



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 9, 2025 – 02:10 PM JST

PDB ID : 8ZVM / pdb_00008zvm
Title : Human citrate synthase intermediate 1
Authors : Yang, L.Y.; Fang, Y.J.
Deposited on : 2024-06-11
Resolution : 2.27 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 Phenix2.0rc1
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

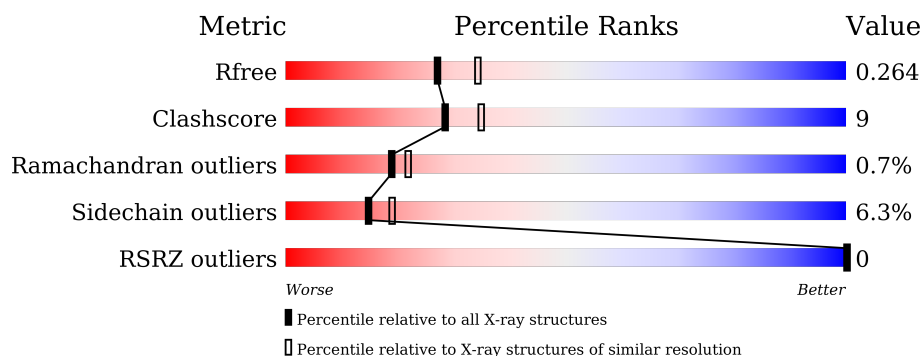
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	8487 (2.30-2.26)
Clashscore	180529	9437 (2.30-2.26)
Ramachandran outliers	177936	9341 (2.30-2.26)
Sidechain outliers	177891	9342 (2.30-2.26)
RSRZ outliers	164620	8487 (2.30-2.26)

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	434	
1	B	434	

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
3	ACE	A	502	-	-	X	-

2 Entry composition [i](#)

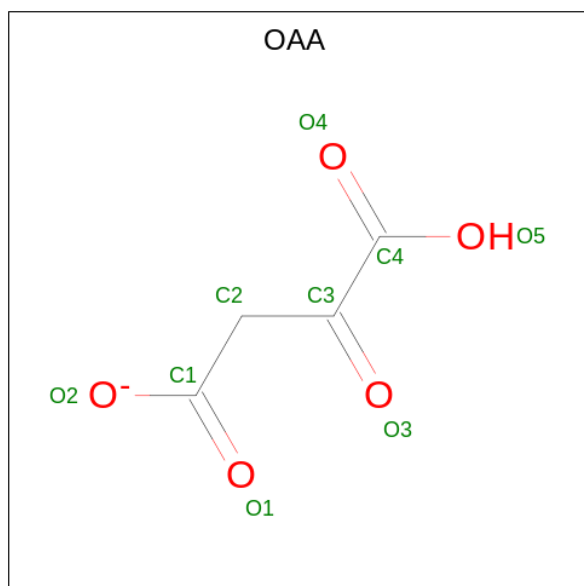
There are 5 unique types of molecules in this entry. The entry contains 6992 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

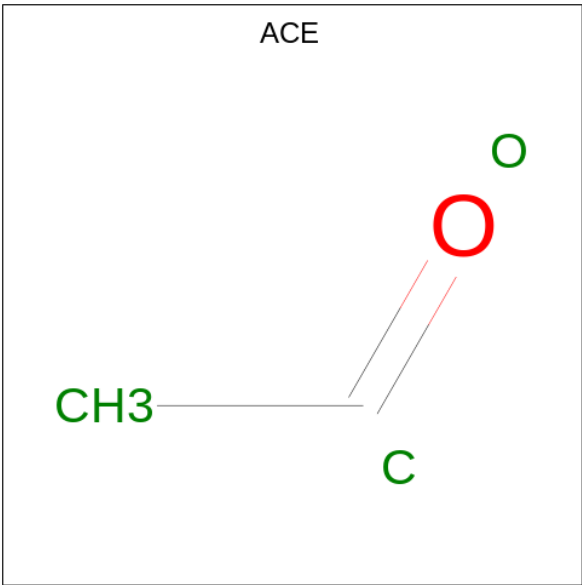
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	1	0
			3416	2184	585	630	17			
1	B	434	Total	C	N	O	S	0	1	0
			3394	2170	578	629	17			

- Molecule 2 is OXALOACETATE ION (CCD ID: OAA) (formula: $C_4H_3O_5$).



