



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 9, 2025 – 02:16 PM JST

PDB ID : 8ZVU / pdb\_00008zvu  
Title : Human citrate synthase intermediate 4  
Authors : Yang, L.Y.; Fang, Y.J.  
Deposited on : 2024-06-12  
Resolution : 1.78 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

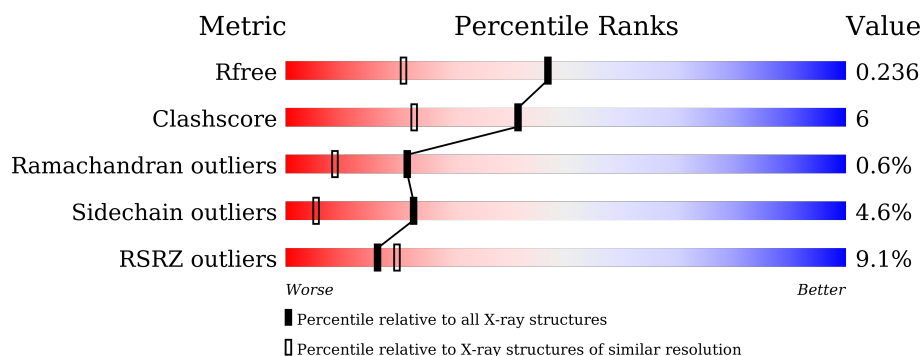
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.78 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	1191 (1.78-1.78)
Clashscore	180529	1282 (1.78-1.78)
Ramachandran outliers	177936	1270 (1.78-1.78)
Sidechain outliers	177891	1270 (1.78-1.78)
RSRZ outliers	164620	1191 (1.78-1.78)

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  $\geq 3$ , 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	434	<div> <div>8%</div> <div>86%</div> <div>12%</div> <div>.</div> </div>
1	B	434	<div> <div>11%</div> <div>84%</div> <div>14%</div> <div>..</div> </div>

## 2 Entry composition [i](#)

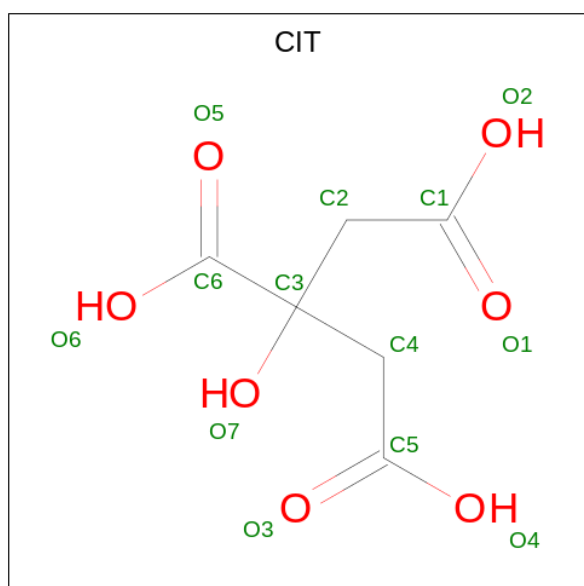
There are 5 unique types of molecules in this entry. The entry contains 7252 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, mitochondrial.

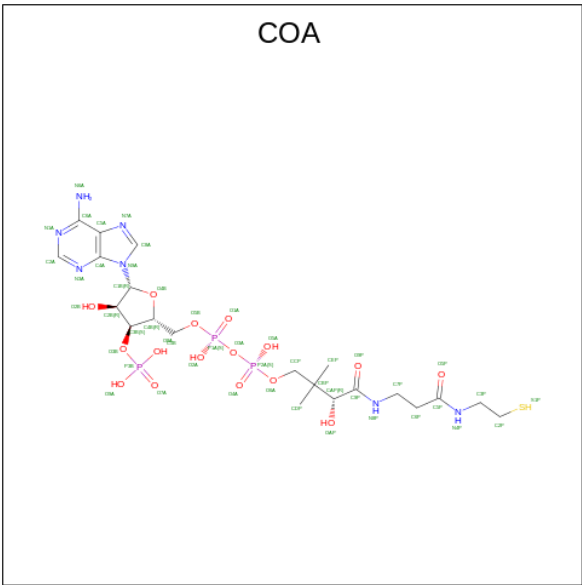
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	1	0
			3416	2184	585	630	17			
1	B	434	Total	C	N	O	S	0	2	0
			3421	2189	584	631	17			

- Molecule 2 is CITRIC ACID (CCD ID: CIT) (formula:  $C_6H_8O_7$ ).



