Full wwPDB X-ray Structure Validation Report (i)

Jan 13, 2025 – 06:09 PM JST

PDB ID	:	8XXD
Title	:	TtCS-citrate-CoA complex
Authors	:	Yang, L.; Fang, Y.J.
Deposited on	:	2024-01-18
Resolution	:	2.32 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

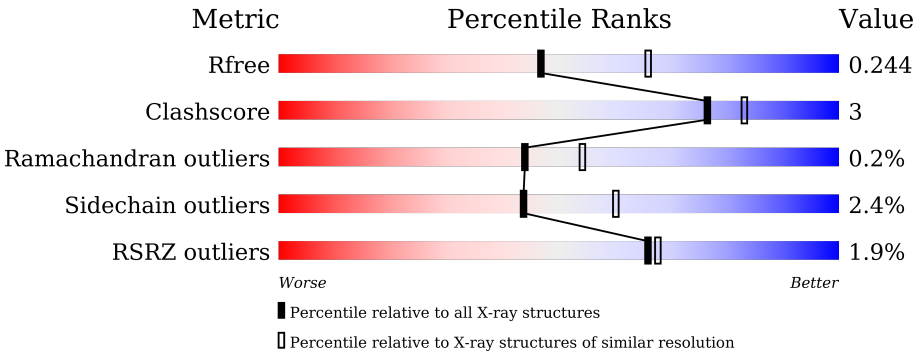
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 2.32 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	7250 (2.34-2.30)
Clashscore	180529	8063 (2.34-2.30)
Ramachandran outliers	177936	7993 (2.34-2.30)
Sidechain outliers	177891	7993 (2.34-2.30)
RSRZ outliers	164620	7250 (2.34-2.30)

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	449	3% 91% 8%
1	B	449	3% 87% 12%
1	C	449	92% 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11035 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.

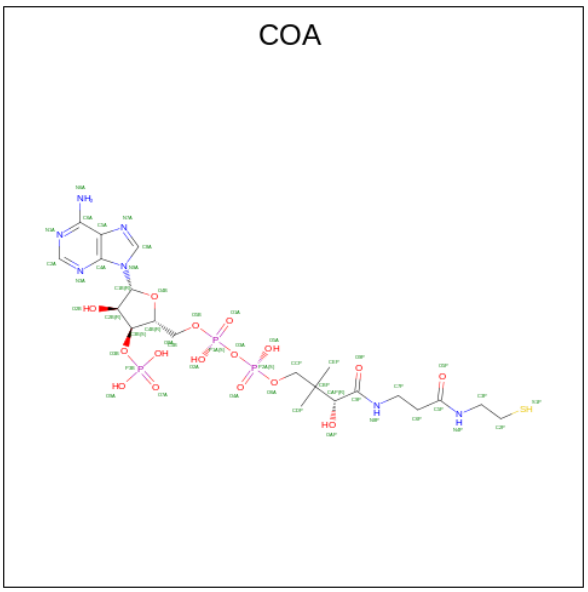
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3576	2298	614	643	21			
1	B	449	Total	C	N	O	S	0	0	0
			3588	2306	615	646	21			
1	C	442	Total	C	N	O	S	0	1	0
			3561	2287	612	641	21			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	443	LYS	-	expression tag	UNP A0A0S3QTD0
A	444	LEU	-	expression tag	UNP A0A0S3QTD0
A	445	ALA	-	expression tag	UNP A0A0S3QTD0
A	446	ALA	-	expression tag	UNP A0A0S3QTD0
A	447	ALA	-	expression tag	UNP A0A0S3QTD0
A	448	LEU	-	expression tag	UNP A0A0S3QTD0
A	449	GLU	-	expression tag	UNP A0A0S3QTD0
B	443	LYS	-	expression tag	UNP A0A0S3QTD0
B	444	LEU	-	expression tag	UNP A0A0S3QTD0
B	445	ALA	-	expression tag	UNP A0A0S3QTD0
B	446	ALA	-	expression tag	UNP A0A0S3QTD0
B	447	ALA	-	expression tag	UNP A0A0S3QTD0
B	448	LEU	-	expression tag	UNP A0A0S3QTD0
B	449	GLU	-	expression tag	UNP A0A0S3QTD0
C	443	LYS	-	expression tag	UNP A0A0S3QTD0
C	444	LEU	-	expression tag	UNP A0A0S3QTD0
C	445	ALA	-	expression tag	UNP A0A0S3QTD0
C	446	ALA	-	expression tag	UNP A0A0S3QTD0
C	447	ALA	-	expression tag	UNP A0A0S3QTD0
C	448	LEU	-	expression tag	UNP A0A0S3QTD0
C	449	GLU	-	expression tag	UNP A0A0S3QTD0

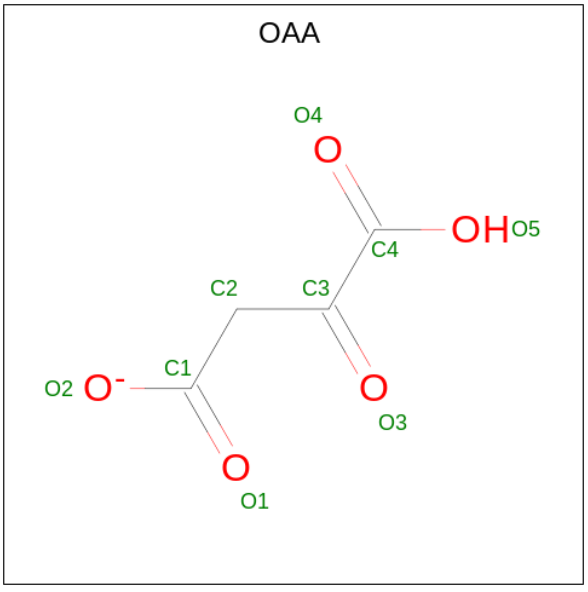
- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled

as "Ligand of Interest" by depositor).