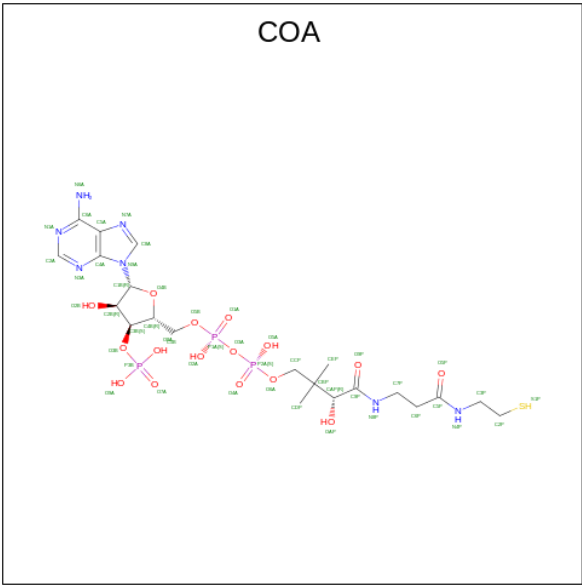
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			9	4	5		

- Molecule 3 is ACETYL GROUP (CCD ID: ACE) (formula: C_2H_4O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			3	2	1		

- Molecule 4 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



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

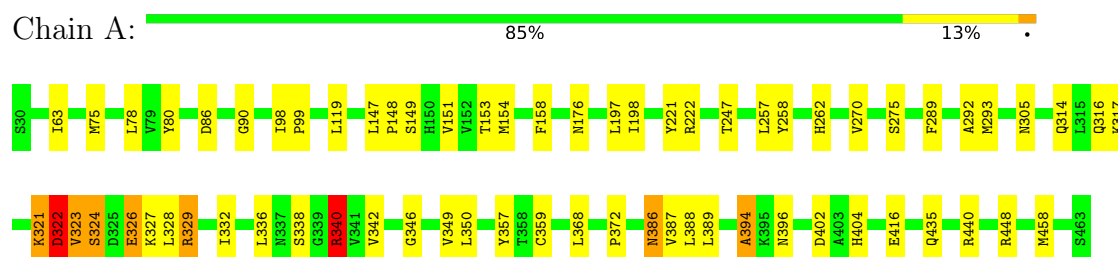
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	68	Total 68	O 68	0	0
5	B	54	Total 54	O 54	0	0