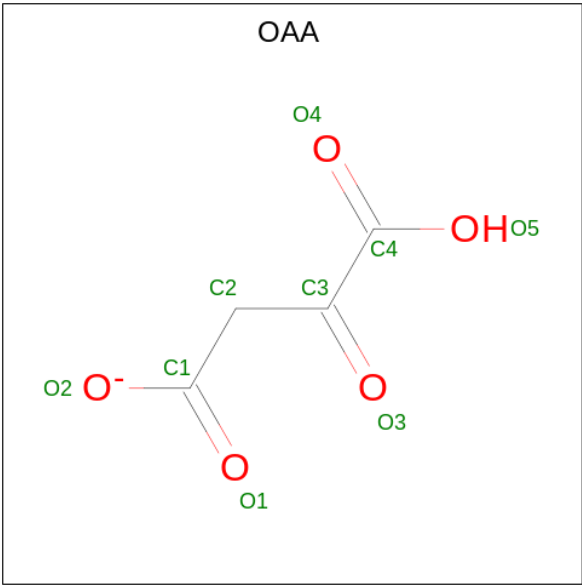
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 3 is COENZYME A (CCD ID: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



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

- Molecule 4 is OXALOACETATE ION (CCD ID: OAA) (formula:  $C_4H_3O_5$ ).



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

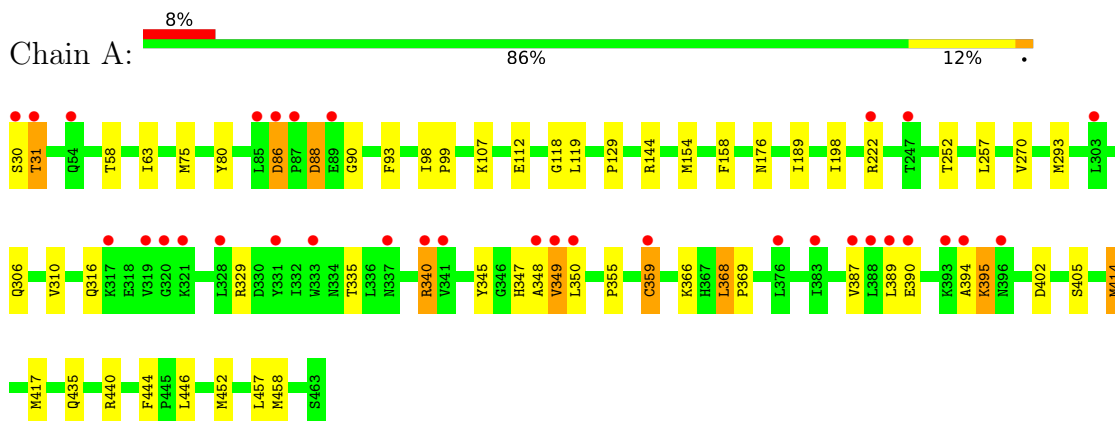
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	172	Total 172	O 172	0	0
5	B	173	Total 173	O 173	0	0