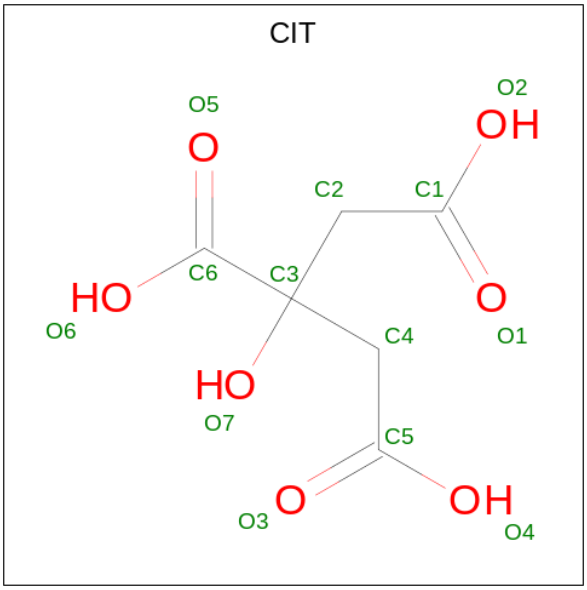
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 3 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 4 5	0	0
3	B	1	Total C O 9 4 5	0	0

- Molecule 4 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
4	C	1	Total C O 13 6 7	0	0

- Molecule 5 is water.

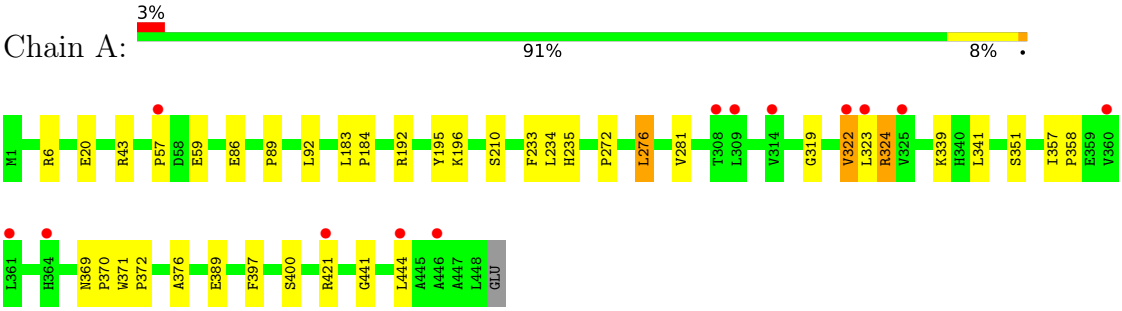
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	63	Total O 63 63	0	0
5	B	49	Total O 49 49	0	0
5	C	71	Total O 71 71	0	0

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.

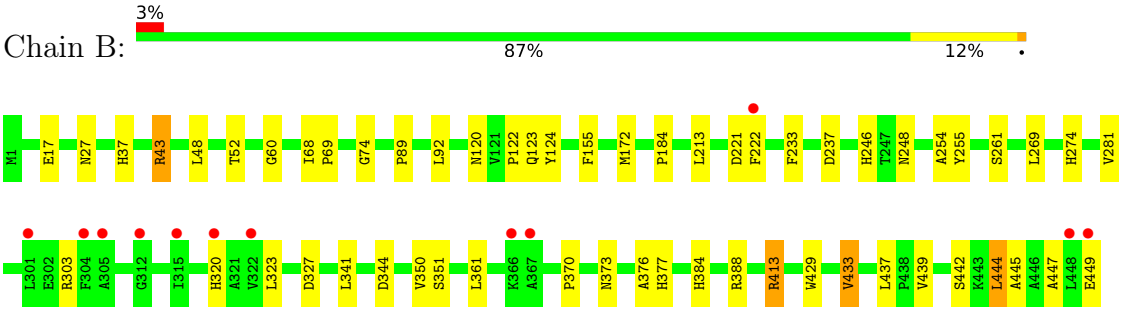
• Molecule 1: Citrate synthase

Chain A:



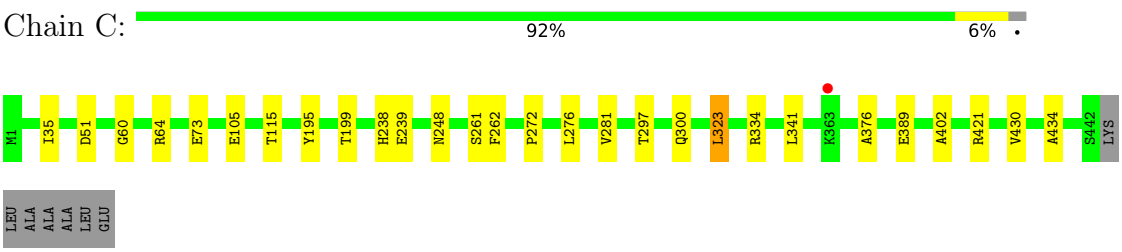
• Molecule 1: Citrate synthase

Chain B:



• Molecule 1: Citrate synthase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	109.56Å 109.56Å 265.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.63 – 2.32 50.63 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.63-2.32) 99.9 (50.63-2.32)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.8.0411	Depositor
R, R_{free}	0.188 , 0.243 0.194 , 0.244	Depositor DCC
R_{free} test set	3548 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	42.5	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11035	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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, COA, OAA

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	0.43	0/3672	0.72	0/4979
1	B	0.44	0/3684	0.76	1/4995 (0.0%)
1	C	0.46	0/3657	0.73	2/4957 (0.0%)
All	All	0.44	0/11013	0.74	3/14931 (0.0%)

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	3
1	C	0	1
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	334	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	334	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	B	388	ARG	CG-CD-NE	-5.02	101.26	111.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	324	ARG	Sidechain
1	A	43	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	6	ARG	Sidechain
1	C	73	GLU	Peptide

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	3576	0	3526	17	0
1	B	3588	0	3541	35	0
1	C	3561	0	3511	11	0
2	A	48	0	32	0	0
2	C	48	0	32	0	0
3	A	9	0	2	0	0
3	B	9	0	2	0	0
4	C	13	0	5	0	0
5	A	63	0	0	2	0
5	B	49	0	0	7	0
5	C	71	0	0	0	0
All	All	11035	0	10651	60	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 3.