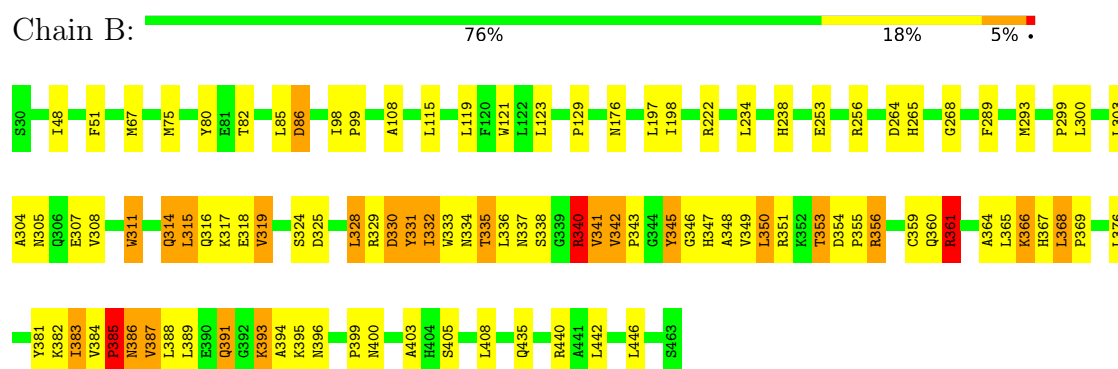
3 Residue-property plots

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, α , β , γ	58.21Å 59.82Å 73.24Å 101.72° 98.66° 116.55°	Depositor
Resolution (Å)	51.00 – 2.27 51.00 – 2.27	Depositor EDS
% Data completeness (in resolution range)	93.2 (51.00-2.27) 83.0 (51.00-2.27)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.219 , 0.268 0.222 , 0.264	Depositor DCC
R_{free} test set	1775 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.111 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6992	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, OAA, COA

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	0.57	1/3504 (0.0%)	1.00	5/4759 (0.1%)
1	B	0.78	7/3482 (0.2%)	1.12	10/4735 (0.2%)
All	All	0.68	8/6986 (0.1%)	1.06	15/9494 (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	2
1	B	0	4
All	All	0	6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	332	ILE	C-N	20.88	1.58	1.33
1	A	322	ASP	C-N	11.71	1.49	1.33
1	B	317	LYS	C-N	8.86	1.45	1.33
1	B	394	ALA	C-N	7.96	1.44	1.33
1	B	300	LEU	C-N	7.68	1.43	1.34
1	B	331	TYR	C-N	6.88	1.43	1.33
1	B	383	ILE	C-N	5.35	1.39	1.33
1	B	395	LYS	C-N	5.16	1.42	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	ASP	CA-C-N	-7.46	108.55	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	322	ASP	C-N-CA	-7.46	108.55	121.97
1	B	316	GLN	CA-C-N	-7.41	111.41	121.71
1	B	316	GLN	C-N-CA	-7.41	111.41	121.71
1	B	332	ILE	O-C-N	7.35	131.76	122.57
1	B	331	TYR	CA-C-N	-7.24	108.93	121.97
1	B	331	TYR	C-N-CA	-7.24	108.93	121.97
1	B	300	LEU	CA-C-N	-6.70	113.59	121.64
1	B	300	LEU	C-N-CA	-6.70	113.59	121.64
1	A	153	THR	CA-CB-OG1	-5.50	101.36	109.60
1	B	332	ILE	CA-C-N	-5.34	113.37	120.79
1	B	332	ILE	C-N-CA	-5.34	113.37	120.79
1	A	247	THR	CA-CB-OG1	-5.30	101.64	109.60
1	B	317	LYS	O-C-N	5.22	128.02	122.38
1	A	86	ASP	CB-CA-C	5.13	118.14	109.67

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	329	ARG	Sidechain
1	A	340	ARG	Sidechain
1	B	340	ARG	Sidechain
1	B	351	ARG	Sidechain
1	B	356	ARG	Sidechain
1	B	361	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	47	0
1	B	3394	0	3332	76	0
2	A	9	0	2	1	0
3	A	3	0	3	6	0
4	A	48	0	32	0	0
5	A	68	0	0	5	0
5	B	54	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6992	0	6751	119	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 9.