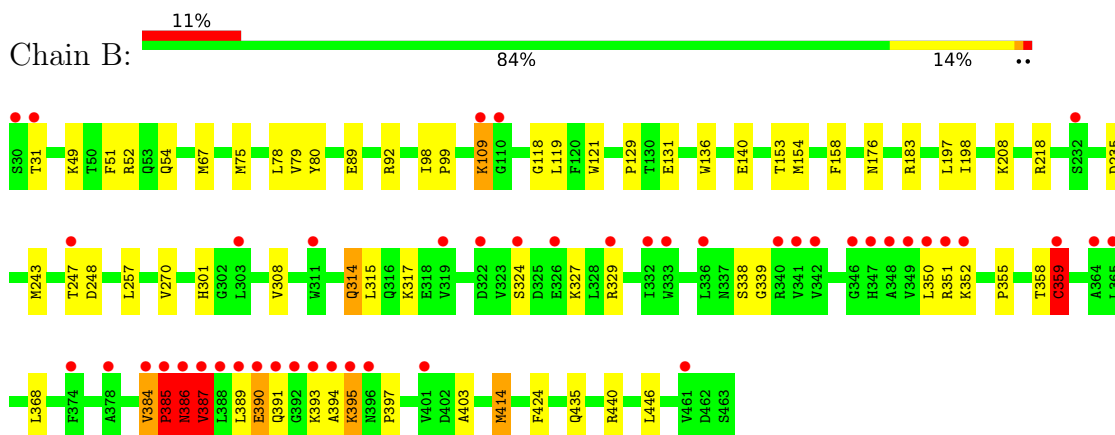
### 3 Residue-property plots

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, mitochondrial



#### • Molecule 1: Citrate synthase, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.91Å 59.69Å 73.43Å 101.45° 98.91° 116.47°	Depositor
Resolution (Å)	50.98 – 1.78 50.98 – 1.78	Depositor EDS
% Data completeness (in resolution range)	88.6 (50.98-1.78) 88.6 (50.98-1.78)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, $R_{free}$	0.183 , 0.233 0.191 , 0.236	Depositor DCC
$R_{free}$ test set	3844 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 34.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7252	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: COA, OAA, 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	0.70	1/3504 (0.0%)	1.15	10/4759 (0.2%)
1	B	0.75	3/3509 (0.1%)	1.23	19/4766 (0.4%)
All	All	0.73	4/7013 (0.1%)	1.19	29/9525 (0.3%)

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	2
1	B	0	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	393	LYS	C-N	15.08	1.54	1.33
1	B	384	VAL	C-N	9.34	1.47	1.33
1	A	348	ALA	C-N	8.37	1.45	1.33
1	B	385	PRO	C-N	7.08	1.43	1.33

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	VAL	CA-C-N	-11.97	105.59	119.47
1	B	384	VAL	C-N-CA	-11.97	105.59	119.47
1	B	109	LYS	CB-CA-C	11.26	127.15	110.26
1	B	390	GLU	N-CA-C	-8.73	102.53	113.01
1	B	414	MET	CG-SD-CE	7.48	117.35	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	359	CYS	CB-CA-C	7.38	122.63	110.81
1	A	414	MET	CG-SD-CE	7.36	117.10	100.90
1	B	424	PHE	CA-CB-CG	6.88	120.68	113.80
1	B	385	PRO	O-C-N	6.81	130.41	122.17
1	B	358	THR	CA-CB-OG1	-6.43	99.95	109.60
1	B	393	LYS	CA-C-N	-6.29	109.53	121.54
1	B	393	LYS	C-N-CA	-6.29	109.53	121.54
1	A	252	THR	CA-CB-OG1	-6.17	100.35	109.60
1	A	58	THR	CA-CB-OG1	-6.08	100.48	109.60
1	B	359	CYS	N-CA-CB	-5.87	101.19	109.94
1	B	153	THR	CA-CB-OG1	-5.84	100.84	109.60
1	B	385	PRO	CA-C-O	-5.79	110.49	119.64
1	A	366	LYS	CB-CA-C	-5.73	101.16	110.79
1	A	31	THR	CA-CB-OG1	-5.64	101.14	109.60
1	B	248	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	444	PHE	CA-CB-CG	5.59	119.39	113.80
1	A	348	ALA	CA-C-N	-5.50	112.06	121.97
1	A	348	ALA	C-N-CA	-5.50	112.06	121.97
1	B	235	ASP	CA-C-N	5.35	127.40	120.44
1	B	235	ASP	C-N-CA	5.35	127.40	120.44
1	B	248	ASP	N-CA-CB	-5.33	100.53	109.28
1	B	54	GLN	CB-CA-C	-5.25	99.11	109.67
1	A	417	MET	CG-SD-CE	-5.18	89.50	100.90
1	A	345	TYR	CB-CA-C	5.07	118.48	109.72

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	ARG	Sidechain
1	A	329	ARG	Sidechain
1	B	52	ARG	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3416	0	3382	40	0
1	B	3421	0	3390	54	0
2	A	13	0	5	3	0
3	A	48	0	32	0	0
4	B	9	0	2	0	0
5	A	172	0	0	0	0
5	B	173	0	0	12	0
All	All	7252	0	6811	86	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 6.

