114	550	604	18			
1	E	423	Total	C	N	O	S	0	0	0
			3338	2150	559	611	18			
1	F	418	Total	C	N	O	S	0	0	0
			3282	2111	549	604	18			
1	G	423	Total	C	N	O	S	0	0	0
			3338	2150	559	611	18			
1	H	418	Total	C	N	O	S	0	0	0
			3286	2114	550	604	18			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	PHE	LEU	engineered mutation	UNP A0A7C2VVZ8
A	48	SER	CYS	engineered mutation	UNP A0A7C2VVZ8
A	99	VAL	ILE	engineered mutation	UNP A0A7C2VVZ8
A	207	LEU	VAL	engineered mutation	UNP A0A7C2VVZ8
A	278	VAL	THR	engineered mutation	UNP A0A7C2VVZ8
A	309	SER	ALA	engineered mutation	UNP A0A7C2VVZ8
A	330	VAL	MET	engineered mutation	UNP A0A7C2VVZ8
B	3	PHE	LEU	engineered mutation	UNP A0A7C2VVZ8
B	48	SER	CYS	engineered mutation	UNP A0A7C2VVZ8
B	99	VAL	ILE	engineered mutation	UNP A0A7C2VVZ8
B	207	LEU	VAL	engineered mutation	UNP A0A7C2VVZ8
B	278	VAL	THR	engineered mutation	UNP A0A7C2VVZ8
B	309	SER	ALA	engineered mutation	UNP A0A7C2VVZ8

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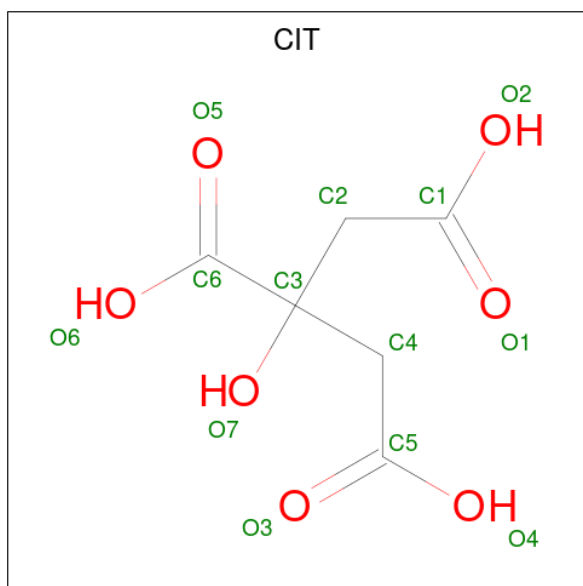
Chain	Residue	Modelled	Actual	Comment	Reference
B	330	VAL	MET	engineered mutation	UNP A0A7C2VVZ8
C	3	PHE	LEU	engineered mutation	UNP A0A7C2VVZ8
C	48	SER	CYS	engineered mutation	UNP A0A7C2VVZ8
C	99	VAL	ILE	engineered mutation	UNP A0A7C2VVZ8
C	207	LEU	VAL	engineered mutation	UNP A0A7C2VVZ8
C	278	VAL	THR	engineered mutation	UNP A0A7C2VVZ8
C	309	SER	ALA	engineered mutation	UNP A0A7C2VVZ8
C	330	VAL	MET	engineered mutation	UNP A0A7C2VVZ8
D	3	PHE	LEU	engineered mutation	UNP A0A7C2VVZ8
D	48	SER	CYS	engineered mutation	UNP A0A7C2VVZ8
D	99	VAL	ILE	engineered mutation	UNP A0A7C2VVZ8
D	207	LEU	VAL	engineered mutation	UNP A0A7C2VVZ8
D	278	VAL	THR	engineered mutation	UNP A0A7C2VVZ8
D	309	SER	ALA	engineered mutation	UNP A0A7C2VVZ8
D	330	VAL	MET	engineered mutation	UNP A0A7C2VVZ8
E	3	PHE	LEU	engineered mutation	UNP A0A7C2VVZ8
E	48	SER	CYS	engineered mutation	UNP A0A7C2VVZ8
E	99	VAL	ILE	engineered mutation	UNP A0A7C2VVZ8
E	207	LEU	VAL	engineered mutation	UNP A0A7C2VVZ8
E	278	VAL	THR	engineered mutation	UNP A0A7C2VVZ8
E	309	SER	ALA	engineered mutation	UNP A0A7C2VVZ8
E	330	VAL	MET	engineered mutation	UNP A0A7C2VVZ8
F	3	PHE	LEU	engineered mutation	UNP A0A7C2VVZ8
F	48	SER	CYS	engineered mutation	UNP A0A7C2VVZ8
F	99	VAL	ILE	engineered mutation	UNP A0A7C2VVZ8
F	207	LEU	VAL	engineered mutation	UNP A0A7C2VVZ8
F	278	VAL	THR	engineered mutation	UNP A0A7C2VVZ8
F	309	SER	ALA	engineered mutation	UNP A0A7C2VVZ8
F	330	VAL	MET	engineered mutation	UNP A0A7C2VVZ8
G	3	PHE	LEU	engineered mutation	UNP A0A7C2VVZ8
G	48	SER	CYS	engineered mutation	UNP A0A7C2VVZ8
G	99	VAL	ILE	engineered mutation	UNP A0A7C2VVZ8
G	207	LEU	VAL	engineered mutation	UNP A0A7C2VVZ8
G	278	VAL	THR	engineered mutation	UNP A0A7C2VVZ8
G	309	SER	ALA	engineered mutation	UNP A0A7C2VVZ8
G	330	VAL	MET	engineered mutation	UNP A0A7C2VVZ8
H	3	PHE	LEU	engineered mutation	UNP A0A7C2VVZ8
H	48	SER	CYS	engineered mutation	UNP A0A7C2VVZ8
H	99	VAL	ILE	engineered mutation	UNP A0A7C2VVZ8
H	207	LEU	VAL	engineered mutation	UNP A0A7C2VVZ8
H	278	VAL	THR	engineered mutation	UNP A0A7C2VVZ8
H	309	SER	ALA	engineered mutation	UNP A0A7C2VVZ8

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Chain	Residue	Modelled	Actual	Comment	Reference
H	330	VAL	MET	engineered mutation	UNP A0A7C2VVZ8

- 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
2	G	1	Total C O 13 6 7	0	0
2	H	1	Total C O 13 6 7	0	0

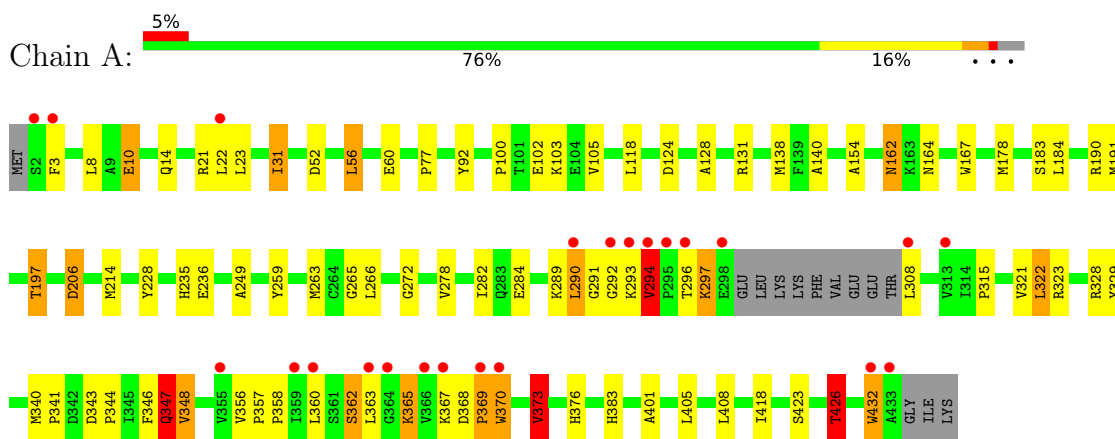
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	123	Total 123	O 123	0	0
3	B	121	Total 121	O 121	0	0
3	C	118	Total 118	O 118	0	0
3	D	122	Total 122	O 122	0	0
3	E	113	Total 113	O 113	0	0
3	F	116	Total 116	O 116	0	0
3	G	120	Total 120	O 120	0	0
3	H	140	Total 140	O 140	0	0

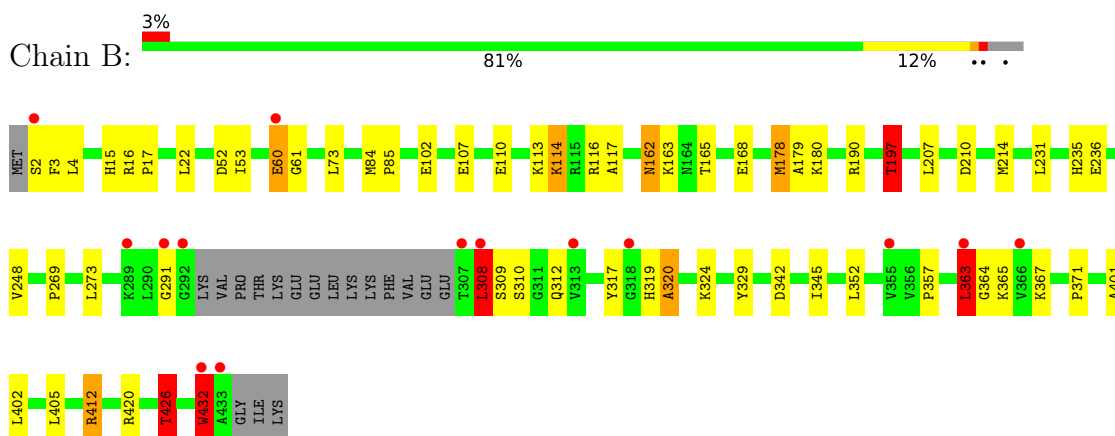
3 Residue-property plots [i](#)

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.

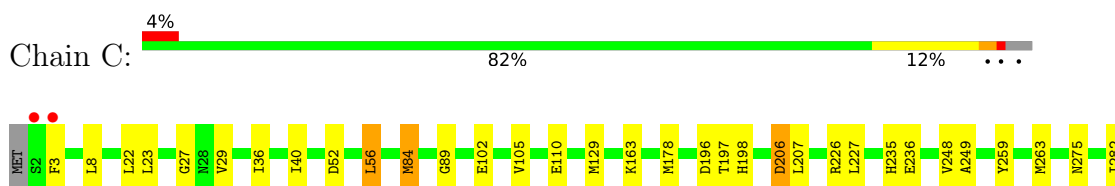
- Molecule 1: Citrate synthase

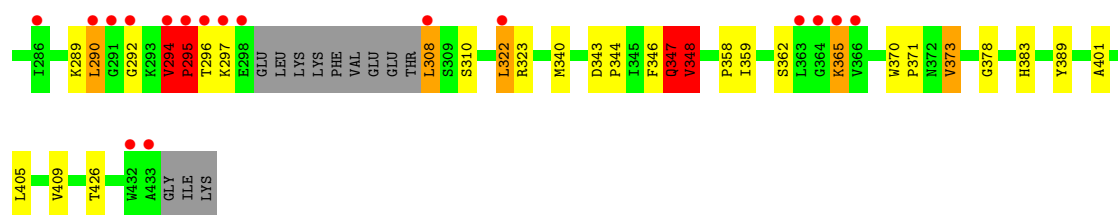


- Molecule 1: Citrate synthase

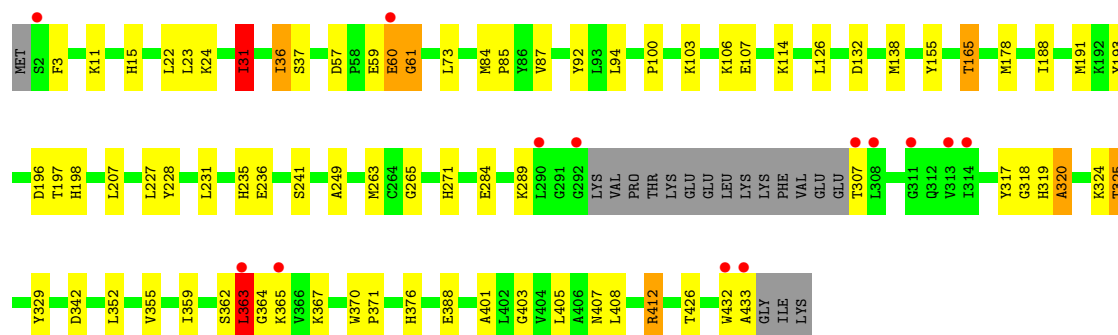
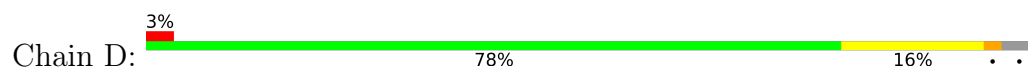


- Molecule 1: Citrate synthase

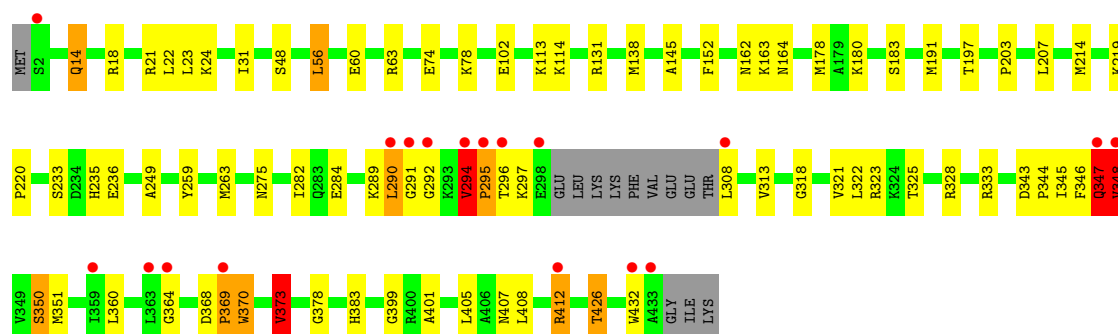
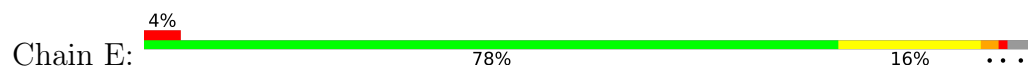