All (60) 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:B:350:VAL:HG11	5:B:631:HOH:O	1.50	1.07
1:B:123:GLN:HG2	5:B:645:HOH:O	1.85	0.74
1:B:377:HIS:HA	5:B:631:HOH:O	1.90	0.72
1:A:370:PRO:HG2	1:A:371:TRP:CD1	2.26	0.69
1:B:350:VAL:HG21	5:B:631:HOH:O	2.02	0.59
1:B:344:ASP:OD2	1:B:384:HIS:ND1	2.35	0.56
1:A:272:PRO:HA	1:A:276:LEU:HD12	1.89	0.55
1:C:262:PHE:CZ	1:C:402:ALA:HB2	2.42	0.55
1:C:35:ILE:HD13	1:C:430:VAL:HG13	1.90	0.54
1:B:120:ASN:HA	1:C:199:THR:HG21	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:LEU:HD13	1:B:370:PRO:HA	1.90	0.52
1:B:439:VAL:HG13	1:B:442:SER:CB	2.38	0.52
1:A:183:LEU:HB2	1:A:184:PRO:HD3	1.92	0.51
1:A:441:GLY:HA2	1:B:449:GLU:HB3	1.92	0.51
1:C:238:HIS:O	1:C:239:GLU:HB2	2.11	0.50
1:B:60:GLY:HA2	1:B:323:LEU:HD21	1.93	0.50
1:B:439:VAL:O	1:B:445:ALA:HB2	2.12	0.50
1:B:413:ARG:NE	1:B:413:ARG:HA	2.27	0.49
1:B:123:GLN:CG	5:B:645:HOH:O	2.53	0.49
1:A:281:VAL:HG11	1:A:376:ALA:HA	1.95	0.48
1:A:371:TRP:HB3	1:A:372:PRO:HD2	1.95	0.48
1:B:444:LEU:O	1:B:447:ALA:HB3	2.14	0.48
1:A:421:ARG:HB3	1:B:43:ARG:NH1	2.28	0.48
1:B:254:ALA:O	1:B:255:TYR:HB2	2.14	0.48
1:A:339:LYS:HD2	5:A:609:HOH:O	2.12	0.48
1:B:281:VAL:HG11	1:B:376:ALA:HA	1.94	0.47
1:C:195:TYR:CG	1:C:389:GLU:HG2	2.51	0.46
5:A:649:HOH:O	1:B:17:GLU:HG2	2.15	0.46
1:B:439:VAL:HG13	1:B:442:SER:HB3	1.97	0.46
1:C:60:GLY:HA2	1:C:323:LEU:HD11	1.97	0.46
1:A:195:TYR:CG	1:A:389:GLU:HG2	2.51	0.46
1:B:52:THR:OG1	1:B:237:ASP:OD2	2.28	0.45
1:B:37:HIS:HE1	5:B:633:HOH:O	2.00	0.44
1:B:68:ILE:HB	1:B:69:PRO:HD3	1.99	0.44
1:B:221:ASP:OD1	1:B:222:PHE:N	2.51	0.44
1:B:327:ASP:CB	1:B:373:ASN:HA	2.46	0.44
1:B:155:PHE:CE2	1:B:172:MET:HE3	2.53	0.44
1:C:51:ASP:O	1:C:64:ARG:HD3	2.18	0.44
1:B:221:ASP:OD1	1:B:221:ASP:C	2.55	0.43
1:A:357:ILE:N	1:A:358:PRO:CD	2.81	0.43
1:B:248:ASN:ND2	1:B:261:SER:OG	2.51	0.43
1:B:184:PRO:HB3	1:B:213:LEU:HB2	2.01	0.43
1:C:430:VAL:O	1:C:434:ALA:HB2	2.19	0.43
1:A:89:PRO:HG3	1:A:210:SER:OG	2.19	0.43
1:A:235:HIS:HB2	1:A:400:SER:OG	2.19	0.43
1:B:89:PRO:HD2	5:B:603:HOH:O	2.17	0.43
1:C:281:VAL:HG11	1:C:376:ALA:HA	1.99	0.42
1:C:248:ASN:ND2	1:C:261:SER:OG	2.52	0.42
1:A:92:LEU:HD22	1:A:233:PHE:CD1	2.54	0.42
1:B:122:PRO:HB3	1:B:124:TYR:CE2	2.53	0.42
1:A:319:GLY:HA2	1:A:369:ASN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:LEU:HA	1:B:274:HIS:CD2	2.55	0.41
1:C:297:THR:OG1	1:C:300:GLN:HG3	2.20	0.41
1:A:233:PHE:CD2	1:A:234:LEU:HD23	2.56	0.41
1:B:48:LEU:HD11	1:B:246:HIS:CD2	2.55	0.41
1:B:92:LEU:HD22	1:B:233:PHE:CD1	2.54	0.41
1:B:429:TRP:O	1:B:433:VAL:HB	2.20	0.41
1:A:192:ARG:HA	1:A:196:LYS:HB2	2.02	0.41
1:B:444:LEU:HD23	1:B:444:LEU:HA	1.92	0.41
1:A:86:GLU:OE2	1:A:86:GLU:HA	2.21	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	446/449 (99%)	433 (97%)	11 (2%)	2 (0%)	30	37
1	B	447/449 (100%)	439 (98%)	7 (2%)	1 (0%)	44	54
1	C	442/449 (98%)	436 (99%)	6 (1%)	0	100	100
All	All	1335/1347 (99%)	1308 (98%)	24 (2%)	3 (0%)	44	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	GLU
1	B	74	GLY
1	A	322	VAL

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	372/376 (99%)	362 (97%)	10 (3%)	40	56
1	B	374/376 (100%)	364 (97%)	10 (3%)	40	56
1	C	373/376 (99%)	366 (98%)	7 (2%)	52	68
All	All	1119/1128 (99%)	1092 (98%)	27 (2%)	44	60

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	57	PRO
1	A	276	LEU
1	A	322	VAL
1	A	323	LEU
1	A	324	ARG
1	A	341	LEU
1	A	351	SER
1	A	397	PHE
1	A	444	LEU
1	B	27	ASN
1	B	43	ARG
1	B	303	ARG
1	B	320	HIS
1	B	341	LEU
1	B	351	SER
1	B	413	ARG
1	B	433	VAL
1	B	437	LEU
1	B	444	LEU
1	C	105	GLU
1	C	115	THR
1	C	272	PRO
1	C	276	LEU
1	C	323	LEU
1	C	341	LEU

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Mol	Chain	Res	Type
1	C	421	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	248	ASN
1	B	27	ASN
1	B	37	HIS
1	B	248	ASN
1	B	313	GLN
1	B	333	GLN
1	B	408	GLN
1	C	120	ASN
1	C	248	ASN
1	C	340	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