All (86) 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:A:154:MET:HE3	1:B:154:MET:HE3	1.26	1.17
1:B:270[B]:VAL:HG23	1:B:301:HIS:CD2	2.05	0.91
1:B:270[B]:VAL:CG2	1:B:301:HIS:CD2	2.64	0.81
1:B:384:VAL:O	1:B:385:PRO:C	2.27	0.78
1:B:385:PRO:O	1:B:387:VAL:N	2.18	0.76
1:A:154:MET:HE2	1:A:158:PHE:HZ	1.55	0.72
1:A:154:MET:CE	1:B:154:MET:HE3	2.14	0.68
1:B:131:GLU:CG	5:B:636:HOH:O	2.43	0.67
1:A:93:PHE:CE2	1:A:98:ILE:HD11	2.31	0.66
1:B:154:MET:HE2	1:B:158:PHE:HZ	1.62	0.64
1:A:93:PHE:CE2	1:A:98:ILE:CD1	2.82	0.62
1:A:222:ARG:HH11	1:A:222:ARG:HG2	1.65	0.62
1:A:446:LEU:HD11	1:B:270[A]:VAL:HG21	1.83	0.61
1:B:98:ILE:HB	1:B:99:PRO:HD3	1.82	0.61
1:B:154:MET:HE2	1:B:158:PHE:CZ	2.36	0.61
1:B:339:GLY:HA3	5:B:632:HOH:O	2.01	0.61
1:A:98:ILE:HB	1:A:99:PRO:HD3	1.84	0.60
1:B:270[B]:VAL:HG23	1:B:301:HIS:HD2	1.67	0.59
1:B:329:ARG:HD3	5:B:740:HOH:O	2.01	0.59
1:A:458:MET:HE2	1:B:51:PHE:HB2	1.85	0.59
1:B:198:ILE:HG13	1:B:440:ARG:HG3	1.86	0.57
1:A:154:MET:HE2	1:A:158:PHE:CZ	2.36	0.57
1:B:131:GLU:CD	5:B:636:HOH:O	2.48	0.57
1:B:131:GLU:HG3	5:B:636:HOH:O	2.02	0.57
1:B:355:PRO:O	1:B:359:CYS:HB3	2.05	0.57
1:A:446:LEU:HD11	1:B:270[A]:VAL:CG2	2.35	0.56
1:B:183:ARG:HB3	5:B:660:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ILE:HG13	1:A:440:ARG:HG3	1.87	0.56
1:A:80:TYR:CE2	1:A:435:GLN:HG2	2.41	0.55
1:A:63:ILE:HD11	1:B:75:MET:HG3	1.89	0.55
1:B:197:LEU:HD22	1:B:197:LEU:N	2.22	0.55
1:B:270[B]:VAL:CG2	1:B:301:HIS:CG	2.89	0.55
2:A:501:CIT:O4	2:A:501:CIT:O7	2.17	0.54
1:A:347:HIS:HD2	1:A:349:VAL:H	1.56	0.54
1:A:119:LEU:C	1:A:119:LEU:HD13	2.31	0.54
1:B:208:LYS:NZ	5:B:601:HOH:O	2.28	0.54
1:A:107:LYS:HE3	1:A:112:GLU:O	2.08	0.53
1:A:222:ARG:HH11	1:A:222:ARG:CG	2.20	0.53
1:B:89:GLU:HG3	1:B:92:ARG:HH21	1.72	0.53
1:A:335:THR:O	1:A:340:ARG:HB2	2.09	0.52
1:A:402:ASP:OD2	2:A:501:CIT:O3	2.28	0.52
1:A:293:MET:HE2	1:A:293:MET:HA	1.93	0.51
1:A:86:ASP:OD1	1:A:86:ASP:N	2.40	0.51
1:A:80:TYR:CD2	1:A:435:GLN:HG2	2.47	0.50
1:B:394:ALA:O	1:B:395:LYS:CB	2.59	0.50
1:B:154:MET:CE	1:B:158:PHE:HZ	2.25	0.49
1:B:257:LEU:HD11	1:B:359:CYS:SG	2.52	0.49
1:B:314:GLN:HA	1:B:317:LYS:HD3	1.94	0.48
1:B:247:THR:HB	5:B:652:HOH:O	2.13	0.48
1:A:349:VAL:O	1:A:350:LEU:C	2.56	0.48
1:B:384:VAL:O	1:B:386:ASN:N	2.47	0.47
1:B:118:GLY:HA3	5:B:661:HOH:O	2.15	0.47
1:B:136:TRP:CH2	1:B:140:GLU:HG3	2.49	0.47
1:B:119:LEU:C	1:B:119:LEU:HD13	2.39	0.47
1:B:324:SER:HB2	5:B:666:HOH:O	2.15	0.46
1:B:218:ARG:HD2	1:B:243:MET:O	2.15	0.46
1:B:308:VAL:HG11	1:B:403:ALA:HA	1.98	0.46
1:B:270[B]:VAL:HG22	1:B:301:HIS:CD2	2.50	0.45
1:A:30:SER:OG	1:A:31:THR:N	2.49	0.45
1:A:394:ALA:O	1:A:395:LYS:CB	2.65	0.45
1:B:67:MET:HB3	1:B:75:MET:CE	2.47	0.45
1:B:80:TYR:CE2	1:B:435:GLN:HG2	2.52	0.45
1:A:86:ASP:C	1:A:88:ASP:H	2.26	0.44
1:A:93:PHE:HE2	1:A:98:ILE:CD1	2.27	0.44
1:A:270:VAL:HG21	1:B:446:LEU:HD11	1.99	0.44
1:B:78:LEU:N	1:B:78:LEU:HD23	2.32	0.44
1:A:90:GLY:HA3	1:A:355:PRO:HG3	1.99	0.44
1:A:88:ASP:OD1	1:A:88:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:PRO:O	1:B:386:ASN:C	2.61	0.44
1:A:347:HIS:HE1	2:A:501:CIT:O7	2.02	0.43
1:B:49:LYS:NZ	5:B:613:HOH:O	2.51	0.43
1:A:306:GLN:O	1:A:310:VAL:HG23	2.18	0.43
1:A:154:MET:HE3	1:B:154:MET:CE	2.19	0.42
1:A:452:MET:O	1:B:79:VAL:HA	2.19	0.42
1:B:121:TRP:CG	1:B:129:PRO:HB3	2.55	0.42
1:B:121:TRP:CD1	1:B:129:PRO:HB3	2.55	0.42
1:B:197:LEU:N	1:B:197:LEU:CD2	2.83	0.42
1:A:257:LEU:HD11	1:A:359:CYS:SG	2.59	0.41
1:B:136:TRP:CZ2	1:B:140:GLU:HG3	2.55	0.41
1:B:270[B]:VAL:HG22	1:B:301:HIS:CG	2.56	0.41
1:B:80:TYR:CD2	1:B:435:GLN:HG2	2.55	0.41
1:A:368:LEU:N	1:A:369:PRO:CD	2.83	0.41
1:A:118:GLY:HA2	1:A:129:PRO:HG3	2.03	0.41
1:B:386:ASN:ND2	5:B:608:HOH:O	2.45	0.40
1:A:347:HIS:CD2	1:A:349:VAL:H	2.36	0.40
1:A:75:MET:HB2	1:A:75:MET:HE3	1.86	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	433/434 (100%)	418 (96%)	14 (3%)	1 (0%)	44	29
1	B	434/434 (100%)	417 (96%)	13 (3%)	4 (1%)	14	4
All	All	867/868 (100%)	835 (96%)	27 (3%)	5 (1%)	22	9