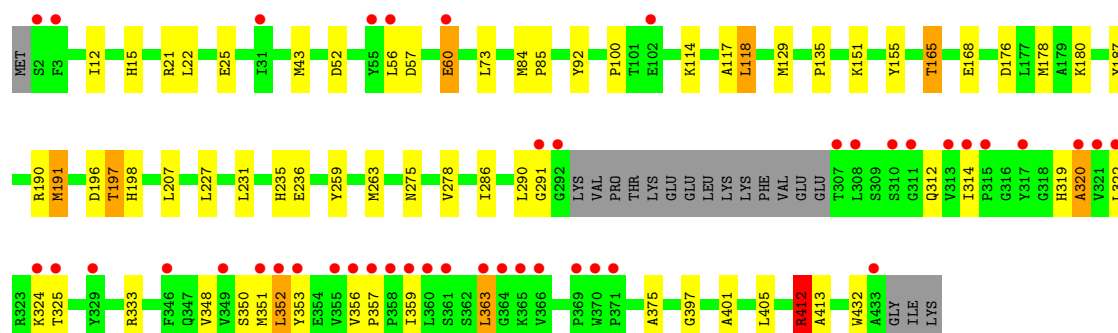
• Molecule 1: Citrate synthase



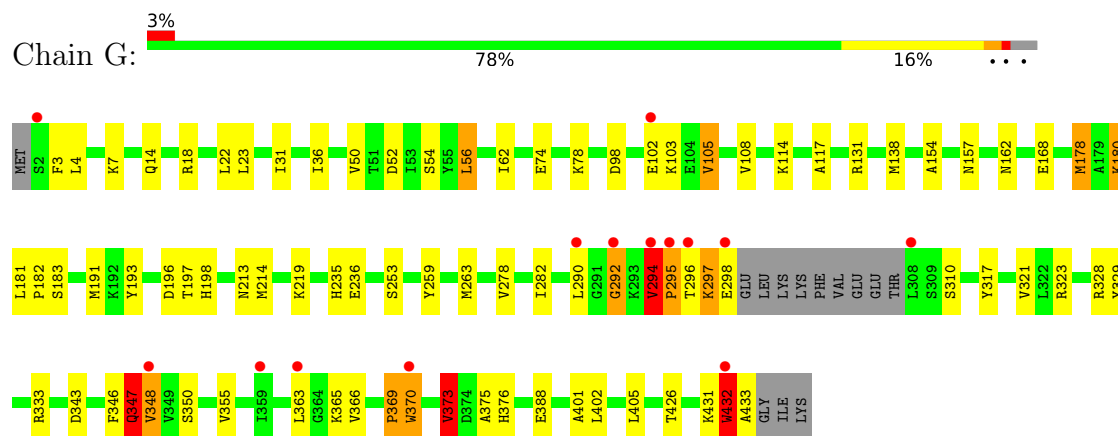
• Molecule 1: Citrate synthase



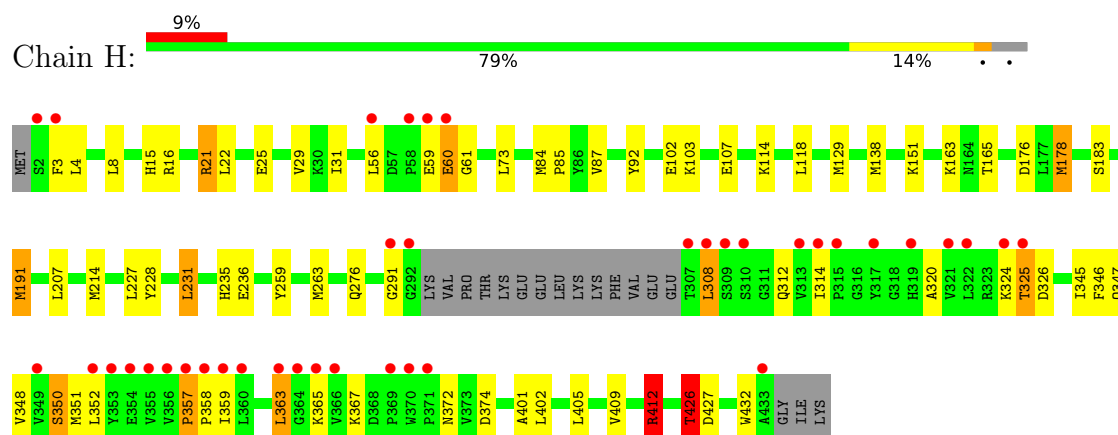
• Molecule 1: Citrate synthase



- Molecule 1: Citrate synthase



- Molecule 1: Citrate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	362.33Å 362.33Å 77.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	181.17 – 2.19 181.17 – 2.19	Depositor EDS
% Data completeness (in resolution range)	97.3 (181.17-2.19) 97.5 (181.17-2.19)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.196 , 0.249 0.202 , 0.253	Depositor DCC
R_{free} test set	9674 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27573	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.6882e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	1.10	4/3424 (0.1%)	1.18	10/4640 (0.2%)
1	B	1.16	7/3375 (0.2%)	1.17	9/4576 (0.2%)
1	C	1.04	0/3424	1.12	9/4640 (0.2%)
1	D	1.04	2/3371 (0.1%)	1.16	8/4572 (0.2%)
1	E	1.14	3/3424 (0.1%)	1.18	9/4640 (0.2%)
1	F	1.12	5/3367 (0.1%)	1.15	9/4568 (0.2%)
1	G	1.17	8/3424 (0.2%)	1.20	14/4640 (0.3%)
1	H	1.18	3/3371 (0.1%)	1.20	13/4572 (0.3%)
All	All	1.12	32/27180 (0.1%)	1.17	81/36848 (0.2%)

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	4
1	B	0	4
1	C	0	3
1	D	0	1
1	E	0	5
1	G	0	4
1	H	0	2
All	All	0	23

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	432	TRP	CA-C	9.27	1.65	1.52
1	E	180	LYS	C-O	-7.53	1.14	1.24
1	F	432	TRP	CA-C	6.93	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	50	VAL	C-O	-6.26	1.17	1.24
1	B	179	ALA	C-O	-6.25	1.16	1.24
1	G	253	SER	C-O	6.12	1.31	1.23
1	G	168	GLU	C-O	-6.04	1.18	1.24
1	E	370	TRP	CA-C	5.88	1.60	1.52
1	A	124	ASP	C-O	-5.60	1.17	1.24
1	A	206	ASP	CG-OD2	5.59	1.35	1.25
1	B	162	ASN	CA-C	-5.59	1.45	1.52
1	B	432	TRP	CA-C	5.58	1.60	1.52
1	G	154	ALA	C-O	-5.55	1.17	1.24
1	H	412	ARG	CD-NE	-5.49	1.38	1.46
1	A	154	ALA	CA-C	5.44	1.59	1.52
1	D	132	ASP	C-O	-5.41	1.16	1.24
1	F	135	PRO	C-O	-5.31	1.17	1.24
1	B	113	LYS	C-O	-5.30	1.18	1.24
1	F	357	PRO	CA-C	5.29	1.57	1.52
1	B	168	GLU	CA-C	5.28	1.58	1.52
1	A	432	TRP	CA-C	5.24	1.59	1.52
1	D	318	GLY	N-CA	5.19	1.51	1.44
1	B	426	THR	CB-CG2	-5.16	1.35	1.52
1	F	118	LEU	C-O	-5.13	1.17	1.24
1	F	397	GLY	N-CA	5.12	1.52	1.45
1	G	105	VAL	C-O	-5.12	1.18	1.24
1	G	405	LEU	N-CA	5.12	1.52	1.46
1	H	357	PRO	CA-C	5.11	1.56	1.52
1	G	213	ASN	CA-C	5.10	1.59	1.52
1	H	3	PHE	N-CA	5.05	1.52	1.46
1	B	214	MET	C-O	-5.04	1.17	1.24
1	E	145	ALA	C-O	-5.02	1.17	1.24

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	373	VAL	CB-CA-C	-11.09	95.86	112.05
1	E	373	VAL	CB-CA-C	-10.93	96.10	112.05
1	E	294	VAL	CA-C-N	8.86	130.91	119.84
1	E	294	VAL	C-N-CA	8.86	130.91	119.84
1	G	373	VAL	CB-CA-C	-8.40	99.78	112.05
1	C	373	VAL	CB-CA-C	-8.31	99.92	112.05
1	E	370	TRP	N-CA-C	8.24	128.02	109.81
1	H	412	ARG	NE-CZ-NH2	-7.31	112.62	119.20
1	B	412	ARG	CG-CD-NE	-7.13	96.31	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	168	GLU	CA-C-N	-7.11	112.38	119.56
1	F	168	GLU	C-N-CA	-7.11	112.38	119.56
1	H	129	MET	CA-C-N	-6.85	112.70	119.76
1	H	129	MET	C-N-CA	-6.85	112.70	119.76
1	C	296	THR	N-CA-C	6.72	119.62	110.35
1	G	370	TRP	N-CA-C	6.69	124.60	109.81
1	D	407	ASN	N-CA-C	6.68	118.57	111.28
1	G	105	VAL	CB-CA-C	-6.59	103.53	111.97
1	C	249	ALA	N-CA-C	6.54	119.23	111.71
1	H	412	ARG	CD-NE-CZ	6.53	133.54	124.40
1	B	412	ARG	NE-CZ-NH2	-6.53	113.33	119.20
1	G	296	THR	N-CA-C	6.45	118.34	110.41
1	G	178	MET	CG-SD-CE	-6.42	86.77	100.90
1	G	105	VAL	N-CA-CB	6.32	117.95	110.55
1	D	87	VAL	N-CA-C	-6.30	103.21	111.09
1	C	129	MET	CA-C-N	-6.21	113.37	119.76
1	C	129	MET	C-N-CA	-6.21	113.37	119.76
1	A	10	GLU	N-CA-CB	6.14	118.92	110.01
1	B	364	GLY	N-CA-C	6.11	123.47	115.40
1	F	412	ARG	CG-CD-NE	-6.09	98.61	112.00
1	G	292	GLY	N-CA-C	-5.89	99.22	113.18
1	H	412	ARG	CG-CD-NE	-5.88	99.06	112.00
1	F	356	VAL	CA-C-N	-5.88	114.33	120.38
1	F	356	VAL	C-N-CA	-5.88	114.33	120.38
1	F	129	MET	CA-C-N	-5.71	113.88	119.76
1	F	129	MET	C-N-CA	-5.71	113.88	119.76
1	H	359	ILE	N-CA-C	5.71	115.90	110.42
1	A	370	TRP	N-CA-C	5.64	122.27	109.81
1	B	178	MET	CG-SD-CE	-5.63	88.51	100.90
1	D	355	VAL	N-CA-C	5.63	115.76	110.30
1	H	178	MET	CG-SD-CE	-5.61	88.56	100.90
1	D	31	ILE	CB-CA-C	5.58	115.97	111.06
1	B	317	TYR	N-CA-C	5.58	120.74	113.88
1	A	376	HIS	N-CA-C	5.56	121.09	113.97
1	G	432	TRP	CB-CA-C	5.52	121.41	110.42
1	F	432	TRP	CA-C-N	5.49	131.58	121.70
1	F	432	TRP	C-N-CA	5.49	131.58	121.70
1	G	432	TRP	CA-C-N	5.48	131.56	121.70
1	G	432	TRP	C-N-CA	5.48	131.56	121.70
1	E	378	GLY	N-CA-C	5.41	118.78	112.50
1	B	412	ARG	CD-NE-CZ	5.39	131.95	124.40
1	H	16	ARG	CA-CB-CG	5.38	124.85	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	292	GLY	N-CA-C	-5.36	100.48	113.18
1	A	140	ALA	CA-C-N	5.32	127.36	120.44
1	A	140	ALA	C-N-CA	5.32	127.36	120.44
1	G	253	SER	N-CA-C	-5.29	101.85	110.20
1	H	87	VAL	CA-C-N	5.28	127.61	120.38
1	H	87	VAL	C-N-CA	5.28	127.61	120.38
1	D	36	ILE	CA-C-N	5.27	127.66	120.54
1	D	36	ILE	C-N-CA	5.27	127.66	120.54
1	A	292	GLY	N-CA-C	-5.27	100.69	113.18
1	H	276	GLN	CB-CA-C	-5.26	101.74	110.68
1	C	389	TYR	N-CA-C	5.26	117.42	111.11
1	G	180	LYS	N-CA-C	5.24	119.73	113.23
1	B	357	PRO	N-CA-C	5.24	117.09	110.70
1	A	426	THR	N-CA-CB	5.23	118.39	110.28
1	G	294	VAL	CA-C-N	5.22	126.36	119.84
1	G	294	VAL	C-N-CA	5.22	126.36	119.84
1	H	426	THR	N-CA-CB	5.22	118.33	110.30
1	A	128	ALA	N-CA-C	-5.21	106.43	112.89
1	H	16	ARG	CB-CA-C	5.19	120.39	110.17
1	B	426	THR	CB-CA-C	5.18	120.62	110.67
1	C	84	MET	N-CA-C	5.16	116.50	110.31
1	C	348	VAL	N-CA-CB	5.13	119.69	111.23
1	D	325	THR	CB-CA-C	5.12	117.88	109.90
1	D	364	GLY	N-CA-C	5.11	122.95	115.08
1	E	373	VAL	N-CA-CB	5.11	118.56	110.54
1	E	348	VAL	N-CA-CB	5.08	119.61	111.23
1	E	407	ASN	N-CA-C	5.07	116.81	111.28
1	B	197	THR	N-CA-C	-5.06	101.91	109.95
1	C	378	GLY	N-CA-C	5.03	118.33	112.50
1	A	357	PRO	N-CA-C	5.00	116.81	110.70