All (119) 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:147:LEU:HB3	5:A:648:HOH:O	1.76	0.84
1:A:402:ASP:OD2	3:A:502:ACE:H3	1.79	0.83
1:B:384:VAL:O	1:B:386:ASN:N	2.18	0.77
1:A:257:LEU:HD11	1:A:359:CYS:SG	2.25	0.76
1:A:402:ASP:OD2	3:A:502:ACE:CH3	2.37	0.72
1:B:361:ARG:HH11	1:B:381:TYR:HD2	1.40	0.70
1:A:151:VAL:HB	5:A:648:HOH:O	1.92	0.69
1:B:332:ILE:HG22	1:B:336:LEU:CD1	2.24	0.68
1:A:389:LEU:HA	5:A:616:HOH:O	1.95	0.66
1:B:383:ILE:O	1:B:384:VAL:C	2.39	0.66
1:B:386:ASN:HD22	1:B:387:VAL:H	1.43	0.65
1:B:332:ILE:HG22	1:B:336:LEU:HD11	1.78	0.64
1:A:458:MET:HE2	1:B:51:PHE:HB2	1.81	0.63
1:A:321:LYS:HD2	1:A:372:PRO:HB3	1.81	0.61
1:B:108:ALA:HB2	1:B:115:LEU:HD21	1.84	0.60
1:A:98:ILE:HB	1:A:99:PRO:HD3	1.83	0.59
1:B:347:HIS:HD2	1:B:350:LEU:H	1.50	0.59
1:A:198:ILE:HG13	1:A:440:ARG:HG3	1.85	0.58
1:B:253:GLU:OE1	1:B:256:ARG:NH1	2.28	0.57
1:A:323:VAL:HG23	1:A:327:LYS:NZ	2.19	0.57
1:B:80:TYR:CE1	1:B:435:GLN:HG2	2.41	0.56
1:B:345:TYR:HA	1:B:399:PRO:HA	1.87	0.56
1:A:402:ASP:CG	3:A:502:ACE:CH3	2.78	0.56
1:B:334:ASN:O	1:B:338:SER:N	2.38	0.56
1:A:221:TYR:CD1	1:A:416:GLU:HG2	2.42	0.55
2:A:501:OAA:O3	3:A:502:ACE:O	2.24	0.55
1:A:63:ILE:HD11	1:B:75:MET:HG3	1.89	0.54
1:A:323:VAL:HG22	1:A:324:SER:H	1.72	0.54
1:B:336:LEU:HD13	1:B:391:GLN:HG3	1.88	0.54
1:B:333:TRP:CZ3	1:B:391:GLN:HG2	2.43	0.53
1:A:338:SER:HB2	1:A:340:ARG:HG3	1.91	0.53
1:B:328:LEU:O	1:B:329:ARG:C	2.52	0.53
1:A:148:PRO:HD2	5:A:648:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:ASN:HD22	1:B:387:VAL:N	2.07	0.52
1:B:299:PRO:HA	1:B:303:LEU:HB2	1.91	0.52
1:B:360:GLN:HB3	1:B:408:LEU:HD11	1.91	0.51
1:A:328:LEU:O	1:A:332:ILE:HG12	2.11	0.51
1:A:323:VAL:HG23	1:A:327:LYS:HZ3	1.74	0.51
1:B:198:ILE:HG13	1:B:440:ARG:HG3	1.93	0.50
1:B:330:ASP:O	1:B:331:TYR:C	2.53	0.50
1:B:332:ILE:HG23	1:B:342:VAL:HG22	1.92	0.50
1:B:311:TRP:HH2	1:B:335:THR:HG21	1.76	0.50
1:A:154:MET:HE3	1:A:158:PHE:HZ	1.75	0.50
1:B:332:ILE:O	1:B:335:THR:N	2.45	0.50
1:B:121:TRP:CD1	1:B:129:PRO:HB3	2.47	0.49
1:B:384:VAL:C	1:B:386:ASN:N	2.69	0.49
1:B:311:TRP:CH2	1:B:335:THR:HG21	2.48	0.49
1:B:347:HIS:CD2	1:B:350:LEU:H	2.31	0.49
1:B:361:ARG:HH21	1:B:365:LEU:HD21	1.78	0.49
1:A:402:ASP:OD1	3:A:502:ACE:CH3	2.61	0.48
1:B:331:TYR:O	1:B:332:ILE:C	2.54	0.48
1:B:364:ALA:O	1:B:368:LEU:N	2.45	0.48
1:B:366:LYS:HB3	1:B:366:LYS:HE3	1.59	0.48
1:A:221:TYR:CG	1:A:416:GLU:HG2	2.49	0.48
1:A:270:VAL:CG2	1:B:446:LEU:HD11	2.44	0.47
1:B:364:ALA:HA	1:B:368:LEU:HG	1.96	0.47
1:B:333:TRP:O	1:B:337:ASN:N	2.45	0.47
1:A:119:LEU:C	1:A:119:LEU:HD13	2.38	0.47
1:B:85:LEU:HD22	1:B:265:HIS:CE1	2.48	0.47
1:A:78:LEU:N	1:A:78:LEU:HD23	2.29	0.47
1:B:354:ASP:HB2	1:B:400:ASN:HA	1.97	0.47
1:A:402:ASP:OD1	3:A:502:ACE:H2	2.15	0.47
1:B:384:VAL:O	1:B:385:PRO:C	2.57	0.47
1:A:387:VAL:HG23	1:A:388:LEU:HG	1.97	0.47
5:A:610:HOH:O	1:B:85:LEU:HD23	2.15	0.46