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	386	ASN
1	B	395	LYS
1	B	387	VAL
1	A	395	LYS
1	B	351	ARG

### 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	367/369 (100%)	352 (96%)	15 (4%)	26	7
1	B	368/369 (100%)	349 (95%)	19 (5%)	19	4
All	All	735/738 (100%)	701 (95%)	34 (5%)	23	5

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ASP
1	A	88	ASP
1	A	176	ASN
1	A	189	ILE
1	A	316	GLN
1	A	340	ARG
1	A	349	VAL
1	A	359	CYS
1	A	368	LEU
1	A	387	VAL
1	A	389	LEU
1	A	390	GLU
1	A	405	SER
1	A	414	MET
1	A	457	LEU
1	B	31	THR
1	B	109	LYS
1	B	176	ASN
1	B	314	GLN

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Mol	Chain	Res	Type
1	B	315	LEU
1	B	327	LYS
1	B	338	SER
1	B	350	LEU
1	B	352	LYS
1	B	359	CYS
1	B	368	LEU
1	B	385	PRO
1	B	386	ASN
1	B	387	VAL
1	B	389	LEU
1	B	390	GLU
1	B	391	GLN
1	B	397	PRO
1	B	414	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	62	GLN
1	A	102	GLN
1	A	127	HIS
1	A	150	HIS
1	A	180	ASN
1	A	314	GLN
1	A	316	GLN
1	A	347	HIS
1	A	391	GLN
1	A	396	ASN
1	B	54	GLN
1	B	62	GLN
1	B	102	GLN
1	B	150	HIS
1	B	249	HIS
1	B	316	GLN
1	B	334	ASN
1	B	386	ASN