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	GLY	Peptide
1	A	294	VAL	Peptide
1	A	347	GLN	Peptide
1	A	369	PRO	Peptide
1	B	2	SER	Peptide
1	B	309	SER	Peptide
1	B	363	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	B	60	GLU	Peptide
1	C	292	GLY	Peptide
1	C	295	PRO	Peptide
1	C	347	GLN	Peptide
1	D	432	TRP	Peptide
1	E	291	GLY	Peptide
1	E	294	VAL	Peptide
1	E	347	GLN	Peptide
1	E	369	PRO	Peptide
1	E	432	TRP	Peptide
1	G	292	GLY	Peptide
1	G	317	TYR	Peptide
1	G	347	GLN	Peptide
1	G	369	PRO	Peptide
1	H	412	ARG	Sidechain
1	H	60	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3338	0	3320	44	1
1	B	3290	0	3252	30	1
1	C	3338	0	3320	31	0
1	D	3286	0	3241	46	0
1	E	3338	0	3320	47	0
1	F	3282	0	3230	39	0
1	G	3338	0	3320	50	1
1	H	3286	0	3241	37	1
2	A	13	0	5	0	0
2	B	13	0	5	0	0
2	C	13	0	5	0	0
2	D	13	0	5	1	0
2	E	13	0	5	0	0
2	F	13	0	5	2	0
2	G	13	0	5	0	0
2	H	13	0	5	0	0
3	A	123	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	121	0	0	2	0
3	C	118	0	0	0	0
3	D	122	0	0	3	0
3	E	113	0	0	2	0
3	F	116	0	0	2	0
3	G	120	0	0	7	0
3	H	140	0	0	2	0
All	All	27573	0	26284	301	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (301) 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:G:432:TRP:C	3:G:602:HOH:O	1.97	1.06
1:H:138:MET:HE1	1:H:191:MET:SD	1.99	1.02
1:G:3:PHE:CG	3:G:650:HOH:O	2.14	0.98
1:G:432:TRP:CA	3:G:602:HOH:O	2.18	0.91
1:F:178:MET:HE2	1:F:405:LEU:HD12	1.51	0.90
1:A:178:MET:CE	1:A:405:LEU:HD12	2.06	0.86
1:C:178:MET:HE2	1:C:405:LEU:HD12	1.56	0.84
1:G:3:PHE:CD2	3:G:650:HOH:O	2.31	0.82
1:G:178:MET:HE1	1:G:402:LEU:HA	1.61	0.81
1:F:178:MET:CE	1:F:405:LEU:HD12	2.10	0.81
1:G:432:TRP:HA	3:G:602:HOH:O	1.80	0.80
1:B:178:MET:HE2	1:B:405:LEU:HD12	1.64	0.79
1:H:178:MET:HE2	1:H:405:LEU:HD12	1.63	0.79
1:B:162:ASN:HD21	1:D:433:ALA:HB1	1.47	0.78
1:E:178:MET:HE1	1:E:401:ALA:CB	2.13	0.78
1:B:178:MET:HE1	1:B:401:ALA:C	2.09	0.77
1:C:178:MET:HE1	1:C:401:ALA:C	2.10	0.77
1:D:60:GLU:OE2	1:D:61:GLY:N	2.18	0.77
1:E:178:MET:HE2	1:E:405:LEU:HD12	1.65	0.77
1:H:178:MET:HE1	1:H:401:ALA:C	2.10	0.76
1:D:178:MET:HE2	1:D:405:LEU:HD12	1.69	0.75
1:E:178:MET:CE	1:E:405:LEU:HD12	2.17	0.74
1:F:190:ARG:HH21	1:F:197:THR:HG22	1.53	0.74
1:G:178:MET:CE	1:G:402:LEU:HA	2.18	0.73
1:A:178:MET:HE1	1:A:401:ALA:CB	2.19	0.72
1:G:138:MET:SD	1:G:191:MET:HE1	2.28	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:259:TYR:CZ	1:H:263:MET:HE3	2.26	0.71
1:A:178:MET:HE1	1:A:401:ALA:HB1	1.73	0.70
1:B:162:ASN:HB3	1:B:165:THR:HG22	1.71	0.70
1:A:138:MET:SD	1:A:191:MET:HE1	2.32	0.69
1:D:178:MET:CE	1:D:405:LEU:HD12	2.22	0.69
1:D:84:MET:HE3	1:D:85:PRO:HD2	1.75	0.68
1:E:14:GLN:HE21	1:E:14:GLN:HA	1.59	0.68
1:F:178:MET:HE1	1:F:401:ALA:C	2.19	0.67
1:D:57:ASP:HB3	1:D:60:GLU:O	1.95	0.67
1:D:138:MET:HE2	1:D:188:ILE:HG23	1.78	0.66
1:B:178:MET:HE1	1:B:401:ALA:O	1.96	0.66
1:A:77:PRO:HG2	1:A:105:VAL:HG21	1.78	0.65
1:C:178:MET:HE1	1:C:401:ALA:O	1.96	0.65
1:A:77:PRO:CG	1:A:105:VAL:HG21	2.27	0.64
1:G:328:ARG:HB2	1:G:373:VAL:HG13	1.79	0.64
1:E:178:MET:HE1	1:E:401:ALA:HB3	1.79	0.64
1:A:178:MET:HE2	1:A:405:LEU:HD12	1.80	0.62
1:G:282:ILE:HG23	1:G:348:VAL:HG11	1.81	0.62
1:G:178:MET:HE1	1:G:402:LEU:CA	2.30	0.62
1:C:36:ILE:HG12	1:D:31:ILE:HD13	1.81	0.61
1:H:73:LEU:HD22	1:H:84:MET:HE1	1.81	0.61
1:D:60:GLU:OE2	1:D:60:GLU:C	2.43	0.61
1:G:56:LEU:HD13	1:G:321:VAL:HG11	1.81	0.61
1:G:328:ARG:CB	1:G:373:VAL:HG13	2.31	0.61
1:C:259:TYR:CZ	1:C:263:MET:HE3	2.36	0.61
1:C:27:GLY:O	1:D:37:SER:HB2	2.01	0.61
1:D:178:MET:HE1	1:D:401:ALA:C	2.25	0.60
1:G:193:TYR:CG	1:G:388:GLU:HG2	2.37	0.60
1:A:190:ARG:HH21	1:A:197:THR:HG22	1.65	0.59
1:B:163:LYS:HD3	3:D:633:HOH:O	2.01	0.59
1:D:178:MET:HE1	1:D:401:ALA:CB	2.32	0.59
1:E:343:ASP:O	1:E:346:PHE:O	2.20	0.59
1:G:56:LEU:HD13	1:G:321:VAL:CG1	2.32	0.59
1:C:344:PRO:HA	1:C:347:GLN:HE22	1.67	0.59
1:F:56:LEU:HD22	1:F:235:HIS:CD2	2.38	0.58
1:B:73:LEU:HD22	1:B:84:MET:HE1	1.85	0.58
1:A:358:PRO:O	1:A:362:SER:N	2.36	0.58
1:C:294:VAL:HG13	1:C:295:PRO:HD3	1.85	0.58
1:E:152:PHE:CZ	1:E:412:ARG:NH1	2.71	0.58
1:E:178:MET:HE1	1:E:401:ALA:C	2.29	0.58
1:E:282:ILE:HG23	1:E:348:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:SER:OG	1:A:214:MET:HE1	2.05	0.57
1:A:282:ILE:HG23	1:A:348:VAL:HG11	1.87	0.57
1:G:157:ASN:HB3	3:G:699:HOH:O	2.05	0.56
1:A:426:THR:HG23	1:B:52:ASP:OD2	2.05	0.56
1:D:138:MET:HE1	1:D:191:MET:SD	2.45	0.56
1:F:151:LYS:NZ	1:F:176:ASP:OD2	2.38	0.56
1:G:18:ARG:NH2	1:H:427:ASP:OD1	2.38	0.56
1:G:343:ASP:O	1:G:346:PHE:O	2.23	0.56
1:D:155:TYR:OH	1:D:165:THR:HG22	2.06	0.56
1:H:84:MET:HE3	1:H:85:PRO:HD2	1.87	0.56
1:D:198:HIS:HD2	3:D:715:HOH:O	1.89	0.56
1:H:178:MET:CE	1:H:405:LEU:HD12	2.33	0.56
1:A:343:ASP:O	1:A:346:PHE:O	2.23	0.55
1:E:360:LEU:O	1:E:364:GLY:HA2	2.07	0.55
1:H:314:ILE:HD12	1:H:314:ILE:N	2.21	0.55
1:G:178:MET:HE3	1:G:402:LEU:HD23	1.89	0.55
1:G:198:HIS:HD2	3:G:713:HOH:O	1.90	0.55
1:C:36:ILE:HG12	1:D:31:ILE:CD1	2.37	0.54
1:E:48:SER:HB2	1:F:43:MET:HG2	1.89	0.54
1:G:131:ARG:NH1	1:G:191:MET:HG2	2.22	0.54
1:H:183:SER:OG	1:H:214:MET:HE1	2.07	0.54
1:F:84:MET:HE3	1:F:85:PRO:HD2	1.90	0.54
1:H:4:LEU:HD13	1:H:92:TYR:CD2	2.43	0.54
1:D:359:ILE:O	1:D:363:LEU:HB2	2.08	0.53
1:D:73:LEU:HD22	1:D:84:MET:HE1	1.90	0.53
1:G:52:ASP:OD2	1:H:426:THR:HG23	2.08	0.53
1:G:131:ARG:HD3	1:G:191:MET:HE3	1.91	0.53
1:F:286:ILE:HD11	1:F:348:VAL:HG21	1.91	0.52
1:E:249:ALA:O	1:E:412:ARG:NH2	2.42	0.52
1:E:259:TYR:CZ	1:E:263:MET:HE3	2.45	0.52
1:H:178:MET:HE1	1:H:401:ALA:O	2.09	0.52
1:A:8:LEU:HD23	1:A:167:TRP:CZ3	2.44	0.52
2:F:501:CIT:H22	3:F:670:HOH:O	2.10	0.52
1:B:84:MET:HE3	1:B:85:PRO:HD2	1.92	0.51
1:E:328:ARG:CB	1:E:373:VAL:HG13	2.40	0.51
1:B:178:MET:CE	1:B:402:LEU:HA	2.40	0.51
1:F:207:LEU:C	1:F:207:LEU:HD23	2.36	0.51
1:H:151:LYS:NZ	1:H:176:ASP:OD2	2.44	0.51
1:A:328:ARG:CB	1:A:373:VAL:HG13	2.41	0.51
1:D:317:TYR:O	1:D:370:TRP:O	2.29	0.51
1:E:249:ALA:CB	1:E:408:LEU:HD22	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:ASP:HB3	1:F:60:GLU:O	2.11	0.51
1:G:131:ARG:CD	1:G:191:MET:HE3	2.41	0.51
1:F:259:TYR:CZ	1:F:263:MET:HE3	2.45	0.51
1:F:319:HIS:CD2	1:F:322:LEU:HD12	2.45	0.51
1:C:343:ASP:O	1:C:346:PHE:O	2.29	0.51
1:C:29:VAL:HB	1:D:36:ILE:HD12	1.91	0.51
1:C:178:MET:CE	1:C:405:LEU:HD12	2.33	0.51
1:C:282:ILE:HG23	1:C:348:VAL:HG11	1.94	0.51
1:F:21:ARG:HD2	1:F:25:GLU:OE1	2.11	0.51
1:C:275:ASN:C	1:C:275:ASN:OD1	2.55	0.50
1:F:325:THR:HG23	1:F:325:THR:O	2.12	0.50
1:C:196:ASP:OD1	1:C:198:HIS:HE1	1.94	0.50
1:F:412:ARG:NH2	3:F:601:HOH:O	2.43	0.50
1:G:329:TYR:CD1	1:G:376:HIS:HB2	2.47	0.50
1:E:113:LYS:HD3	1:E:203:PRO:O	2.11	0.50
1:E:207:LEU:C	1:E:207:LEU:HD23	2.36	0.50
1:H:228:TYR:CD1	1:H:228:TYR:C	2.90	0.49
1:C:52:ASP:OD2	1:D:426:THR:HG23	2.13	0.49
1:C:206:ASP:OD2	1:C:226:ARG:NE	2.39	0.49
1:E:249:ALA:HB1	1:E:412:ARG:HH21	1.78	0.49
1:E:333:ARG:HH12	1:E:350:SER:HG	1.58	0.49
1:B:319:HIS:O	1:B:320:ALA:HB2	2.13	0.49
1:D:178:MET:HE1	1:D:401:ALA:HB1	1.93	0.49
1:F:12:ILE:HG12	1:F:413:ALA:HB1	1.94	0.49
1:H:325:THR:HG23	1:H:325:THR:O	2.12	0.49
1:E:178:MET:HE1	1:E:401:ALA:HB1	1.94	0.48
1:A:343:ASP:OD2	1:A:383:HIS:HD2	1.95	0.48
1:D:412:ARG:NH1	3:D:605:HOH:O	2.46	0.48
1:F:319:HIS:O	1:F:320:ALA:HB2	2.13	0.48
1:G:7:LYS:NZ	1:G:98:ASP:OD2	2.45	0.48
1:D:207:LEU:HD23	1:D:207:LEU:C	2.39	0.48
1:B:319:HIS:O	1:B:320:ALA:CB	2.62	0.48
1:C:344:PRO:O	1:C:347:GLN:O	2.32	0.48
1:G:196:ASP:OD1	1:G:198:HIS:HE1	1.96	0.48
1:B:178:MET:HE1	1:B:402:LEU:N	2.29	0.48
1:E:56:LEU:HD13	1:E:321:VAL:CG1	2.44	0.48
1:G:294:VAL:HG13	1:G:295:PRO:HD3	1.96	0.48
1:A:293:LYS:O	1:A:294:VAL:HB	2.14	0.48
1:A:344:PRO:O	1:A:347:GLN:O	2.32	0.47
1:C:40:ILE:HB	1:D:23:LEU:HD21	1.96	0.47
1:G:138:MET:HE1	1:G:191:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:73:LEU:HD22	1:H:84:MET:CE	2.44	0.47
1:F:196:ASP:OD1	1:F:198:HIS:HE1	1.97	0.47
1:B:178:MET:HE3	1:B:402:LEU:HA	1.97	0.47
1:G:431:LYS:O	1:G:433:ALA:N	2.47	0.47
1:H:372:ASN:OD1	1:H:374:ASP:HB2	2.14	0.47
1:F:73:LEU:HD22	1:F:84:MET:HE1	1.96	0.47
1:G:178:MET:HE1	1:G:401:ALA:C	2.40	0.47
1:G:328:ARG:HB3	1:G:373:VAL:CG1	2.45	0.47
1:A:52:ASP:OD2	1:B:426:THR:CG2	2.62	0.47
1:A:60:GLU:HG3	3:A:712:HOH:O	2.14	0.47
1:A:77:PRO:HG3	1:A:105:VAL:HG21	1.95	0.47
1:D:263:MET:HA	1:D:263:MET:HE2	1.96	0.47
1:G:259:TYR:CZ	1:G:263:MET:HE3	2.49	0.47
1:E:138:MET:SD	1:E:191:MET:HE1	2.55	0.47
1:A:322:LEU:O	1:A:368:ASP:HB2	2.15	0.47
1:A:259:TYR:CZ	1:A:263:MET:HE3	2.50	0.47
1:C:343:ASP:OD2	1:C:383:HIS:CD2	2.68	0.47
1:E:21:ARG:HD2	3:E:681:HOH:O	2.14	0.47
1:E:295:PRO:C	1:E:351:MET:HE1	2.40	0.47
1:A:178:MET:HE1	1:A:401:ALA:C	2.40	0.46
1:F:314:ILE:N	1:F:314:ILE:HD12	2.30	0.46
1:F:412:ARG:HA	1:F:412:ARG:HD3	1.68	0.46
1:A:328:ARG:HB2	1:A:373:VAL:HG13	1.97	0.46
1:H:138:MET:CE	1:H:191:MET:SD	2.90	0.46
1:C:8:LEU:HD21	1:C:409:VAL:HG11	1.97	0.46
1:C:84:MET:HE3	1:C:227:LEU:HD22	1.98	0.46
1:D:138:MET:CE	1:D:188:ILE:HG12	2.46	0.46
1:E:162:ASN:ND2	1:E:164:ASN:H	2.14	0.46
1:E:328:ARG:HB2	1:E:373:VAL:HG13	1.98	0.46
1:E:426:THR:HG23	1:F:52:ASP:OD2	2.15	0.46
1:A:266:LEU:O	1:A:272:GLY:HA3	2.16	0.46
1:H:350:SER:O	1:H:351:MET:C	2.59	0.46
1:A:162:ASN:HD22	1:A:164:ASN:H	1.63	0.46
1:E:233:SER:HA	1:E:399:GLY:O	2.16	0.46
1:E:259:TYR:CZ	1:E:401:ALA:HB2	2.51	0.45
1:E:289:LYS:O	1:E:290:LEU:HD23	2.16	0.45
1:E:318:GLY:HA2	1:E:368:ASP:HB3	1.99	0.45
1:A:92:TYR:CD1	1:A:100:PRO:HB3	2.51	0.45
1:A:131:ARG:NH1	1:A:191:MET:HG2	2.31	0.45
1:C:248:VAL:HG13	1:D:265:GLY:HA2	1.98	0.45
1:H:308:LEU:HG	1:H:312:GLN:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:TYR:CG	1:D:388:GLU:HG2	2.51	0.45
1:G:333:ARG:HA	1:G:376:HIS:NE2	2.31	0.45
1:E:18:ARG:O	1:E:22:LEU:HD13	2.15	0.45
1:F:178:MET:HE2	1:F:405:LEU:CD1	2.36	0.45
1:C:308:LEU:HD12	1:C:308:LEU:C	2.42	0.45
1:E:183:SER:OG	1:E:214:MET:HE1	2.16	0.45
1:F:178:MET:HE1	1:F:401:ALA:O	2.16	0.45
1:A:340:MET:N	1:A:341:PRO:CD	2.80	0.45
1:G:52:ASP:OD2	1:H:426:THR:CG2	2.65	0.45
1:A:228:TYR:CD1	1:A:228:TYR:C	2.94	0.45
1:B:117:ALA:O	1:B:180:LYS:HE3	2.16	0.45
1:E:219:LYS:HG3	1:E:220:PRO:HA	1.99	0.45
1:F:92:TYR:CD1	1:F:100:PRO:HB3	2.51	0.45
1:G:138:MET:CE	1:G:191:MET:HE1	2.47	0.45
1:G:278:VAL:HG11	1:G:375:ALA:HA	1.97	0.45
1:B:116:ARG:HD3	1:B:210:ASP:OD2	2.16	0.45
1:A:56:LEU:HD13	1:A:321:VAL:CG1	2.47	0.44
1:B:16:ARG:NH2	3:B:603:HOH:O	2.43	0.44
1:D:196:ASP:OD1	1:D:198:HIS:HE1	1.99	0.44
1:B:110:GLU:O	1:B:114:LYS:HD2	2.18	0.44
1:B:190:ARG:HH21	1:B:197:THR:HG22	1.82	0.44
1:H:348:VAL:O	1:H:352:LEU:HB2	2.16	0.44
1:D:84:MET:HE2	1:D:227:LEU:HB2	2.00	0.44
1:E:275:ASN:C	1:E:275:ASN:OD1	2.60	0.44
1:F:348:VAL:HG12	1:F:352:LEU:CD2	2.48	0.44
1:B:207:LEU:C	1:B:207:LEU:HD23	2.42	0.44
1:F:319:HIS:CE1	2:F:501:CIT:H41	2.52	0.44
1:A:426:THR:HG21	1:B:15:HIS:CE1	2.52	0.44
1:H:207:LEU:C	1:H:207:LEU:HD23	2.42	0.44
1:C:426:THR:HG21	1:D:15:HIS:CE1	2.53	0.44
1:A:265:GLY:HA2	1:B:248:VAL:HG13	1.99	0.43
1:D:235:HIS:HD2	2:D:501:CIT:O3	2.01	0.43
1:E:426:THR:CG2	1:F:52:ASP:OD2	2.66	0.43
1:G:426:THR:HG22	3:H:614:HOH:O	2.18	0.43
1:H:178:MET:HE3	1:H:402:LEU:HA	1.99	0.43
1:E:131:ARG:NH1	1:E:191:MET:HG2	2.33	0.43
1:H:227:LEU:HG	1:H:231:LEU:HD22	2.00	0.43
1:E:60:GLU:OE2	1:E:63:ARG:NH1	2.51	0.43
1:G:178:MET:HE1	1:G:401:ALA:O	2.19	0.43
1:D:241:SER:H	1:D:271:HIS:HE1	1.65	0.43
1:F:275:ASN:OD1	1:F:275:ASN:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:PHE:HD1	1:B:4:LEU:N	2.16	0.43
1:C:370:TRP:HB3	1:C:371:PRO:HD2	2.01	0.43
1:E:56:LEU:HD13	1:E:321:VAL:HG11	2.00	0.43
1:A:356:VAL:HG12	1:A:360:LEU:HD12	2.01	0.43
1:D:241:SER:H	1:D:271:HIS:CE1	2.36	0.43
1:D:329:TYR:CD2	1:D:371:PRO:HB2	2.53	0.43
1:F:155:TYR:OH	1:F:165:THR:HG22	2.19	0.42
1:G:4:LEU:HD22	1:G:108:VAL:HG22	2.01	0.42
1:G:117:ALA:O	1:G:180:LYS:HE3	2.19	0.42
1:H:56:LEU:HD22	1:H:235:HIS:CD2	2.54	0.42
1:C:89:GLY:HA2	1:C:105:VAL:HG22	2.02	0.42
1:D:94:LEU:HD13	1:D:403:GLY:HA2	2.01	0.42
1:F:278:VAL:HG11	1:F:375:ALA:HA	2.00	0.42
1:H:84:MET:CE	1:H:227:LEU:HD13	2.49	0.42
1:D:249:ALA:CB	1:D:408:LEU:HD22	2.49	0.42
1:E:14:GLN:HE21	1:E:14:GLN:CA	2.31	0.42
1:E:131:ARG:CD	1:E:191:MET:HE3	2.48	0.42
1:D:3:PHE:HA	1:D:107:GLU:OE2	2.19	0.42
1:H:178:MET:CE	1:H:402:LEU:HA	2.50	0.42
1:A:249:ALA:CB	1:A:408:LEU:HD22	2.49	0.42
1:B:308:LEU:HG	3:B:695:HOH:O	2.19	0.42
1:G:426:THR:CG2	3:H:614:HOH:O	2.67	0.42
1:A:289:LYS:O	1:A:290:LEU:HD23	2.19	0.42
1:E:426:THR:HG21	1:F:15:HIS:CE1	2.53	0.42
1:C:56:LEU:HD21	1:C:322:LEU:HD13	2.01	0.42
1:F:117:ALA:O	1:F:180:LYS:HE3	2.20	0.42
1:G:426:THR:HG21	1:H:15:HIS:CE1	2.54	0.42
1:A:178:MET:HE2	1:A:178:MET:HA	2.02	0.42
1:A:263:MET:HE2	1:A:263:MET:HA	2.02	0.42
1:E:333:ARG:NH1	1:E:350:SER:OG	2.42	0.42
1:G:346:PHE:O	1:G:347:GLN:HG2	2.19	0.42
1:D:126:LEU:HD22	1:D:138:MET:HB3	2.01	0.42
1:E:344:PRO:HA	1:E:347:GLN:HE22	1.85	0.42
1:G:52:ASP:CG	1:H:426:THR:HG23	2.44	0.42
1:A:329:TYR:C	1:A:329:TYR:CD1	2.97	0.41
1:D:92:TYR:CD1	1:D:100:PRO:HB3	2.55	0.41
1:C:358:PRO:O	1:C:362:SER:N	2.50	0.41
1:F:319:HIS:O	1:F:320:ALA:CB	2.69	0.41
1:D:73:LEU:HD22	1:D:84:MET:CE	2.50	0.41
1:D:319:HIS:O	1:D:320:ALA:CB	2.68	0.41
1:H:346:PHE:O	1:H:347:GLN:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:MET:HE2	1:E:263:MET:HA	2.02	0.41
1:F:84:MET:HE2	1:F:227:LEU:HB2	2.02	0.41
1:B:329:TYR:CD2	1:B:371:PRO:HB2	2.56	0.41
1:D:60:GLU:OE2	1:D:60:GLU:CA	2.69	0.41
1:E:78:LYS:HD2	3:E:689:HOH:O	2.20	0.41
1:G:54:SER:HB2	1:G:62:ILE:HD11	2.03	0.41
1:B:84:MET:HE3	1:B:85:PRO:CD	2.49	0.41
1:A:278:VAL:HG22	1:A:315:PRO:HB2	2.03	0.41
1:D:228:TYR:CD1	1:D:228:TYR:C	2.99	0.41
1:F:187:TYR:HE2	1:F:191:MET:HE3	1.86	0.41
1:G:181:LEU:N	1:G:182:PRO:CD	2.84	0.41
1:G:183:SER:OG	1:G:214:MET:HE1	2.21	0.41
1:H:8:LEU:HD21	1:H:409:VAL:HG11	2.02	0.41
1:H:21:ARG:HD2	1:H:25:GLU:OE1	2.21	0.41
1:H:325:THR:O	1:H:326:ASP:C	2.64	0.41
1:B:16:ARG:HB3	1:B:17:PRO:HD3	2.03	0.41
1:A:60:GLU:CG	3:A:712:HOH:O	2.69	0.40
1:D:342:ASP:OD1	1:D:342:ASP:N	2.52	0.40
1:F:350:SER:O	1:F:353:TYR:HB3	2.22	0.40
1:F:351:MET:HE2	1:F:351:MET:HB3	2.00	0.40
1:A:31:ILE:HD11	1:B:432:TRP:CE3	2.57	0.40
1:A:118:LEU:HD11	1:A:184:LEU:HA	2.02	0.40
1:C:289:LYS:C	1:C:290:LEU:HD23	2.46	0.40
1:G:7:LYS:CE	1:G:98:ASP:OD2	2.69	0.40
1:B:269:PRO:HA	1:B:273:LEU:HD22	2.04	0.40
1:C:207:LEU:HD23	1:C:207:LEU:C	2.46	0.40
1:E:343:ASP:OD2	1:E:383:HIS:HD2	2.04	0.40
1:G:36:ILE:HD12	1:H:29:VAL:HB	2.04	0.40
1:H:357:PRO:O	1:H:358:PRO:C	2.63	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:102:GLU:OE1	1:H:102:GLU:OE1[1_554]	2.03	0.17
1:A:102:GLU:OE1	1:B:102:GLU:OE1[1_556]	2.11	0.09