5 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	$\#\|Z\|>2$
3	OAA	B	501	-	8,8,8	5.47	4 (50%)	9,10,10	2.25	4 (44%)
2	COA	C	501	-	41,50,50	0.70	0	52,75,75	0.85	2 (3%)
4	CIT	C	502	-	12,12,12	1.06	1 (8%)	17,17,17	1.59	3 (17%)
3	OAA	A	502	-	8,8,8	5.45	2 (25%)	9,10,10	1.36	0
2	COA	A	501	-	41,50,50	0.70	1 (2%)	52,75,75	0.76	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OAA	B	501	-	-	2/8/8/8	-
2	COA	C	501	-	-	3/44/64/64	0/3/3/3
4	CIT	C	502	-	-	10/16/16/16	-
3	OAA	A	502	-	-	0/8/8/8	-
2	COA	A	501	-	-	3/44/64/64	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	OAA	C3-C4	-15.04	1.33	1.53
3	B	501	OAA	C3-C4	-14.92	1.33	1.53
3	B	501	OAA	C2-C1	2.34	1.54	1.51
4	C	502	CIT	C3-C6	2.18	1.55	1.53
2	A	501	COA	P3B-O3B	2.08	1.63	1.59
3	B	501	OAA	O1-C1	2.05	1.28	1.22
3	A	502	OAA	O5-C4	-2.03	1.24	1.30
3	B	501	OAA	O5-C4	-2.01	1.24	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	OAA	C2-C3-C4	4.89	126.10	117.85
4	C	502	CIT	O5-C6-C3	-3.18	117.74	122.25
4	C	502	CIT	O3-C5-C4	-2.76	114.89	122.94
3	B	501	OAA	O3-C3-C4	-2.63	115.62	119.43
2	C	501	COA	O5A-P2A-O4A	2.50	124.61	112.24
4	C	502	CIT	C4-C3-C6	-2.49	104.75	110.11
2	C	501	COA	O6A-CCP-CBP	-2.27	106.90	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	COA	O4B-C1B-C2B	-2.27	103.61	106.93
3	B	501	OAA	O5-C4-C3	2.12	119.78	113.97
3	B	501	OAA	O4-C4-C3	-2.10	118.92	121.72

There are no chirality outliers.

All (18) torsion outliers are listed below:

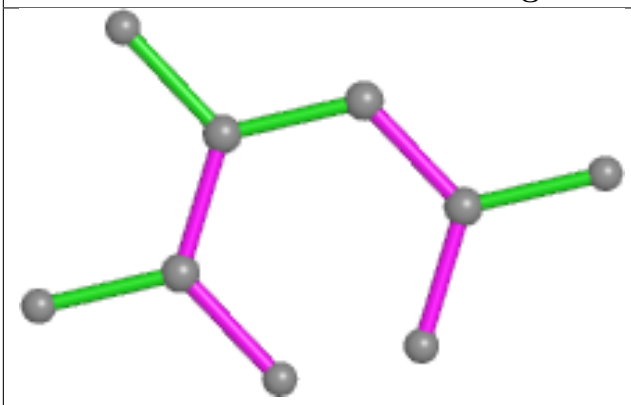
Mol	Chain	Res	Type	Atoms
2	A	501	COA	C3B-O3B-P3B-O9A
2	A	501	COA	C5B-O5B-P1A-O1A
2	C	501	COA	C5B-O5B-P1A-O1A
4	C	502	CIT	C2-C3-C6-O5
4	C	502	CIT	C2-C3-C6-O6
4	C	502	CIT	O7-C3-C6-O5
4	C	502	CIT	O7-C3-C6-O6
4	C	502	CIT	O1-C1-C2-C3
4	C	502	CIT	O2-C1-C2-C3
3	B	501	OAA	C1-C2-C3-O3
4	C	502	CIT	C2-C3-C4-C5
4	C	502	CIT	C3-C4-C5-O3
4	C	502	CIT	C3-C4-C5-O4
3	B	501	OAA	C2-C3-C4-O5
2	A	501	COA	C5B-O5B-P1A-O3A
2	C	501	COA	C3B-O3B-P3B-O8A
2	C	501	COA	C5B-O5B-P1A-O3A
4	C	502	CIT	C6-C3-C4-C5

There are no ring outliers.

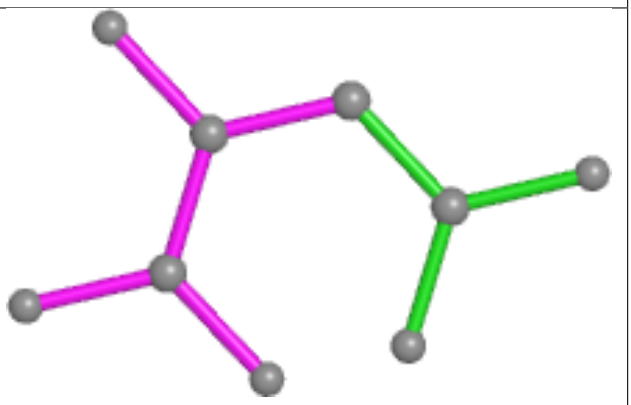
No monomer is involved in short contacts.

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.