### 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 ⓘ

3 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
4	OAA	B	501	-	8,8,8	5.27	2 (25%)	9,10,10	1.61	2 (22%)
2	CIT	A	501	-	12,12,12	1.27	1 (8%)	17,17,17	1.48	3 (17%)
3	COA	A	502	-	41,50,50	0.65	0	52,75,75	0.79	2 (3%)

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
4	OAA	B	501	-	-	2/8/8/8	-
2	CIT	A	501	-	-	10/16/16/16	-
3	COA	A	502	-	-	12/44/64/64	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	501	OAA	C3-C4	-14.44	1.34	1.53
2	A	501	CIT	C3-C6	2.83	1.56	1.53
4	B	501	OAA	O5-C4	-2.74	1.22	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	CIT	O5-C6-C3	-3.73	116.97	122.25
4	B	501	OAA	C2-C3-C4	3.23	123.30	117.85
2	A	501	CIT	O6-C6-C3	3.18	118.58	113.05
3	A	502	COA	P2A-O3A-P1A	2.40	141.05	132.83
2	A	501	CIT	O3-C5-C4	-2.20	116.50	122.94
3	A	502	COA	C5A-C6A-N6A	2.20	123.69	120.35
4	B	501	OAA	O3-C3-C2	-2.01	117.66	120.58

There are no chirality outliers.

All (24) torsion outliers are listed below:

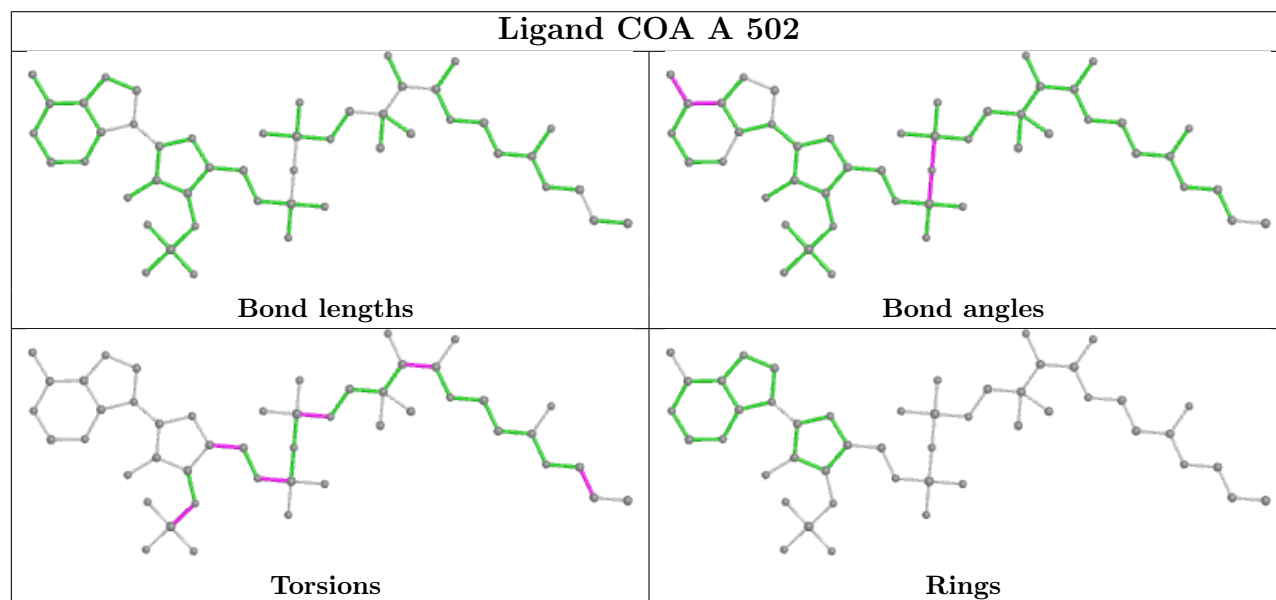
Mol	Chain	Res	Type	Atoms
2	A	501	CIT	C2-C3-C4-C5
2	A	501	CIT	O7-C3-C4-C5
2	A	501	CIT	C6-C3-C4-C5
2	A	501	CIT	C2-C3-C6-O5
2	A	501	CIT	C2-C3-C6-O6
3	A	502	COA	C5B-O5B-P1A-O1A
3	A	502	COA	CCP-O6A-P2A-O4A
3	A	502	COA	CCP-O6A-P2A-O5A
3	A	502	COA	N8P-C9P-CAP-OAP
3	A	502	COA	S1P-C2P-C3P-N4P
4	B	501	OAA	C2-C3-C4-O5
3	A	502	COA	C3B-C4B-C5B-O5B
3	A	502	COA	O4B-C4B-C5B-O5B
3	A	502	COA	O9P-C9P-CAP-OAP
2	A	501	CIT	O7-C3-C6-O6
3	A	502	COA	C5B-O5B-P1A-O3A
4	B	501	OAA	C2-C3-C4-O4
2	A	501	CIT	C4-C3-C6-O5
2	A	501	CIT	C4-C3-C6-O6
2	A	501	CIT	C3-C4-C5-O4
2	A	501	CIT	C3-C4-C5-O3
3	A	502	COA	C3B-O3B-P3B-O7A
3	A	502	COA	C3B-O3B-P3B-O8A
3	A	502	COA	CCP-O6A-P2A-O3A