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	419/436 (96%)	388 (93%)	18 (4%)	13 (3%)	3	1
1	B	414/436 (95%)	393 (95%)	13 (3%)	8 (2%)	6	4
1	C	419/436 (96%)	389 (93%)	21 (5%)	9 (2%)	5	3
1	D	414/436 (95%)	391 (94%)	18 (4%)	5 (1%)	10	8
1	E	419/436 (96%)	393 (94%)	19 (4%)	7 (2%)	7	5
1	F	414/436 (95%)	381 (92%)	26 (6%)	7 (2%)	7	5
1	G	419/436 (96%)	393 (94%)	16 (4%)	10 (2%)	4	3
1	H	414/436 (95%)	386 (93%)	19 (5%)	9 (2%)	5	3
All	All	3332/3488 (96%)	3114 (94%)	150 (4%)	68 (2%)	6	4

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	VAL
1	A	296	THR
1	A	297	LYS
1	A	365	LYS
1	A	369	PRO
1	A	370	TRP
1	B	236	GLU
1	B	312	GLN
1	B	363	LEU
1	C	163	LYS
1	D	61	GLY
1	E	294	VAL
1	E	295	PRO
1	E	369	PRO
1	E	370	TRP
1	F	290	LEU
1	G	294	VAL

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Mol	Chain	Res	Type
1	G	295	PRO
1	G	363	LEU
1	G	370	TRP
1	G	432	TRP
1	H	291	GLY
1	H	363	LEU
1	A	362	SER
1	A	363	LEU
1	A	432	TRP
1	B	291	GLY
1	B	320	ALA
1	B	432	TRP
1	C	206	ASP
1	C	348	VAL
1	D	320	ALA
1	D	363	LEU
1	E	236	GLU
1	F	291	GLY
1	F	320	ALA
1	F	363	LEU
1	G	297	LYS
1	G	369	PRO
1	H	61	GLY
1	H	308	LEU
1	H	320	ALA
1	H	325	THR
1	A	3	PHE
1	A	236	GLU
1	A	347	GLN
1	B	308	LEU
1	C	236	GLU
1	C	294	VAL
1	C	310	SER
1	C	347	GLN
1	D	289	LYS
1	E	347	GLN
1	F	236	GLU
1	G	236	GLU
1	G	347	GLN
1	H	432	TRP
1	C	295	PRO
1	E	348	VAL

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Mol	Chain	Res	Type
1	H	236	GLU
1	H	350	SER
1	B	61	GLY
1	C	365	LYS
1	D	236	GLU
1	F	312	GLN
1	A	348	VAL
1	F	359	ILE
1	G	348	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	352/366 (96%)	327 (93%)	25 (7%)	13	16
1	B	345/366 (94%)	325 (94%)	20 (6%)	18	22
1	C	352/366 (96%)	333 (95%)	19 (5%)	20	25
1	D	344/366 (94%)	321 (93%)	23 (7%)	15	17
1	E	352/366 (96%)	326 (93%)	26 (7%)	13	14
1	F	343/366 (94%)	330 (96%)	13 (4%)	29	40
1	G	352/366 (96%)	326 (93%)	26 (7%)	13	14
1	H	344/366 (94%)	324 (94%)	20 (6%)	18	22
All	All	2784/2928 (95%)	2612 (94%)	172 (6%)	16	20

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	14	GLN
1	A	21	ARG
1	A	22	LEU
1	A	23	LEU
1	A	31	ILE

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Mol	Chain	Res	Type
1	A	56	LEU
1	A	103	LYS
1	A	162	ASN
1	A	197	THR
1	A	206	ASP
1	A	235	HIS
1	A	284	GLU
1	A	290	LEU
1	A	297	LYS
1	A	308	LEU
1	A	322	LEU
1	A	323	ARG
1	A	347	GLN
1	A	365	LYS
1	A	367	LYS
1	A	373	VAL
1	A	418	ILE
1	A	423	SER
1	A	426	THR
1	B	22	LEU
1	B	53	ILE
1	B	60	GLU
1	B	107	GLU
1	B	114	LYS
1	B	197	THR
1	B	231	LEU
1	B	235	HIS
1	B	308	LEU
1	B	310	SER
1	B	324	LYS
1	B	342	ASP
1	B	345	ILE
1	B	352	LEU
1	B	363	LEU
1	B	365	LYS
1	B	367	LYS
1	B	412	ARG
1	B	420	ARG
1	B	426	THR
1	C	3	PHE
1	C	22	LEU
1	C	23	LEU

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Mol	Chain	Res	Type
1	C	56	LEU
1	C	102	GLU
1	C	110	GLU
1	C	197	THR
1	C	235	HIS
1	C	290	LEU
1	C	294	VAL
1	C	297	LYS
1	C	308	LEU
1	C	322	LEU
1	C	323	ARG
1	C	340	MET
1	C	347	GLN
1	C	359	ILE
1	C	365	LYS
1	C	373	VAL
1	D	11	LYS
1	D	22	LEU
1	D	24	LYS
1	D	31	ILE
1	D	59	GLU
1	D	60	GLU
1	D	103	LYS
1	D	106	LYS
1	D	114	LYS
1	D	165	THR
1	D	197	THR
1	D	231	LEU
1	D	284	GLU
1	D	307	THR
1	D	324	LYS
1	D	325	THR
1	D	352	LEU
1	D	362	SER
1	D	363	LEU
1	D	365	LYS
1	D	367	LYS
1	D	376	HIS
1	D	412	ARG
1	E	14	GLN
1	E	23	LEU
1	E	24	LYS

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Mol	Chain	Res	Type
1	E	31	ILE
1	E	56	LEU
1	E	74	GLU
1	E	102	GLU
1	E	114	LYS
1	E	163	LYS
1	E	197	THR
1	E	235	HIS
1	E	284	GLU
1	E	290	LEU
1	E	296	THR
1	E	297	LYS
1	E	308	LEU
1	E	313	VAL
1	E	322	LEU
1	E	323	ARG
1	E	325	THR
1	E	345	ILE
1	E	347	GLN
1	E	350	SER
1	E	373	VAL
1	E	412	ARG
1	E	426	THR
1	F	22	LEU
1	F	60	GLU
1	F	114	LYS
1	F	118	LEU
1	F	165	THR
1	F	191	MET
1	F	197	THR
1	F	231	LEU
1	F	324	LYS
1	F	333	ARG
1	F	352	LEU
1	F	363	LEU
1	F	412	ARG
1	G	14	GLN
1	G	22	LEU
1	G	23	LEU
1	G	31	ILE
1	G	56	LEU
1	G	74	GLU

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Mol	Chain	Res	Type
1	G	78	LYS
1	G	103	LYS
1	G	105	VAL
1	G	114	LYS
1	G	162	ASN
1	G	197	THR
1	G	219	LYS
1	G	235	HIS
1	G	290	LEU
1	G	294	VAL
1	G	297	LYS
1	G	298	GLU
1	G	310	SER
1	G	323	ARG
1	G	347	GLN
1	G	350	SER
1	G	355	VAL
1	G	365	LYS
1	G	366	VAL
1	G	373	VAL
1	H	21	ARG
1	H	22	LEU
1	H	31	ILE
1	H	59	GLU
1	H	60	GLU
1	H	103	LYS
1	H	107	GLU
1	H	114	LYS
1	H	118	LEU
1	H	163	LYS
1	H	165	THR
1	H	191	MET
1	H	231	LEU
1	H	324	LYS
1	H	345	ILE
1	H	363	LEU
1	H	365	LYS
1	H	367	LYS
1	H	412	ARG
1	H	426	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	162	ASN
1	A	271	HIS
1	A	332	GLN
1	A	383	HIS
1	B	15	HIS
1	B	147	GLN
1	B	235	HIS
1	B	271	HIS
1	C	14	GLN
1	C	198	HIS
1	C	271	HIS
1	C	347	GLN
1	C	381	GLN
1	C	383	HIS
1	D	14	GLN
1	D	147	GLN
1	D	198	HIS
1	D	235	HIS
1	D	271	HIS
1	D	381	GLN
1	E	14	GLN
1	E	164	ASN
1	E	271	HIS
1	E	312	GLN
1	E	347	GLN
1	E	381	GLN
1	E	383	HIS
1	F	15	HIS
1	F	147	GLN
1	F	164	ASN
1	F	198	HIS
1	F	235	HIS
1	F	271	HIS
1	F	332	GLN
1	F	376	HIS
1	F	381	GLN
1	G	14	GLN
1	G	162	ASN
1	G	198	HIS
1	G	271	HIS
1	H	15	HIS
1	H	147	GLN

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Mol	Chain	Res	Type
1	H	157	ASN
1	H	198	HIS
1	H	235	HIS
1	H	271	HIS

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](#)

8 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	C	501	-	12,12,12	1.44	1 (8%)	17,17,17	2.03	6 (35%)
2	CIT	H	501	-	12,12,12	2.64	3 (25%)	17,17,17	4.66	10 (58%)
2	CIT	G	501	-	12,12,12	1.45	1 (8%)	17,17,17	1.57	3 (17%)
2	CIT	D	501	-	12,12,12	1.43	1 (8%)	17,17,17	1.91	2 (11%)
2	CIT	A	501	-	12,12,12	1.47	2 (16%)	17,17,17	1.86	5 (29%)
2	CIT	B	501	-	12,12,12	1.36	2 (16%)	17,17,17	1.73	4 (23%)
2	CIT	F	501	-	12,12,12	1.37	1 (8%)	17,17,17	2.32	6 (35%)
2	CIT	E	501	-	12,12,12	1.17	1 (8%)	17,17,17	1.85	5 (29%)

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	C	501	-	-	10/16/16/16	-
2	CIT	H	501	-	-	8/16/16/16	-
2	CIT	G	501	-	-	3/16/16/16	-
2	CIT	D	501	-	-	7/16/16/16	-
2	CIT	A	501	-	-	7/16/16/16	-
2	CIT	B	501	-	-	5/16/16/16	-
2	CIT	F	501	-	-	13/16/16/16	-
2	CIT	E	501	-	-	4/16/16/16	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	501	CIT	C3-C6	7.69	1.61	1.53
2	A	501	CIT	C3-C6	-3.46	1.49	1.53
2	C	501	CIT	C3-C6	-3.30	1.50	1.53
2	G	501	CIT	C4-C3	2.80	1.57	1.54
2	H	501	CIT	C4-C3	-2.60	1.50	1.54
2	F	501	CIT	C4-C3	2.53	1.57	1.54
2	B	501	CIT	C3-C6	-2.43	1.50	1.53
2	H	501	CIT	C2-C3	2.34	1.56	1.54
2	D	501	CIT	O6-C6	-2.20	1.22	1.30
2	A	501	CIT	O6-C6	-2.08	1.23	1.30
2	B	501	CIT	O6-C6	-2.04	1.23	1.30
2	E	501	CIT	O5-C6	2.02	1.28	1.22