1:B:384:VAL:C	1:B:386:ASN:H	2.23	0.46
1:A:388:LEU:HB3	1:A:394:ALA:HB2	1.96	0.46
1:A:80:TYR:CE2	1:A:435:GLN:HG2	2.50	0.46
1:B:98:ILE:HB	1:B:99:PRO:HD3	1.96	0.46
1:A:90:GLY:HA2	1:A:350:LEU:HD21	1.98	0.46
1:A:323:VAL:HG22	1:A:327:LYS:HD3	1.97	0.46
1:B:353:THR:O	1:B:354:ASP:C	2.59	0.46
1:B:341:VAL:O	1:B:342:VAL:C	2.58	0.45
1:B:289:PHE:CE1	1:B:293:MET:HE3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:GLY:HA2	1:B:396:ASN:HB3	1.98	0.45
1:B:367:HIS:O	1:B:369:PRO:HD3	2.17	0.45
1:A:321:LYS:O	1:A:322:ASP:C	2.58	0.45
1:A:357:TYR:CD1	1:A:404:HIS:HB2	2.51	0.45
1:B:384:VAL:O	1:B:386:ASN:ND2	2.50	0.45
1:A:222:ARG:HH11	1:A:222:ARG:HG2	1.82	0.45
1:A:275:SER:HB3	1:A:292:ALA:HB2	1.99	0.45
1:A:270:VAL:HG21	1:B:446:LEU:HD11	1.98	0.44
1:B:121:TRP:CG	1:B:129:PRO:HB3	2.52	0.44
1:A:289:PHE:CE1	1:A:293:MET:HE3	2.53	0.44
1:A:98:ILE:HB	1:A:99:PRO:CD	2.48	0.43
1:B:197:LEU:HD22	1:B:197:LEU:N	2.33	0.43
1:B:332:ILE:CG2	1:B:336:LEU:HD11	2.47	0.43
1:B:311:TRP:CE3	1:B:343:PRO:HD3	2.53	0.43
1:B:340:ARG:HE	1:B:340:ARG:HB2	1.66	0.43
1:B:222:ARG:HH11	1:B:222:ARG:HG2	1.84	0.42
1:B:314:GLN:O	1:B:318:GLU:HG2	2.19	0.42
1:A:336:LEU:HD21	1:A:342:VAL:HG23	2.01	0.42
1:B:67:MET:HB3	1:B:75:MET:HE3	2.01	0.42
1:B:119:LEU:C	1:B:119:LEU:HD13	2.44	0.42
1:B:234:LEU:HD22	1:B:238:HIS:ND1	2.35	0.42
1:B:331:TYR:O	1:B:335:THR:HB	2.20	0.42
1:B:82:THR:OG1	1:B:264:ASP:OD2	2.35	0.42
1:B:356:ARG:O	1:B:360:GLN:HG3	2.19	0.41
1:B:367:HIS:C	1:B:369:PRO:HD3	2.45	0.41
1:A:346:GLY:HA2	1:A:396:ASN:O	2.21	0.41
1:A:448:ARG:NH2	1:B:268:GLY:HA3	2.36	0.41
1:B:393:LYS:H	1:B:393:LYS:HG2	1.60	0.41
1:A:63:ILE:HG12	1:A:75:MET:HE2	2.01	0.41
1:B:354:ASP:HA	1:B:355:PRO:HD3	1.87	0.41
1:A:305:ASN:OD1	1:A:305:ASN:C	2.63	0.41
1:B:48:ILE:CD1	1:B:442:LEU:HD13	2.51	0.41
1:B:86:ASP:OD1	1:B:86:ASP:N	2.48	0.41
1:B:119:LEU:HD11	1:B:123:LEU:HD11	2.03	0.41
1:B:304:ALA:O	1:B:305:ASN:C	2.64	0.41
1:A:154:MET:HE3	1:A:158:PHE:CZ	2.55	0.41
1:B:80:TYR:CD1	1:B:435:GLN:HG2	2.55	0.41
1:A:258:TYR:CE2	1:A:262:HIS:CE1	3.08	0.40
1:A:326:GLU:H	1:A:326:GLU:HG3	1.51	0.40
1:A:80:TYR:CD2	1:A:435:GLN:HG2	2.57	0.40
1:B:308:VAL:HG21	1:B:403:ALA:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:LEU:O	1:B:319:VAL:HG22	2.22	0.40
1:B:347:HIS:CG	1:B:348:ALA:H	2.40	0.40
1:B:333:TRP:O	1:B:334:ASN:C	2.65	0.40
1:B:337:ASN:HB3	5:B:552:HOH:O	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	433/434 (100%)	415 (96%)	15 (4%)	3 (1%)	19	22
1	B	433/434 (100%)	404 (93%)	26 (6%)	3 (1%)	19	22
All	All	866/868 (100%)	819 (95%)	41 (5%)	6 (1%)	19	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	387	VAL
1	A	386	ASN
1	A	394	ALA
1	B	385	PRO
1	B	330	ASP
1	A	323	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	367/369 (100%)	352 (96%)	15 (4%)	26	36
1	B	362/369 (98%)	331 (91%)	31 (9%)	8	10
All	All	729/738 (99%)	683 (94%)	46 (6%)	15	19