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	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 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	434/434 (100%)	0.48	33 (7%) 21 25	16, 31, 74, 102	1 (0%)
1	B	434/434 (100%)	0.56	46 (10%) 13 15	11, 31, 78, 161	2 (0%)
All	All	868/868 (100%)	0.52	79 (9%) 16 20	11, 31, 75, 161	3 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	350	LEU	8.9
1	B	349	VAL	7.5
1	B	388	LEU	7.5
1	B	348	ALA	5.6
1	B	387	VAL	5.4
1	A	31	THR	5.3
1	A	394	ALA	5.2
1	A	389	LEU	5.2
1	B	389	LEU	5.0
1	B	303	LEU	4.5
1	B	386	ASN	4.4
1	B	347	HIS	4.4
1	A	333	TRP	4.2
1	B	392	GLY	3.9
1	A	349	VAL	3.6
1	B	461	VAL	3.6
1	B	30	SER	3.6
1	B	31	THR	3.5
1	A	87	PRO	3.5
1	A	359	CYS	3.5
1	B	110	GLY	3.4
1	A	30	SER	3.4
1	B	333	TRP	3.4
1	A	387	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	385	PRO	3.2
1	B	109	LYS	3.2
1	B	394	ALA	3.2
1	A	341	VAL	3.1
1	A	350	LEU	3.1
1	B	341	VAL	3.1
1	B	342	VAL	3.0
1	A	383	ILE	2.9
1	B	232	SER	2.9
1	B	336	LEU	2.9
1	B	391	GLN	2.8
1	B	396	ASN	2.8
1	B	395	LYS	2.8
1	B	351	ARG	2.8
1	B	247	THR	2.7
1	B	374	PHE	2.7
1	A	388	LEU	2.7
1	B	390	GLU	2.6
1	A	331	TYR	2.6
1	A	319	VAL	2.5
1	A	393	LYS	2.5
1	A	340	ARG	2.5
1	A	86	ASP	2.5
1	B	384	VAL	2.4
1	A	303	LEU	2.4
1	B	359	CYS	2.4
1	B	332	ILE	2.4
1	A	337	ASN	2.4
1	A	247	THR	2.4
1	A	54	GLN	2.4
1	A	348	ALA	2.4
1	B	378	ALA	2.4
1	B	393	LYS	2.3
1	A	321	LYS	2.3
1	B	401	VAL	2.3
1	B	319	VAL	2.2
1	A	328	LEU	2.2
1	A	376	LEU	2.2
1	B	365	LEU	2.2
1	A	222	ARG	2.2
1	B	311	TRP	2.2
1	A	320	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	89	GLU	2.2
1	A	85	LEU	2.2
1	B	364	ALA	2.1
1	A	390	GLU	2.1
1	B	322	ASP	2.1
1	B	340	ARG	2.1
1	B	352	LYS	2.1
1	A	396	ASN	2.1
1	A	317	LYS	2.1
1	B	329	ARG	2.0
1	B	326	GLU	2.0
1	B	346	GLY	2.0
1	B	324	SER	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](#)