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	501	CIT	O7-C3-C6	-12.96	90.57	108.96
2	H	501	CIT	C4-C3-C6	-7.93	92.50	110.03
2	F	501	CIT	O7-C3-C2	-5.68	96.42	109.38
2	H	501	CIT	O6-C6-C3	5.41	123.52	113.14
2	H	501	CIT	O7-C3-C4	5.38	121.65	109.38
2	H	501	CIT	O7-C3-C2	5.18	121.19	109.38
2	E	501	CIT	C4-C3-C6	4.61	120.23	110.03
2	F	501	CIT	C4-C3-C2	4.54	120.96	109.31
2	D	501	CIT	C2-C3-C6	-4.39	100.33	110.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	CIT	C4-C3-C6	4.24	119.41	110.03
2	C	501	CIT	O7-C3-C6	-3.94	103.36	108.96
2	C	501	CIT	C2-C3-C6	-3.75	101.74	110.03
2	H	501	CIT	C3-C4-C5	-3.68	103.86	113.92
2	B	501	CIT	C2-C3-C6	-3.65	101.97	110.03
2	H	501	CIT	C2-C3-C6	-3.64	101.99	110.03
2	B	501	CIT	C4-C3-C6	3.61	118.02	110.03
2	A	501	CIT	O3-C5-C4	-3.40	113.33	122.95
2	C	501	CIT	C4-C3-C6	3.35	117.44	110.03
2	H	501	CIT	O6-C6-O5	-3.22	113.55	123.86
2	A	501	CIT	C4-C3-C6	3.21	117.13	110.03
2	A	501	CIT	O7-C3-C6	-3.14	104.50	108.96
2	F	501	CIT	C3-C2-C1	3.01	122.14	113.92
2	G	501	CIT	O6-C6-C3	2.99	118.88	113.14
2	F	501	CIT	O6-C6-C3	2.93	118.75	113.14
2	G	501	CIT	O7-C3-C6	-2.93	104.81	108.96
2	E	501	CIT	C3-C4-C5	2.85	121.72	113.92
2	E	501	CIT	C2-C3-C6	-2.70	104.07	110.03
2	E	501	CIT	O7-C3-C4	-2.67	103.28	109.38
2	F	501	CIT	C2-C3-C6	2.64	115.88	110.03
2	A	501	CIT	O2-C1-C2	2.50	122.28	114.35
2	C	501	CIT	O3-C5-C4	-2.47	115.96	122.95
2	C	501	CIT	O1-C1-C2	-2.44	116.04	122.95
2	F	501	CIT	O5-C6-C3	-2.43	117.39	122.09
2	B	501	CIT	O6-C6-C3	2.25	117.46	113.14
2	E	501	CIT	O6-C6-C3	2.24	117.43	113.14
2	G	501	CIT	O5-C6-C3	-2.23	117.78	122.09
2	H	501	CIT	C4-C3-C2	2.20	114.96	109.31
2	A	501	CIT	O1-C1-C2	-2.16	116.83	122.95
2	B	501	CIT	C3-C4-C5	2.16	119.82	113.92
2	H	501	CIT	O1-C1-C2	-2.15	116.85	122.95
2	C	501	CIT	O7-C3-C4	2.03	114.01	109.38

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	CIT	O7-C3-C6-O5
2	A	501	CIT	O7-C3-C6-O6
2	A	501	CIT	C4-C3-C6-O5
2	A	501	CIT	C4-C3-C6-O6
2	C	501	CIT	O7-C3-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	501	CIT	C4-C3-C6-O5
2	C	501	CIT	C4-C3-C6-O6
2	F	501	CIT	C1-C2-C3-O7
2	F	501	CIT	C1-C2-C3-C4
2	F	501	CIT	O7-C3-C4-C5
2	H	501	CIT	C2-C3-C6-O5
2	H	501	CIT	C2-C3-C6-O6
2	H	501	CIT	O7-C3-C6-O5
2	H	501	CIT	O7-C3-C6-O6
2	H	501	CIT	O7-C3-C4-C5
2	F	501	CIT	C2-C3-C4-C5
2	F	501	CIT	C6-C3-C4-C5
2	H	501	CIT	C1-C2-C3-O7
2	D	501	CIT	C4-C3-C6-O5
2	D	501	CIT	C4-C3-C6-O6
2	A	501	CIT	C3-C4-C5-O4
2	A	501	CIT	C3-C4-C5-O3
2	C	501	CIT	O7-C3-C6-O5
2	F	501	CIT	O7-C3-C6-O5
2	A	501	CIT	C1-C2-C3-C4
2	C	501	CIT	C3-C4-C5-O4
2	B	501	CIT	C4-C3-C6-O5
2	D	501	CIT	C2-C3-C6-O6
2	C	501	CIT	C3-C4-C5-O3
2	H	501	CIT	O2-C1-C2-C3
2	D	501	CIT	C2-C3-C6-O5
2	E	501	CIT	C2-C3-C6-O5
2	F	501	CIT	C4-C3-C6-O5
2	F	501	CIT	C4-C3-C6-O6
2	G	501	CIT	C2-C3-C6-O6
2	F	501	CIT	C1-C2-C3-C6
2	H	501	CIT	O1-C1-C2-C3
2	F	501	CIT	C3-C4-C5-O4
2	C	501	CIT	C1-C2-C3-C4
2	B	501	CIT	C2-C3-C6-O5
2	B	501	CIT	C2-C3-C6-O6
2	B	501	CIT	C4-C3-C6-O6
2	C	501	CIT	C2-C3-C6-O6
2	E	501	CIT	C2-C3-C6-O6
2	F	501	CIT	C2-C3-C6-O6
2	G	501	CIT	C4-C3-C6-O6
2	F	501	CIT	C3-C4-C5-O3

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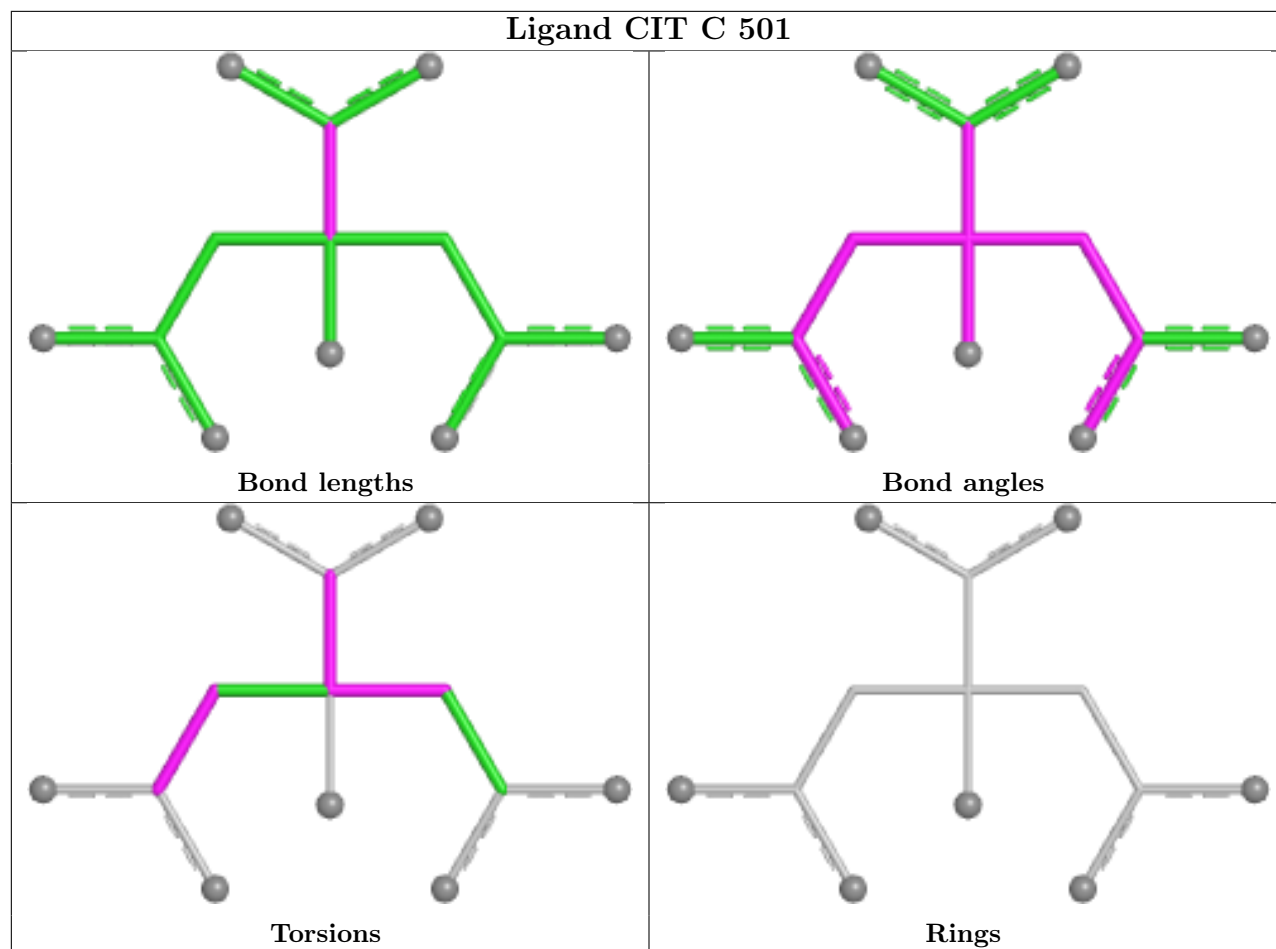
Mol	Chain	Res	Type	Atoms
2	D	501	CIT	C1-C2-C3-C4
2	E	501	CIT	C1-C2-C3-C4
2	G	501	CIT	C1-C2-C3-C4
2	D	501	CIT	O7-C3-C6-O5
2	D	501	CIT	O7-C3-C6-O6
2	E	501	CIT	O7-C3-C6-O5
2	C	501	CIT	C2-C3-C6-O5
2	B	501	CIT	C1-C2-C3-C4
2	C	501	CIT	C1-C2-C3-O7
2	F	501	CIT	O1-C1-C2-C3

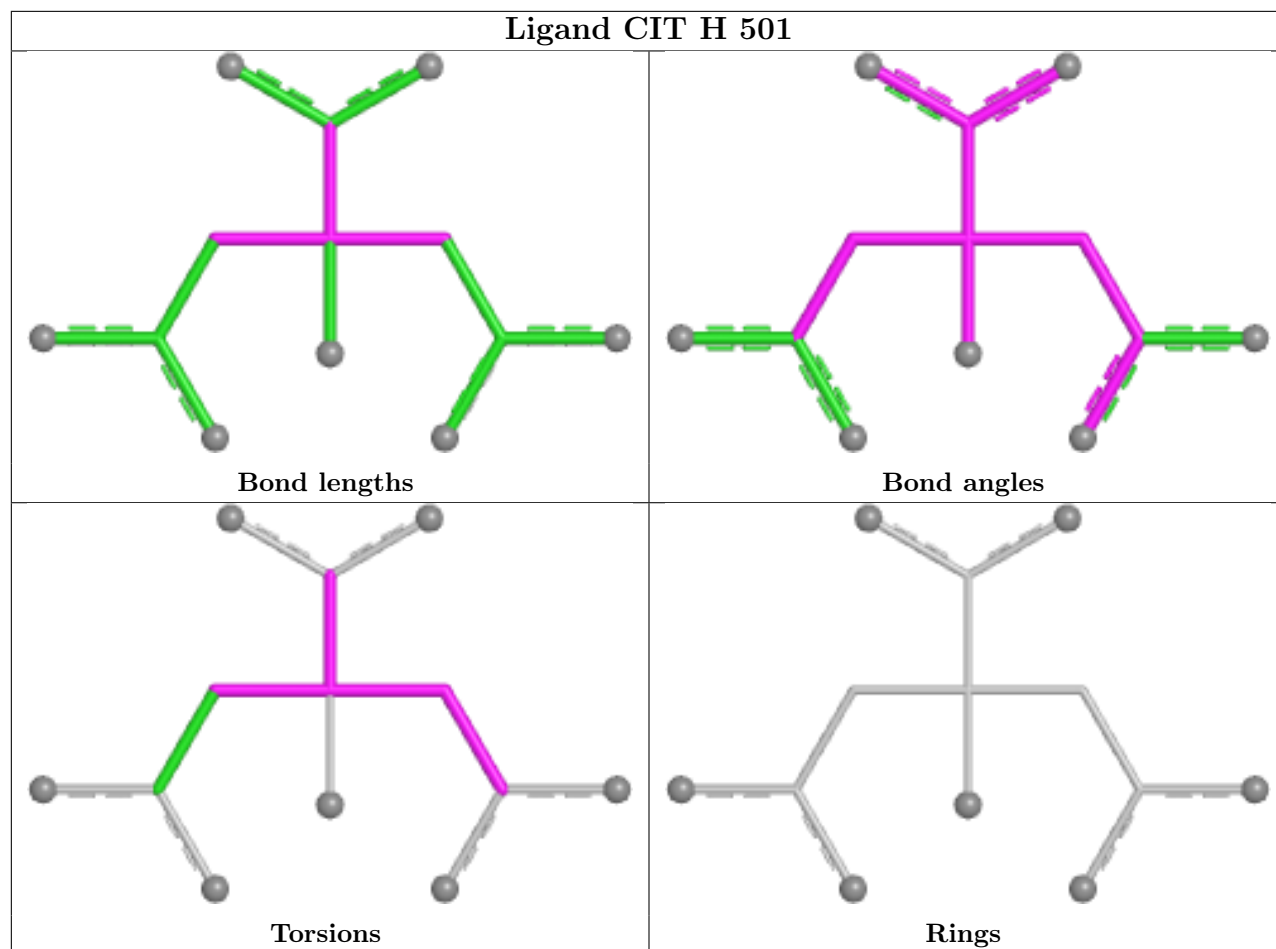
There are no ring outliers.

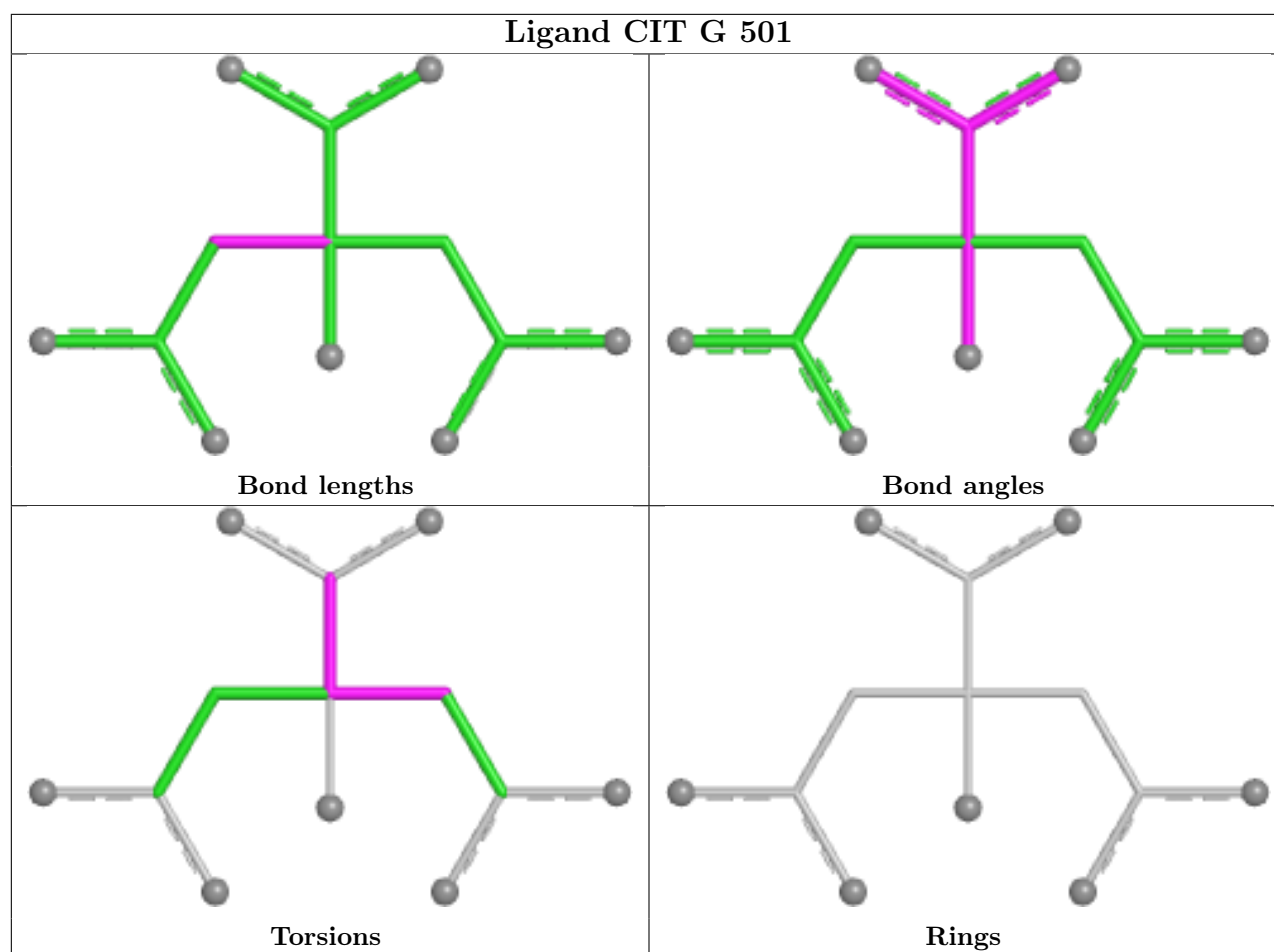
2 monomers are involved in 3 short contacts:

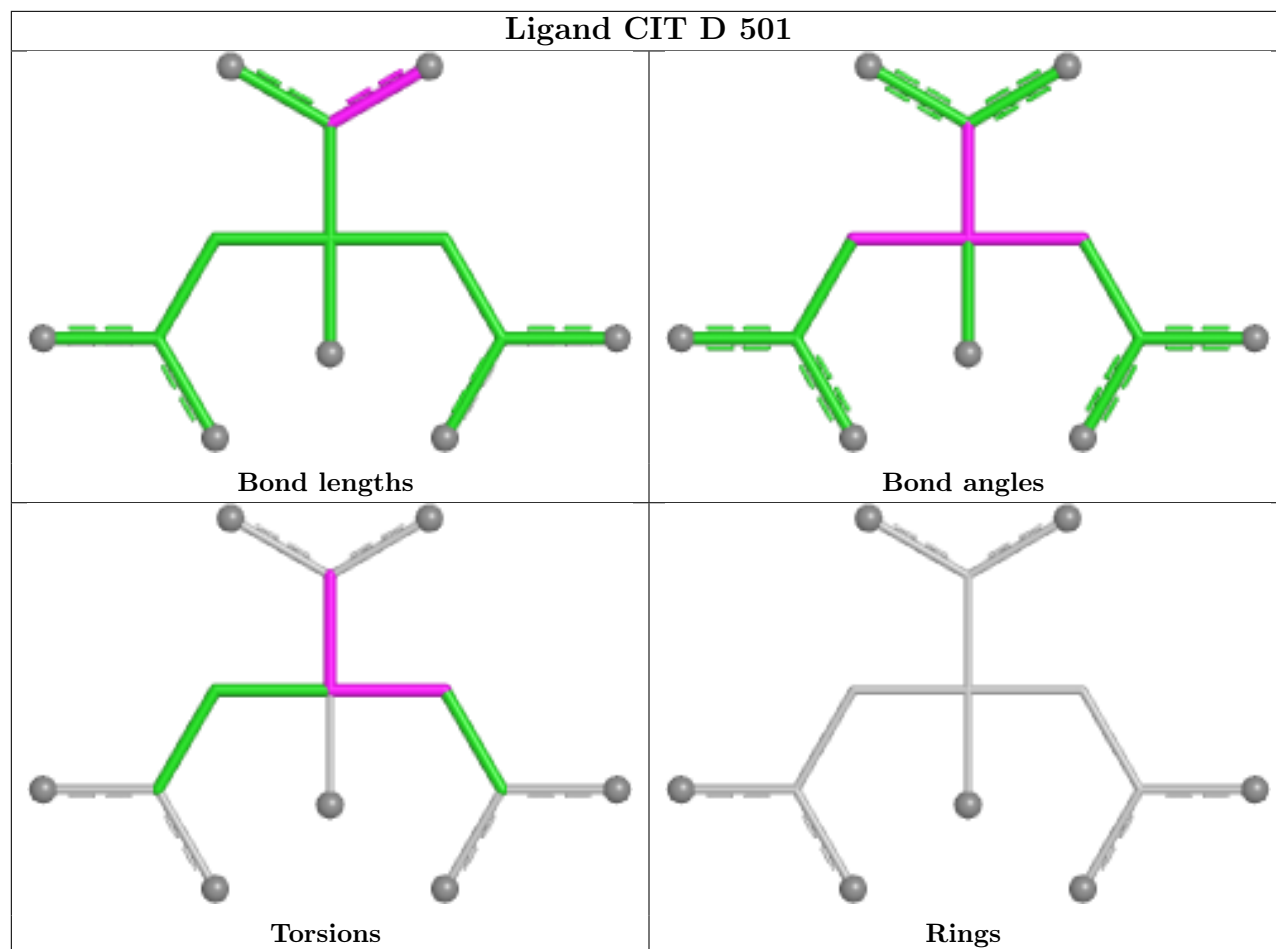
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	CIT	1	0
2	F	501	CIT	2	0

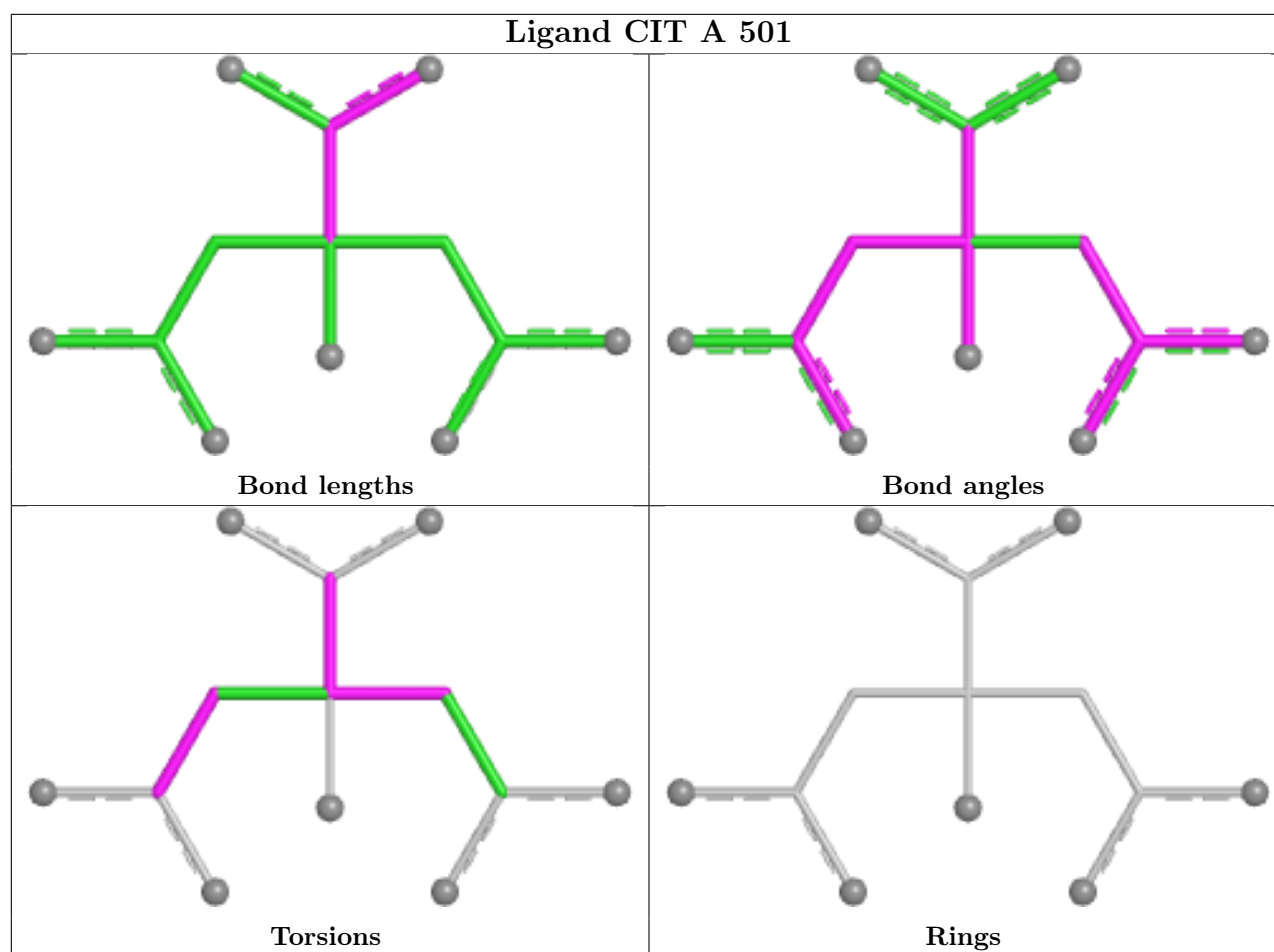
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