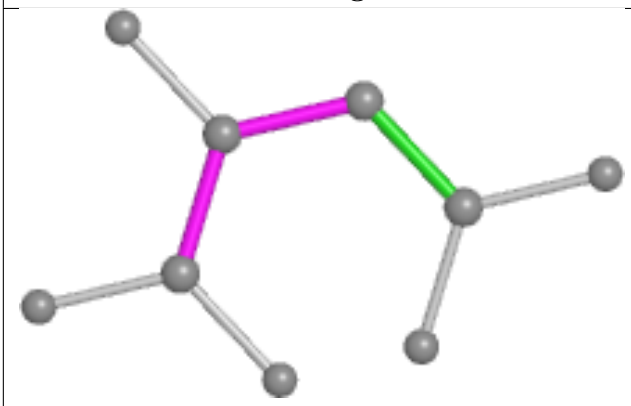
Ligand OAA B 501



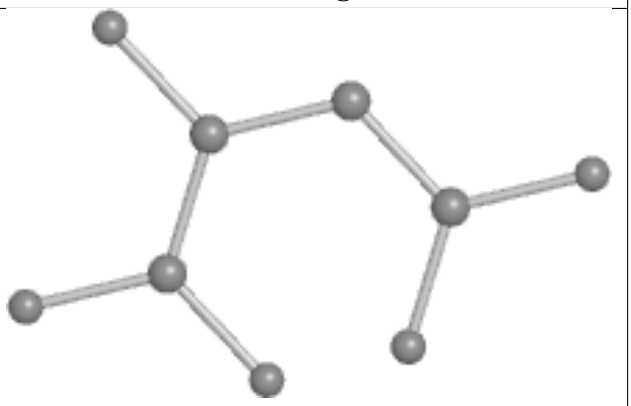
Bond lengths



Bond angles

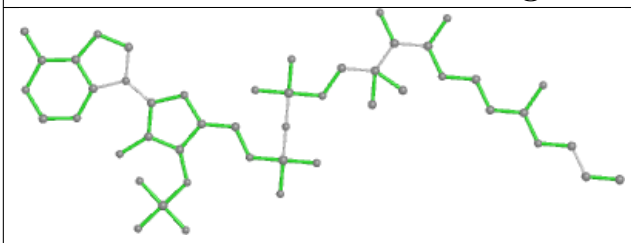


Torsions

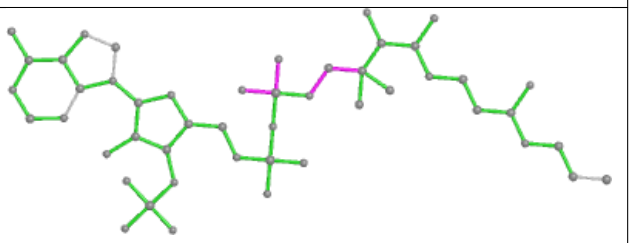


Rings

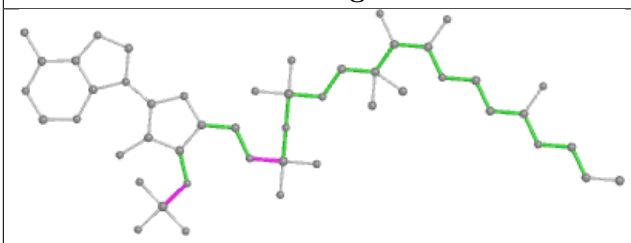
Ligand COA C 501



Bond lengths



Bond angles



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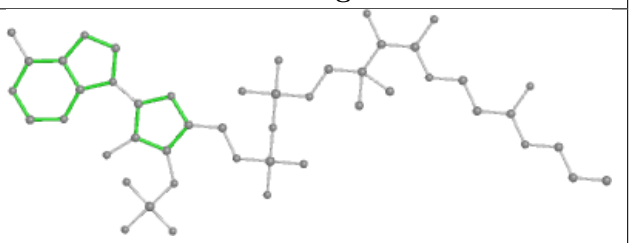
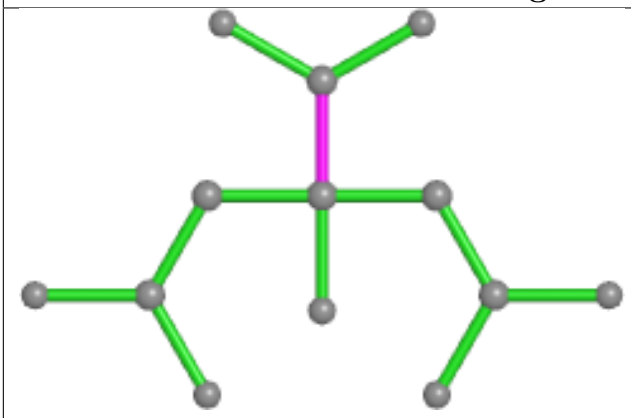
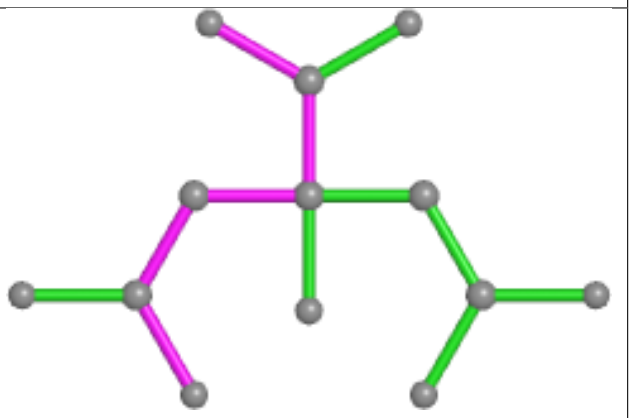