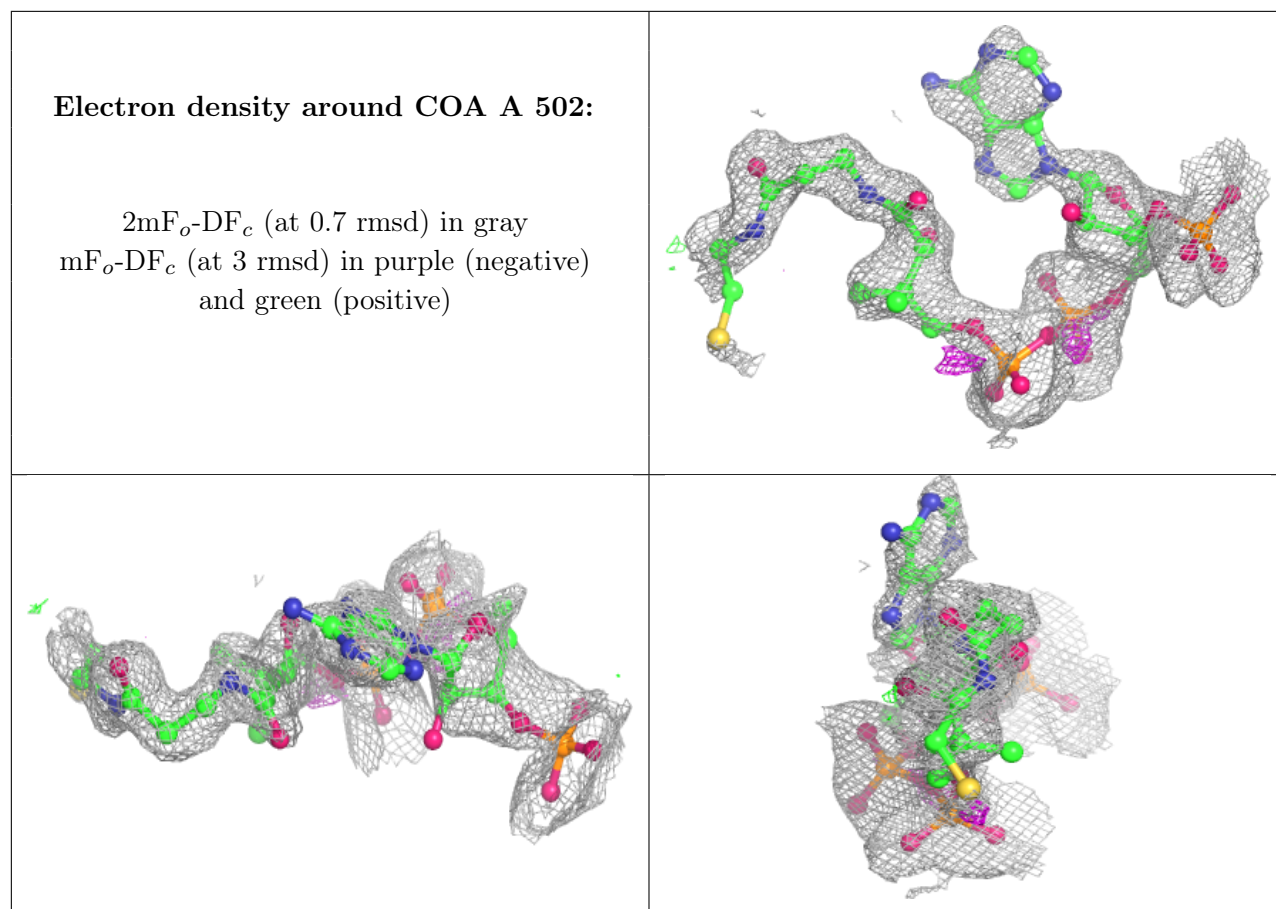
There are no monosaccharides in this entry.

## 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<sup>th</sup> 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
4	OAA	B	501	9/9	0.79	0.14	32,59,70,73	0
3	COA	A	502	48/48	0.81	0.12	49,85,111,118	0
2	CIT	A	501	13/13	0.84	0.11	34,47,59,59	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.



## 6.5 Other polymers ⓘ

There are no such residues in this entry.