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	SER
1	A	176	ASN
1	A	197	LEU
1	A	314	GLN
1	A	316	GLN
1	A	317	LYS
1	A	321	LYS
1	A	322	ASP
1	A	324	SER
1	A	326	GLU
1	A	329	ARG
1	A	340	ARG
1	A	349	VAL
1	A	368	LEU
1	A	386	ASN
1	B	86	ASP
1	B	176	ASN
1	B	307	GLU
1	B	311	TRP
1	B	314	GLN
1	B	315	LEU
1	B	319	VAL
1	B	324	SER
1	B	325	ASP
1	B	328	LEU
1	B	335	THR
1	B	340	ARG
1	B	341	VAL
1	B	342	VAL
1	B	345	TYR
1	B	349	VAL
1	B	350	LEU
1	B	353	THR
1	B	359	CYS

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Mol	Chain	Res	Type
1	B	361	ARG
1	B	366	LYS
1	B	368	LEU
1	B	376	LEU
1	B	382	LYS
1	B	385	PRO
1	B	386	ASN
1	B	388	LEU
1	B	389	LEU
1	B	391	GLN
1	B	393	LYS
1	B	405	SER

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	54	GLN
1	A	102	GLN
1	A	262	HIS
1	A	347	HIS
1	B	55	HIS
1	B	102	GLN
1	B	180	ASN
1	B	347	HIS
1	B	386	ASN
1	B	391	GLN
1	B	410	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
2	OAA	A	501	-	8,8,8	5.58	2 (25%)	9,10,10	1.86	3 (33%)
3	ACE	A	502	-	1,2,2	0.13	0	1,1,1	0.58	0
4	COA	A	503	-	41,50,50	0.60	0	52,75,75	0.73	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
2	OAA	A	501	-	-	0/8/8/8	-
4	COA	A	503	-	-	10/44/64/64	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	OAA	C3-C4	-15.42	1.32	1.53
2	A	501	OAA	O5-C4	-2.35	1.23	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	OAA	C2-C3-C4	3.29	123.41	117.85
2	A	501	OAA	O4-C4-C3	-2.95	117.79	121.72
4	A	503	COA	C5A-C6A-N6A	2.36	123.94	120.35
2	A	501	OAA	O5-C4-C3	2.32	120.32	113.97
4	A	503	COA	O4B-C1B-C2B	-2.30	103.57	106.93

There are no chirality outliers.