Rings

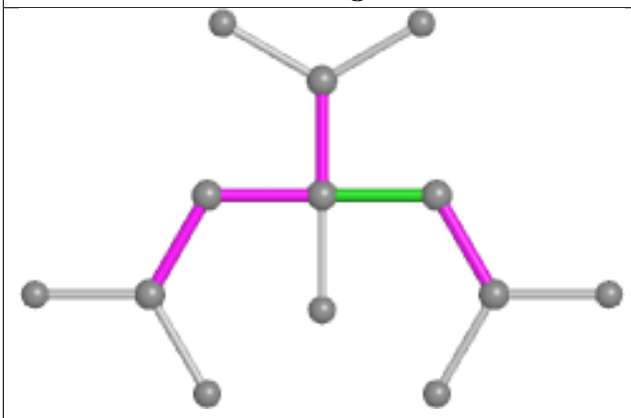
Ligand CIT C 502



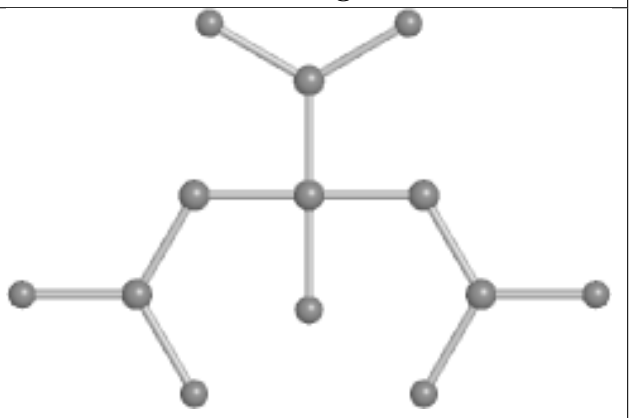
Bond lengths



Bond angles

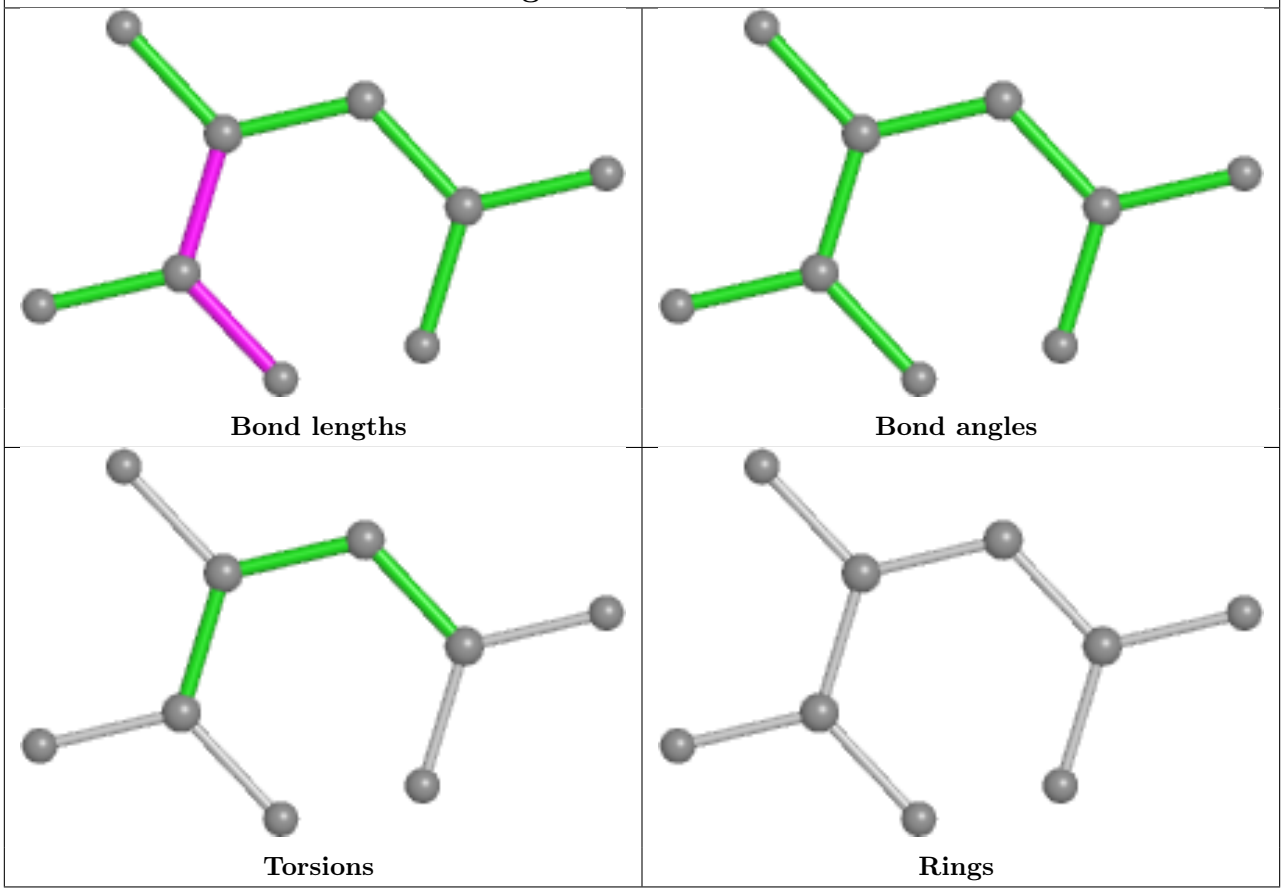


Torsions

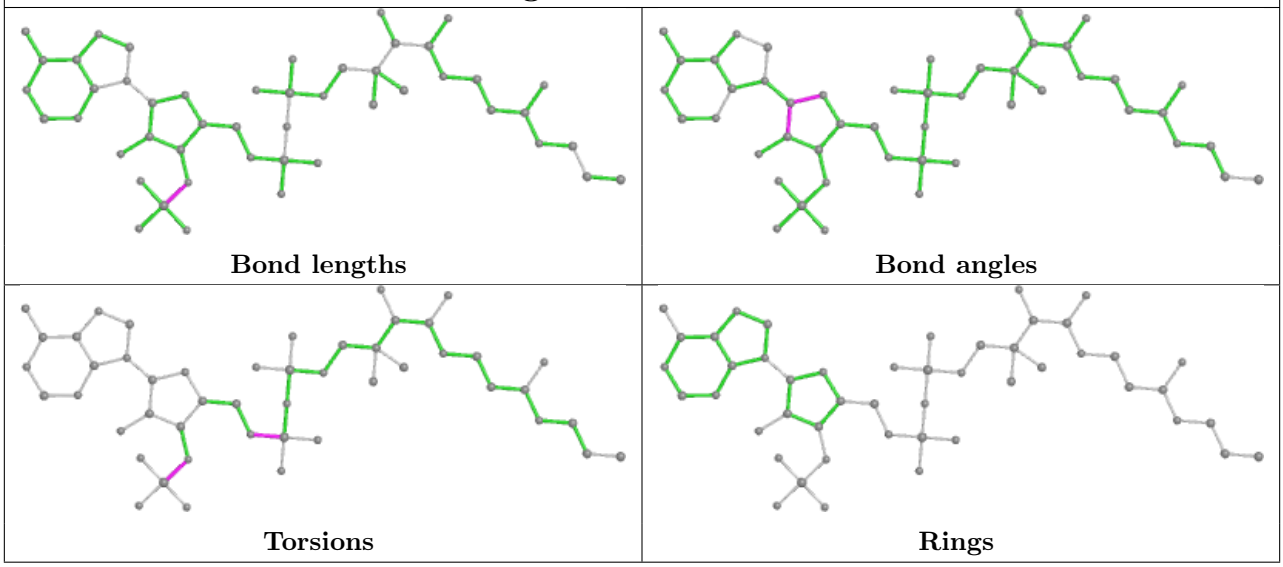


Rings

Ligand OAA A 502



Ligand COA A 501



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	448/449 (99%)	-0.01	13 (2%)	54	56	32, 51, 94, 118	0
1	B	449/449 (100%)	0.14	12 (2%)	56	58	32, 53, 85, 144	0
1	C	442/449 (98%)	-0.26	1 (0%)	92	92	11, 46, 74, 99	1 (0%)
All	All	1339/1347 (99%)	-0.04	26 (1%)	66	68	11, 50, 86, 144	1 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	314	VAL	4.7
1	A	444	LEU	4.6
1	A	325	VAL	4.5
1	B	322	VAL	3.8
1	B	304	PHE	3.3
1	A	446	ALA	3.2
1	B	320	HIS	3.2
1	B	367	ALA	3.1
1	A	57	PRO	2.9
1	B	305	ALA	2.8
1	A	364	HIS	2.6
1	B	366	LYS	2.6
1	A	322	VAL	2.5
1	A	309	LEU	2.4
1	A	308	THR	2.4
1	C	363	LYS	2.4
1	B	449	GLU	2.4
1	A	361	LEU	2.4
1	A	360	VAL	2.3
1	B	448	LEU	2.3
1	B	301	LEU	2.2
1	B	222	PHE	2.1
1	A	421	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	312	GLY	2.1
1	B	315	ILE	2.1
1	A	323	LEU	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)