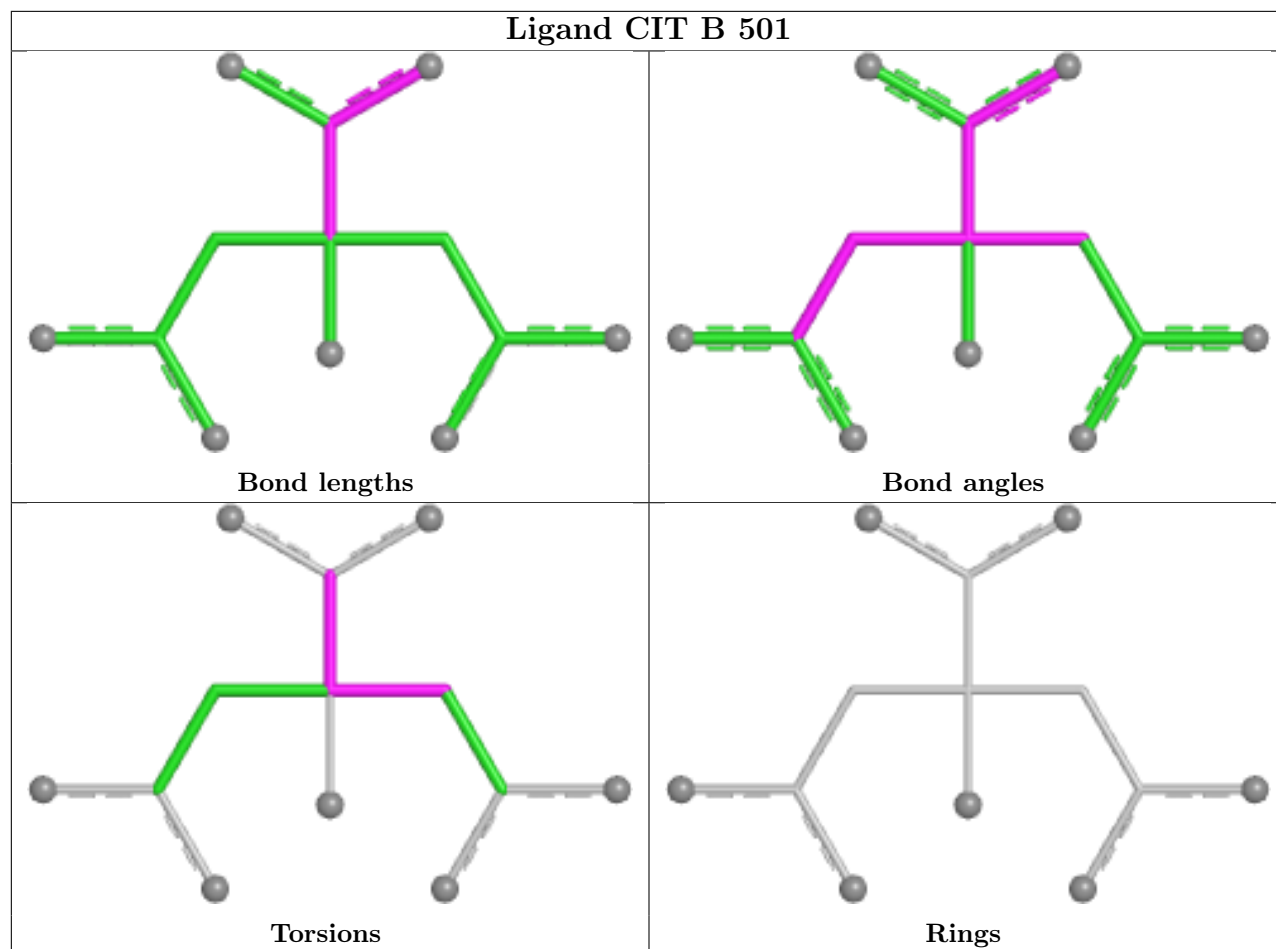


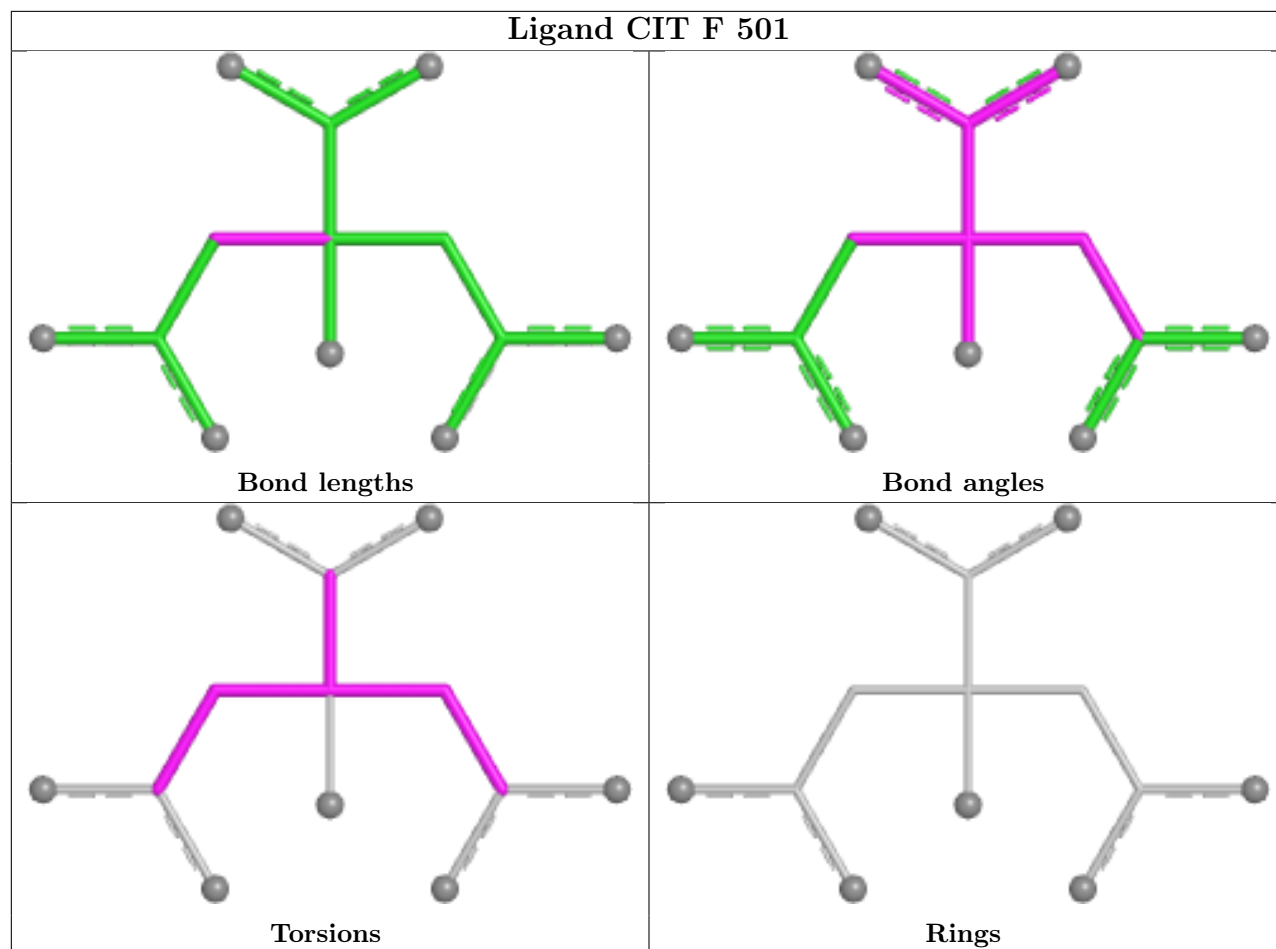


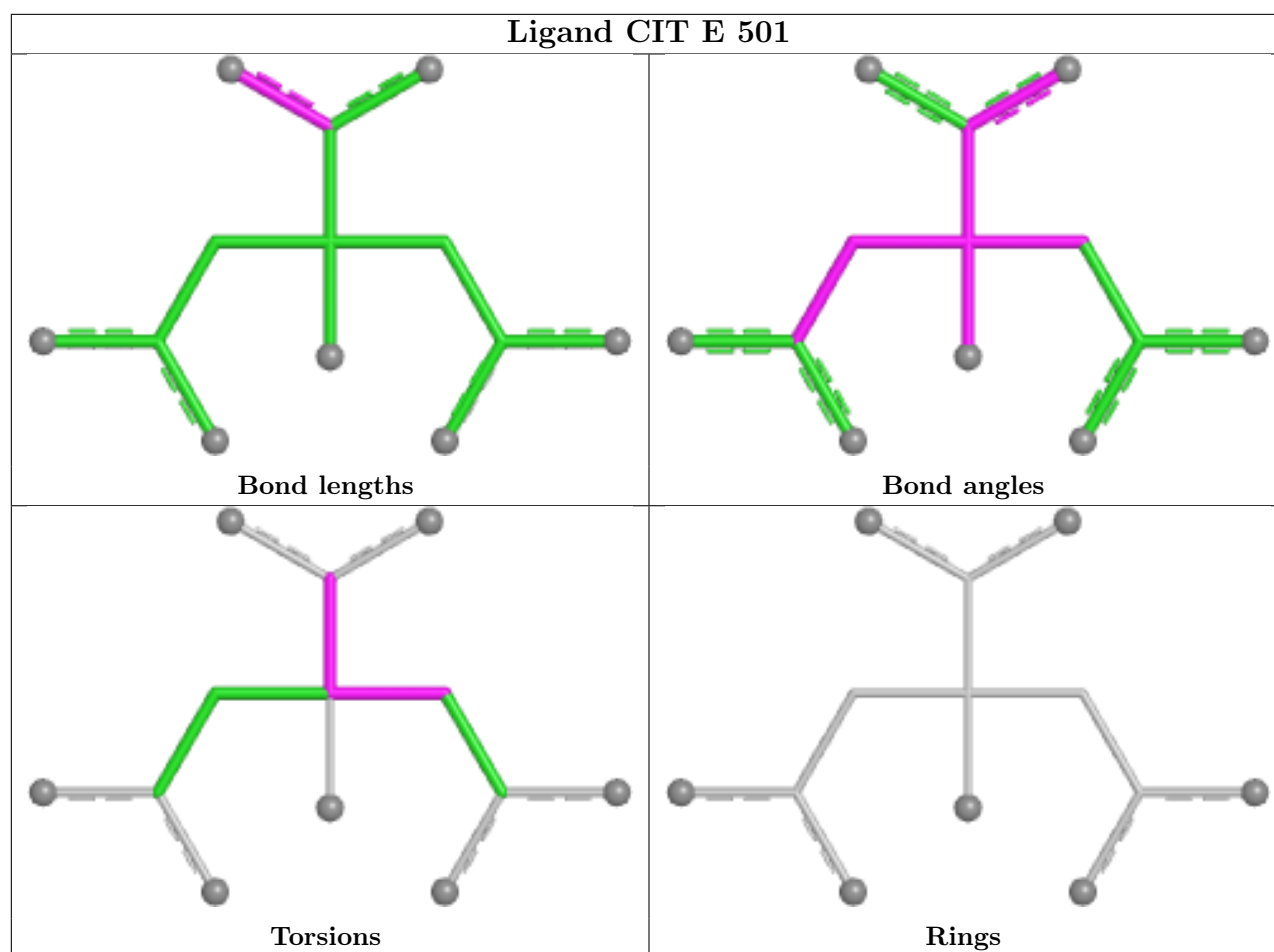












5.7 Other polymers [i](#)

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	423/436 (97%)	0.09	23 (5%)	31	28	16, 31, 70, 114	0
1	B	418/436 (95%)	-0.00	14 (3%)	49	46	16, 29, 66, 93	0
1	C	423/436 (97%)	0.16	19 (4%)	38	35	19, 35, 70, 110	0
1	D	418/436 (95%)	0.08	13 (3%)	51	48	18, 33, 66, 94	0
1	E	423/436 (97%)	0.07	18 (4%)	40	36	16, 31, 73, 116	0
1	F	418/436 (95%)	0.37	43 (10%)	12	9	16, 34, 85, 133	0
1	G	423/436 (97%)	-0.03	14 (3%)	49	46	16, 28, 66, 116	0
1	H	418/436 (95%)	0.12	39 (9%)	14	12	14, 28, 73, 115	0
All	All	3364/3488 (96%)	0.11	183 (5%)	31	28	14, 32, 73, 133	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	363	LEU	6.3
1	F	366	VAL	6.1
1	A	2	SER	5.8
1	H	308	LEU	5.8
1	C	2	SER	5.3
1	B	308	LEU	5.2
1	H	366	VAL	5.2
1	D	432	TRP	5.0
1	G	363	LEU	4.9
1	D	2	SER	4.8
1	F	370	TRP	4.8
1	F	355	VAL	4.7
1	D	307	THR	4.5
1	F	307	THR	4.5
1	E	292	GLY	4.5
1	E	294	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	308	LEU	4.5
1	H	370	TRP	4.5
1	F	308	LEU	4.4
1	F	311	GLY	4.3
1	F	313	VAL	4.3
1	A	296	THR	4.3
1	A	294	VAL	4.2
1	F	325	THR	4.2
1	D	308	LEU	4.2
1	H	359	ILE	4.2
1	C	432	TRP	4.1
1	E	2	SER	4.1
1	F	292	GLY	4.1
1	B	2	SER	4.1
1	F	369	PRO	4.1
1	C	363	LEU	4.0
1	H	314	ILE	4.0
1	F	314	ILE	4.0
1	E	298	GLU	3.9
1	G	2	SER	3.8
1	A	298	GLU	3.8
1	H	313	VAL	3.8
1	H	356	VAL	3.8
1	D	363	LEU	3.7
1	F	365	LYS	3.7
1	H	322	LEU	3.7
1	A	290	LEU	3.6
1	C	366	VAL	3.6
1	B	307	THR	3.6
1	H	292	GLY	3.6
1	C	294	VAL	3.5
1	A	363	LEU	3.4
1	B	292	GLY	3.4
1	F	2	SER	3.4
1	B	313	VAL	3.4
1	G	294	VAL	3.4
1	C	295	PRO	3.4
1	A	292	GLY	3.4
1	E	295	PRO	3.3
1	F	363	LEU	3.3
1	C	290	LEU	3.3
1	D	313	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	363	LEU	3.2
1	E	363	LEU	3.2
1	H	2	SER	3.2
1	D	60	GLU	3.2
1	F	360	LEU	3.2
1	G	308	LEU	3.2
1	G	295	PRO	3.2
1	G	298	GLU	3.2
1	F	357	PRO	3.2
1	B	355	VAL	3.1
1	B	432	TRP	3.1
1	E	432	TRP	3.1
1	A	308	LEU	3.1
1	F	364	GLY	3.1
1	C	292	GLY	3.1
1	H	325	THR	3.1
1	A	433	ALA	3.1
1	F	352	LEU	3.0
1	C	296	THR	2.9
1	A	295	PRO	2.9
1	G	432	TRP	2.9
1	H	355	VAL	2.9
1	E	359	ILE	2.9
1	D	433	ALA	2.9
1	F	31	ILE	2.8
1	C	3	PHE	2.8
1	F	356	VAL	2.8
1	G	102	GLU	2.8
1	D	290	LEU	2.8
1	F	371	PRO	2.8
1	D	292	GLY	2.7
1	F	433	ALA	2.7
1	H	317	TYR	2.7
1	H	315	PRO	2.7
1	H	357	PRO	2.7
1	H	309	SER	2.7
1	A	22	LEU	2.7
1	H	352	LEU	2.7
1	H	369	PRO	2.7
1	F	291	GLY	2.7
1	E	290	LEU	2.6
1	F	353	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	102	GLU	2.6
1	F	358	PRO	2.6
1	C	365	LYS	2.6
1	E	433	ALA	2.6
1	C	308	LEU	2.6
1	A	3	PHE	2.6
1	A	313	VAL	2.6
1	C	433	ALA	2.6
1	H	358	PRO	2.6
1	H	59	GLU	2.5
1	A	366	VAL	2.5
1	F	317	TYR	2.5
1	H	307	THR	2.5
1	F	322	LEU	2.5
1	C	291	GLY	2.5
1	G	296	THR	2.5
1	E	369	PRO	2.5
1	F	315	PRO	2.5
1	F	3	PHE	2.5
1	F	321	VAL	2.5
1	F	320	ALA	2.5
1	C	364	GLY	2.5
1	G	292	GLY	2.5
1	A	355	VAL	2.4
1	F	349	VAL	2.4
1	H	321	VAL	2.4
1	B	289	LYS	2.4
1	F	329	TYR	2.4
1	H	353	TYR	2.4
1	A	369	PRO	2.4
1	H	291	GLY	2.4
1	H	371	PRO	2.4
1	H	324	LYS	2.4
1	B	433	ALA	2.3
1	G	290	LEU	2.3
1	F	351	MET	2.3
1	H	310	SER	2.3
1	E	296	THR	2.3
1	H	364	GLY	2.3
1	A	359	ILE	2.3
1	G	348	VAL	2.3
1	A	293	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	3	PHE	2.3
1	F	359	ILE	2.3
1	E	412	ARG	2.3
1	E	291	GLY	2.3
1	H	365	LYS	2.3
1	B	366	VAL	2.2
1	C	286	ILE	2.2
1	D	311	GLY	2.2
1	H	433	ALA	2.2
1	A	367	LYS	2.2
1	A	364	GLY	2.2
1	F	60	GLU	2.2
1	C	322	LEU	2.2
1	F	56	LEU	2.2
1	F	310	SER	2.2
1	H	60	GLU	2.1
1	B	291	GLY	2.1
1	E	364	GLY	2.1
1	C	297	LYS	2.1
1	F	346	PHE	2.1
1	G	359	ILE	2.1
1	E	347	GLN	2.1
1	A	432	TRP	2.1
1	H	349	VAL	2.1
1	A	360	LEU	2.1
1	F	361	SER	2.1
1	H	56	LEU	2.1
1	H	360	LEU	2.1
1	B	60	GLU	2.1
1	C	298	GLU	2.1
1	H	354	GLU	2.1
1	H	319	HIS	2.1
1	B	318	GLY	2.1
1	D	365	LYS	2.1
1	A	370	TRP	2.1
1	G	370	TRP	2.1
1	F	55	TYR	2.0
1	F	324	LYS	2.0
1	D	314	ILE	2.0
1	E	348	VAL	2.0
1	H	58	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

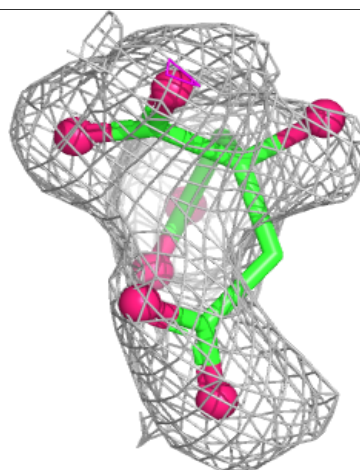
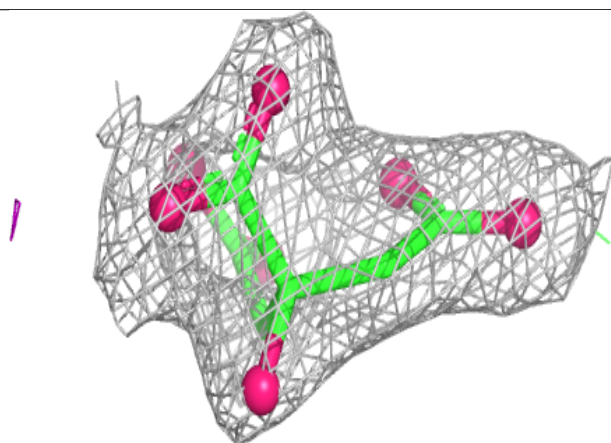
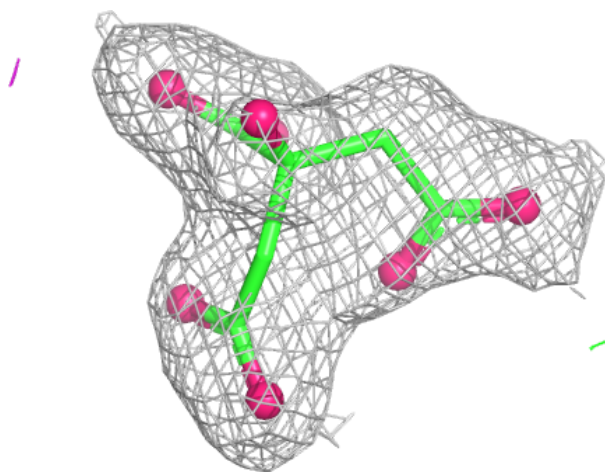
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CIT	F	501	13/13	0.88	0.11	35,45,56,56	0
2	CIT	H	501	13/13	0.91	0.08	22,33,42,48	0
2	CIT	D	501	13/13	0.93	0.07	24,28,37,41	0
2	CIT	A	501	13/13	0.95	0.06	24,29,37,38	0
2	CIT	E	501	13/13	0.95	0.06	24,28,32,34	0
2	CIT	B	501	13/13	0.95	0.06	23,26,34,40	0
2	CIT	C	501	13/13	0.95	0.06	25,33,36,36	0
2	CIT	G	501	13/13	0.96	0.06	22,24,31,35	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.

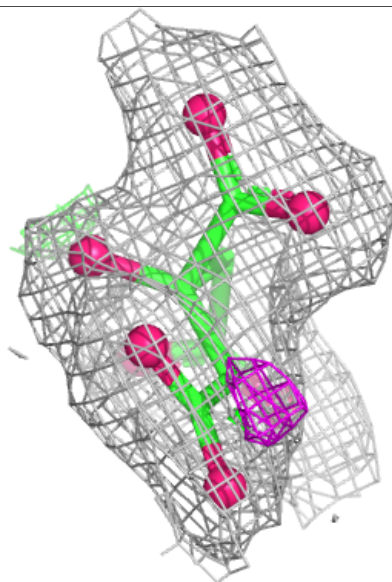
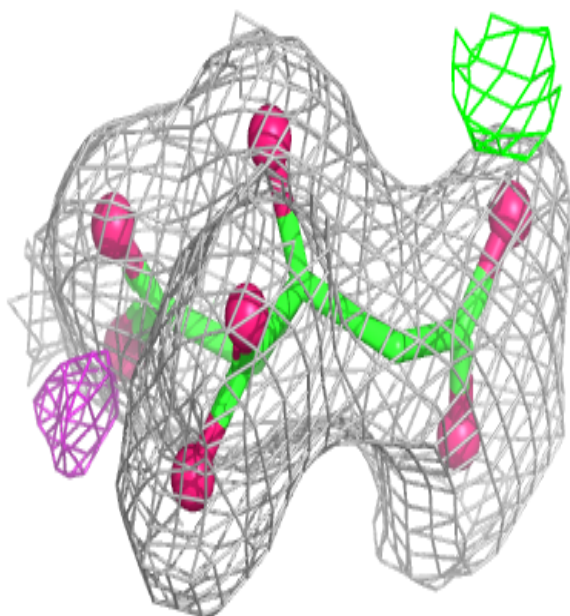
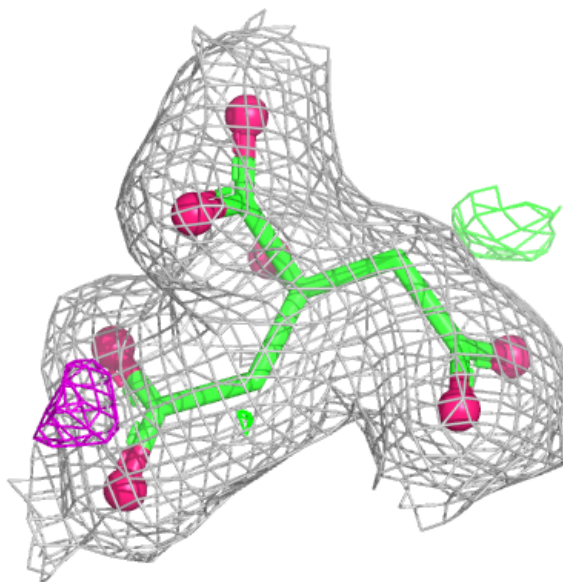
Electron density around CIT F 501:

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



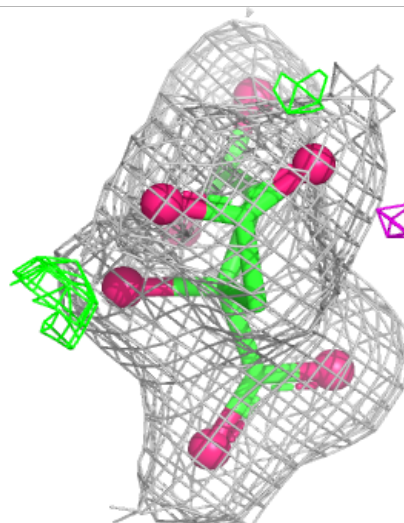
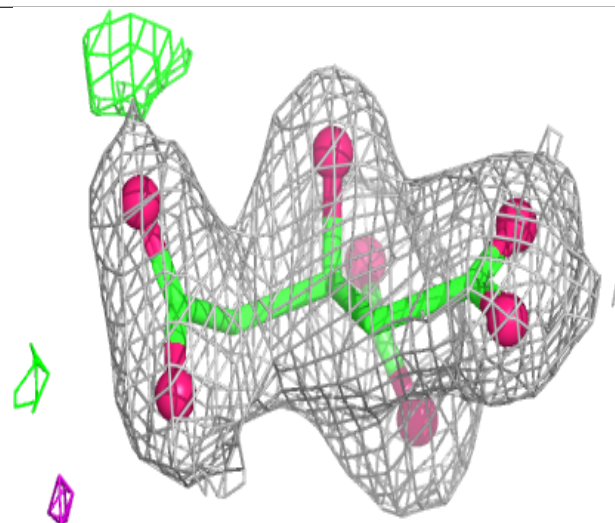
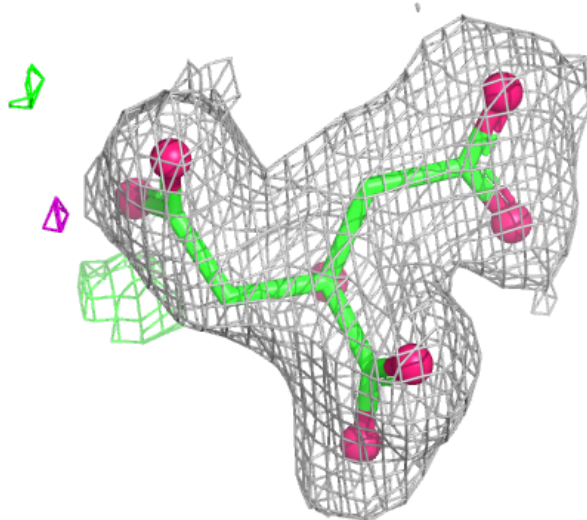
Electron density around CIT H 501:

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



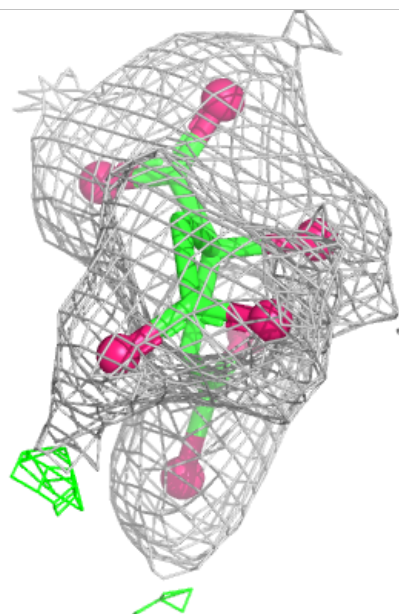
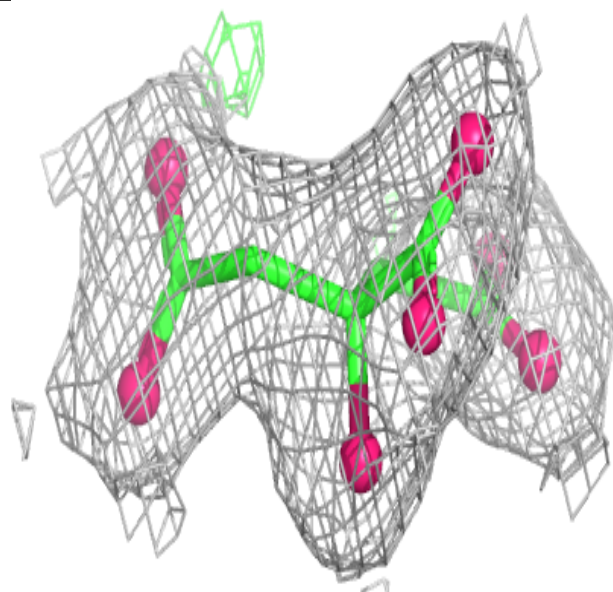
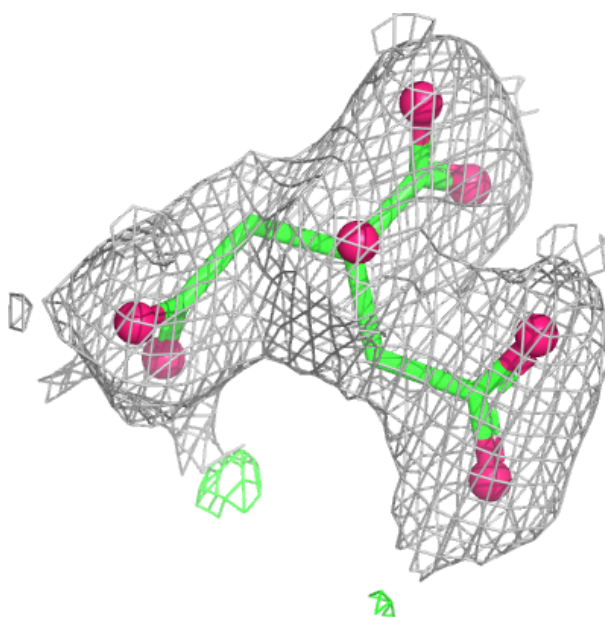
Electron density around CIT D 501:

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



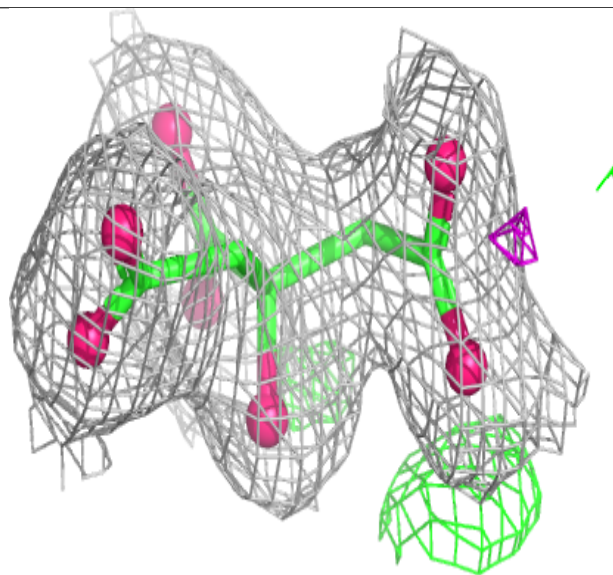
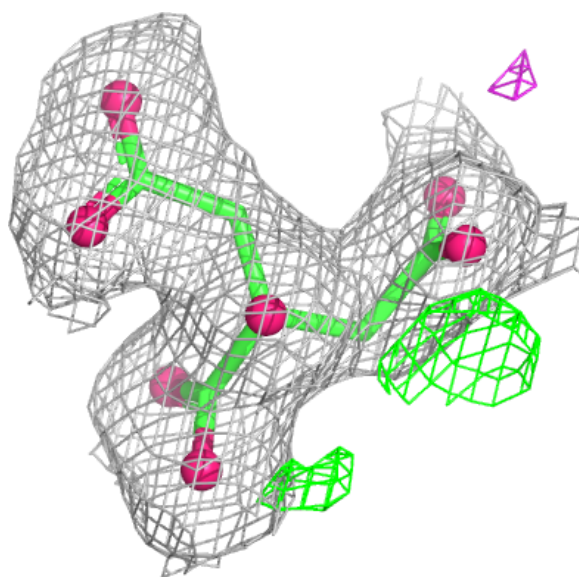
Electron density around CIT A 501:

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



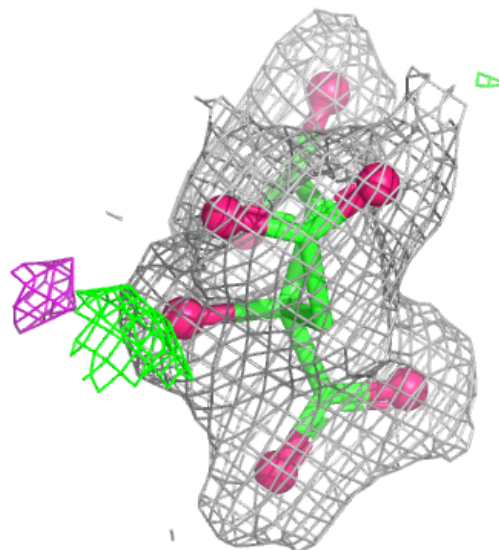
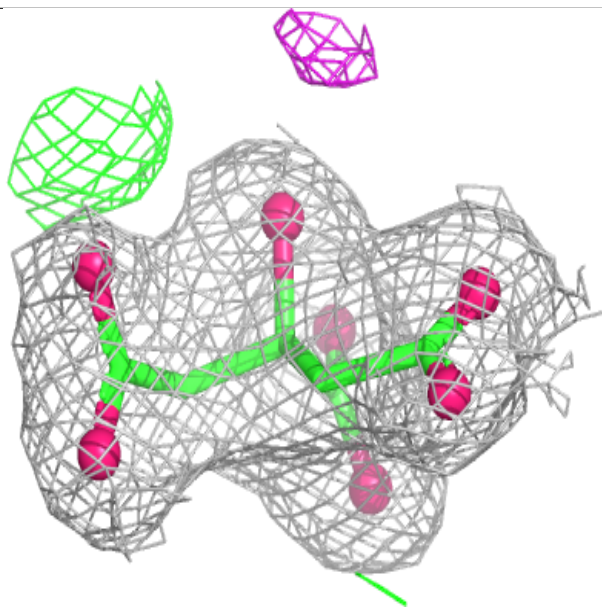
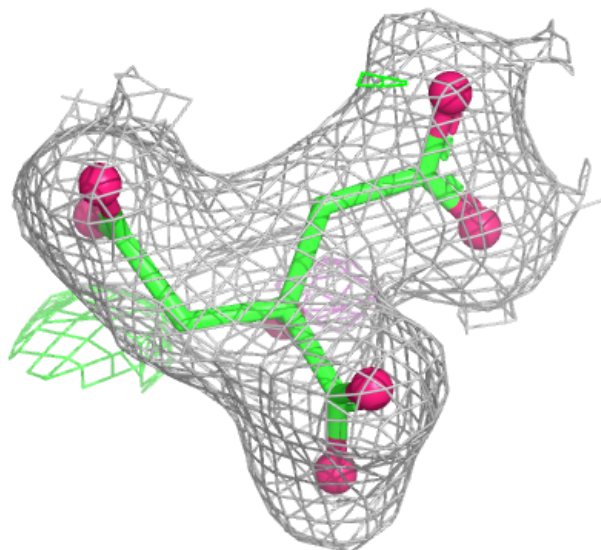
Electron density around CIT E 501:

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



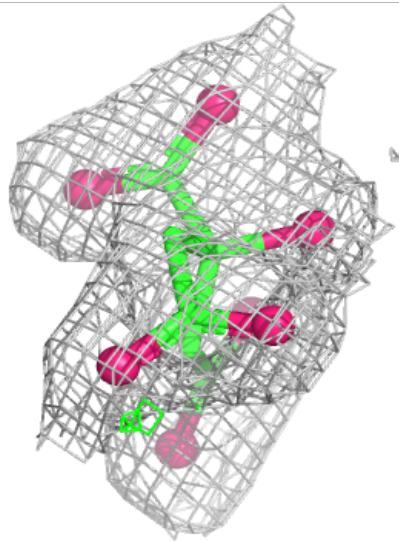
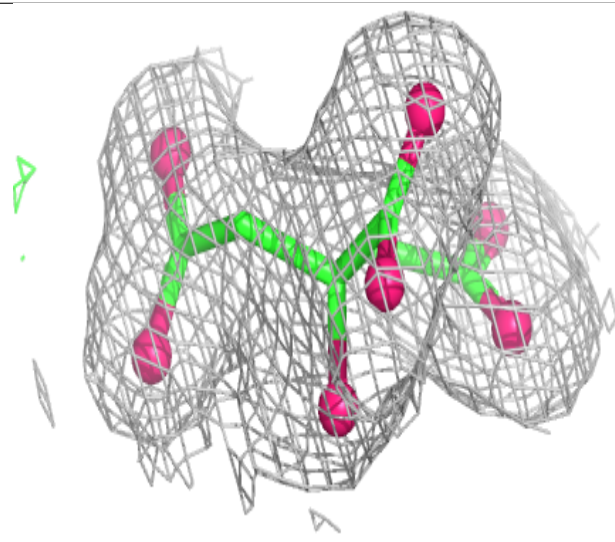
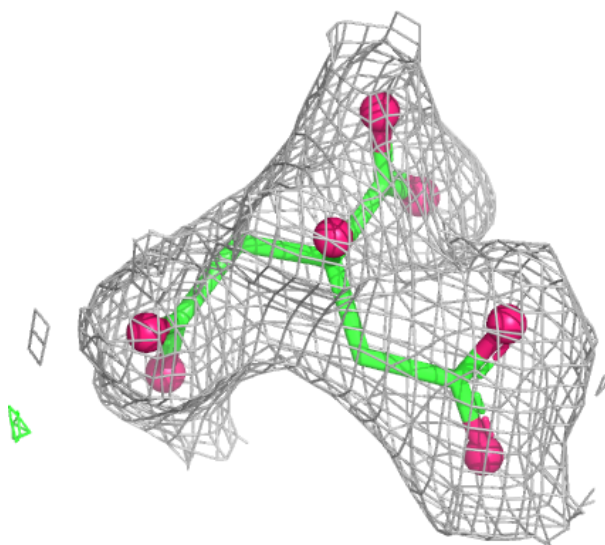
Electron density around CIT B 501:

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



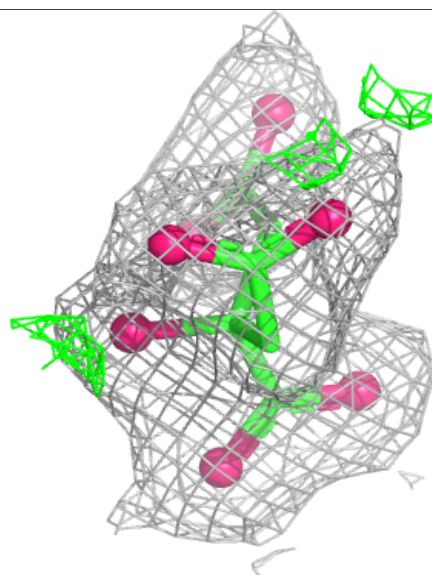
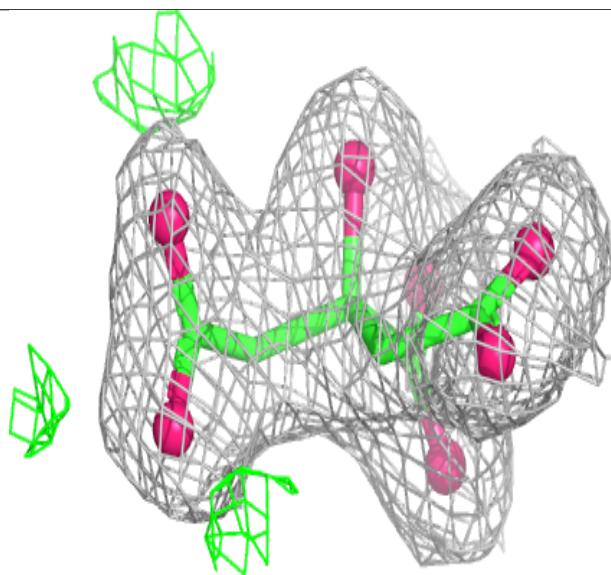
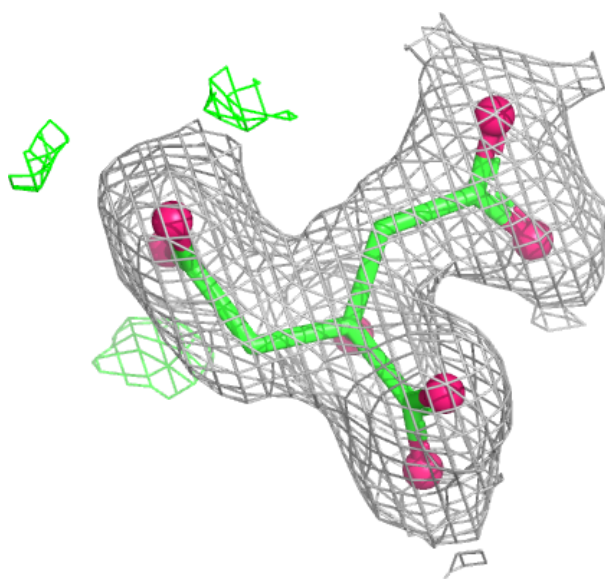
Electron density around CIT C 501:

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



Electron density around CIT G 501:

$2mF_o-DF_c$ (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.