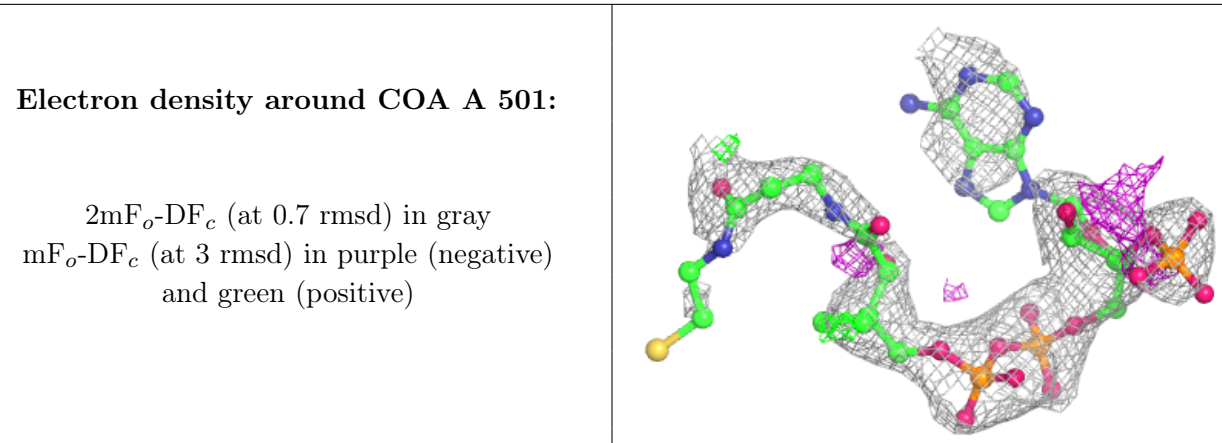
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	COA	A	501	48/48	0.77	0.14	72,106,142,148	0
3	OAA	B	501	9/9	0.81	0.14	66,88,95,95	0
4	CIT	C	502	13/13	0.86	0.13	54,62,89,90	0
3	OAA	A	502	9/9	0.87	0.10	57,64,74,75	0
2	COA	C	501	48/48	0.92	0.08	49,61,82,85	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.

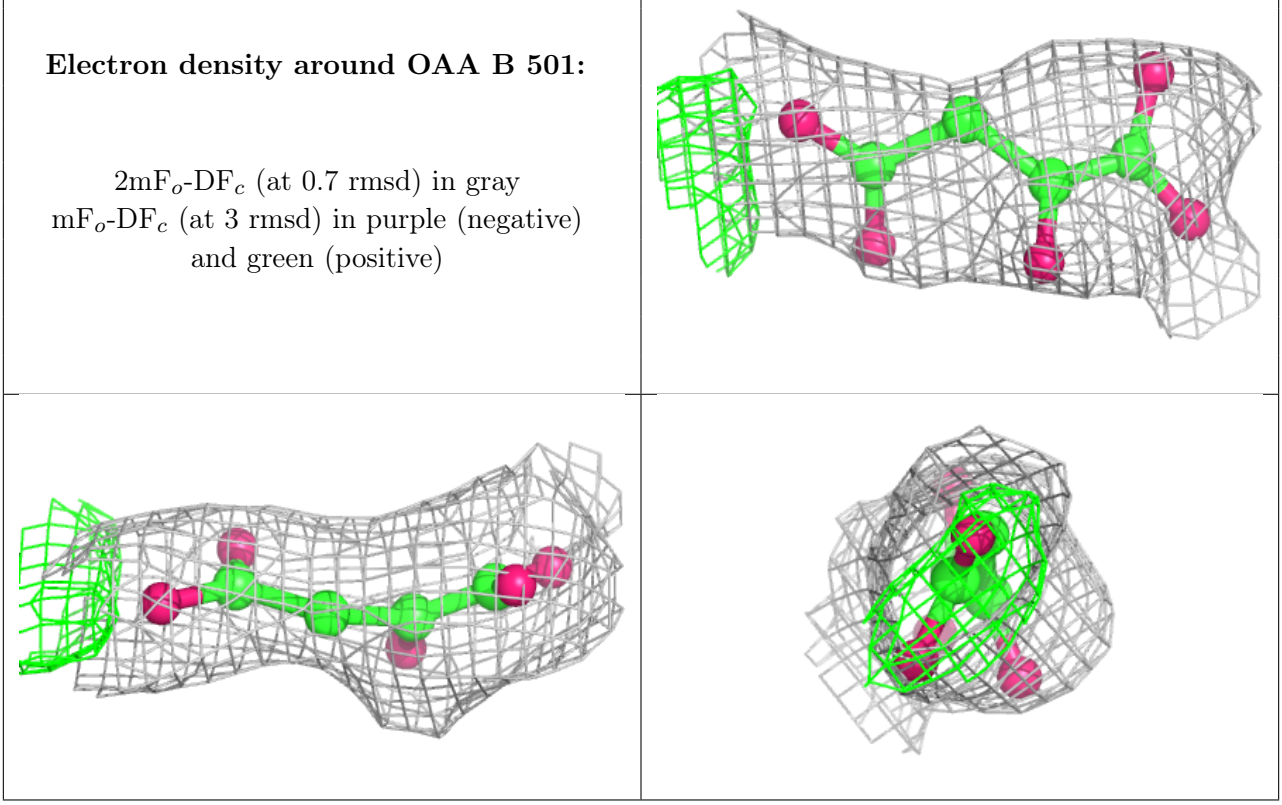
Electron density around COA A 501:

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



Electron density around OAA 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 502:

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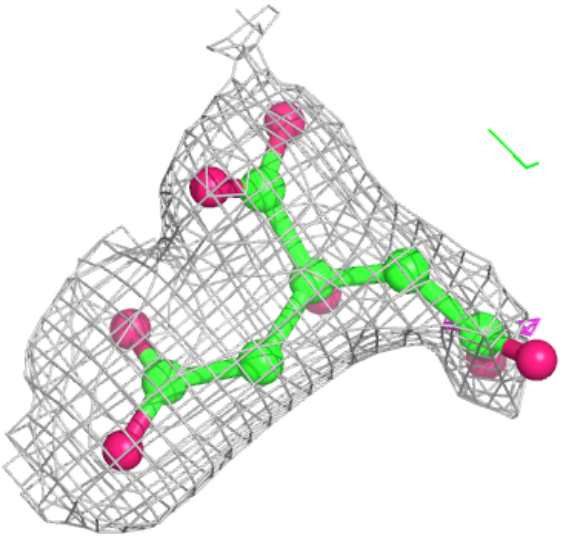
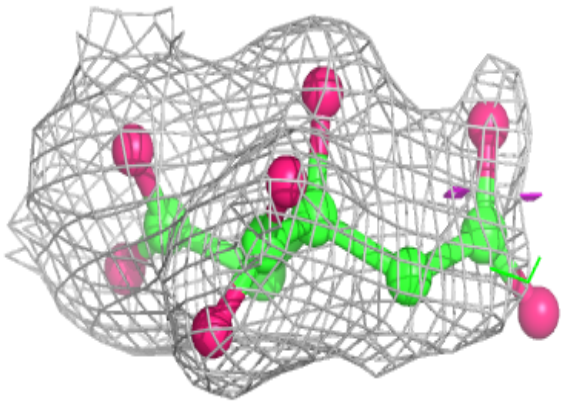
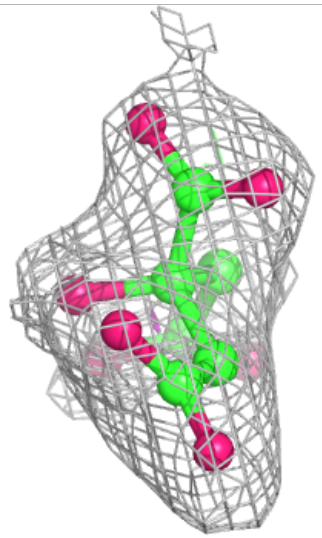
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

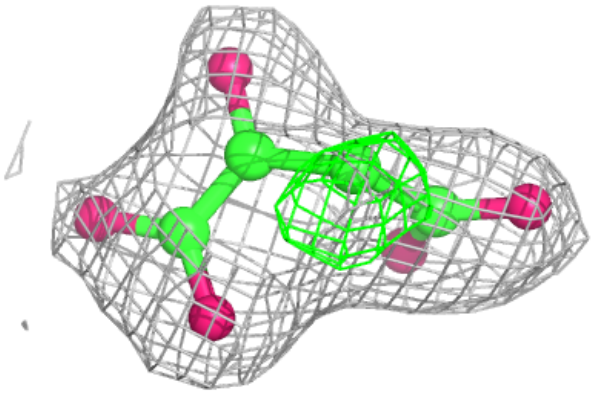


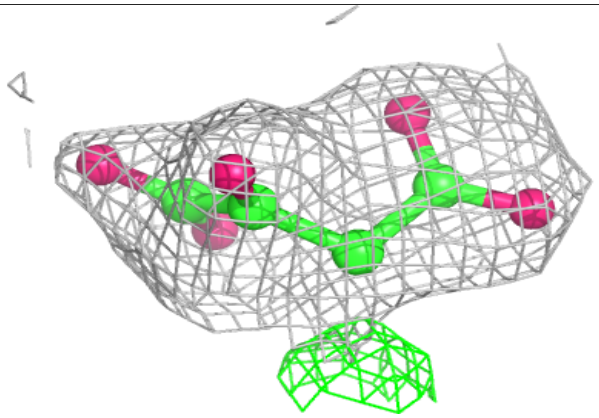


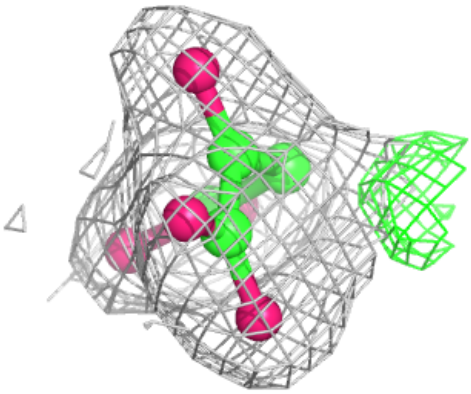


Electron density around OAA A 502:

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

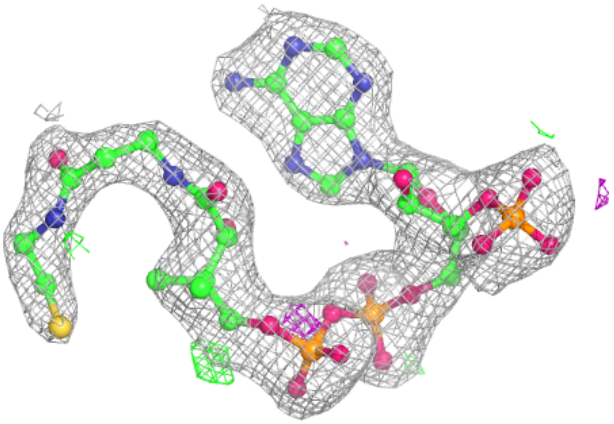


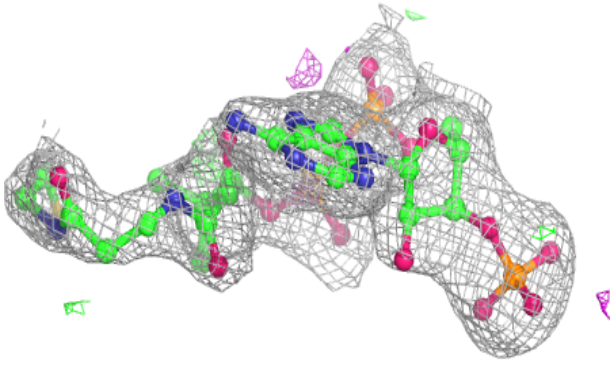


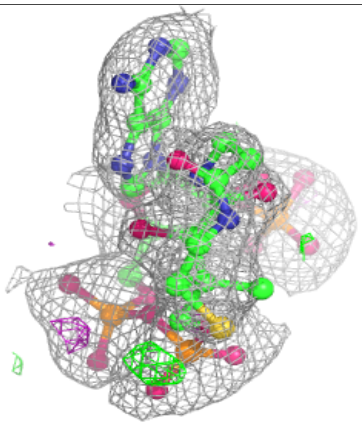


Electron density around COA C 501:

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







6.5 Other polymers (i)

There are no such residues in this entry.