All (10) torsion outliers are listed below:

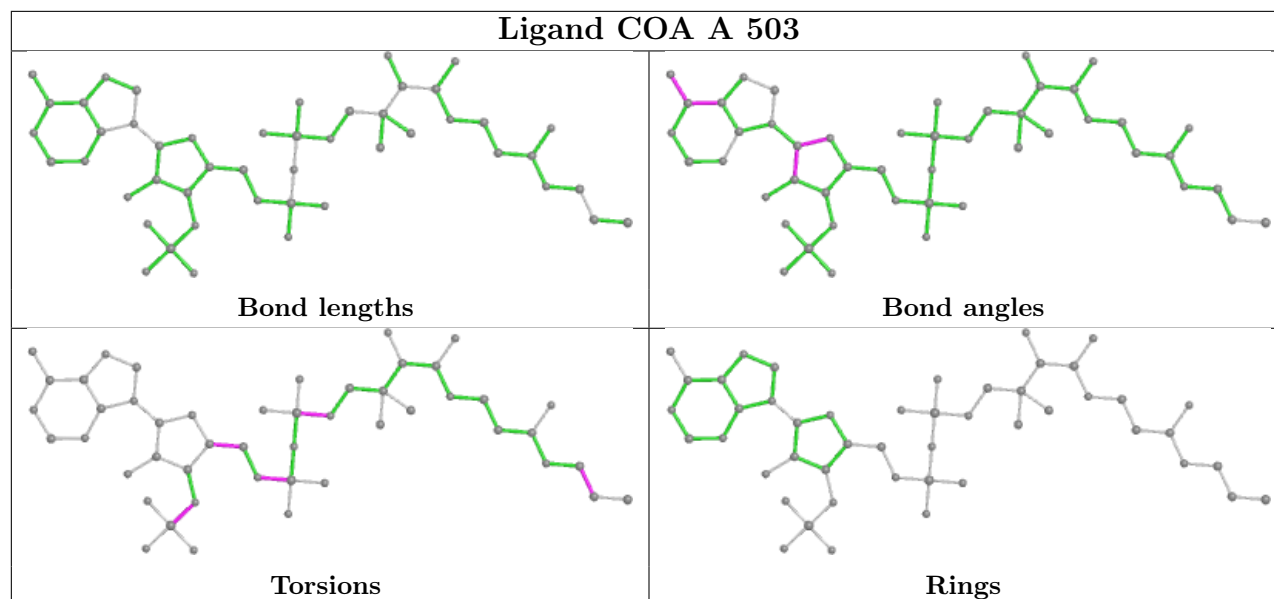
Mol	Chain	Res	Type	Atoms
4	A	503	COA	C5B-O5B-P1A-O3A
4	A	503	COA	CCP-O6A-P2A-O4A
4	A	503	COA	S1P-C2P-C3P-N4P
4	A	503	COA	O4B-C4B-C5B-O5B
4	A	503	COA	C3B-C4B-C5B-O5B
4	A	503	COA	C3B-O3B-P3B-O7A
4	A	503	COA	CCP-O6A-P2A-O3A
4	A	503	COA	C5B-O5B-P1A-O1A
4	A	503	COA	CCP-O6A-P2A-O5A
4	A	503	COA	C3B-O3B-P3B-O9A

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	OAA	1	0
3	A	502	ACE	6	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	434/434 (100%)	-1.69	0 100 100	17, 36, 83, 119	1 (0%)
1	B	434/434 (100%)	-1.61	0 100 100	16, 38, 131, 199	1 (0%)
All	All	868/868 (100%)	-1.65	0 100 100	16, 37, 113, 199	2 (0%)

There are no RSRZ outliers to report.

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.

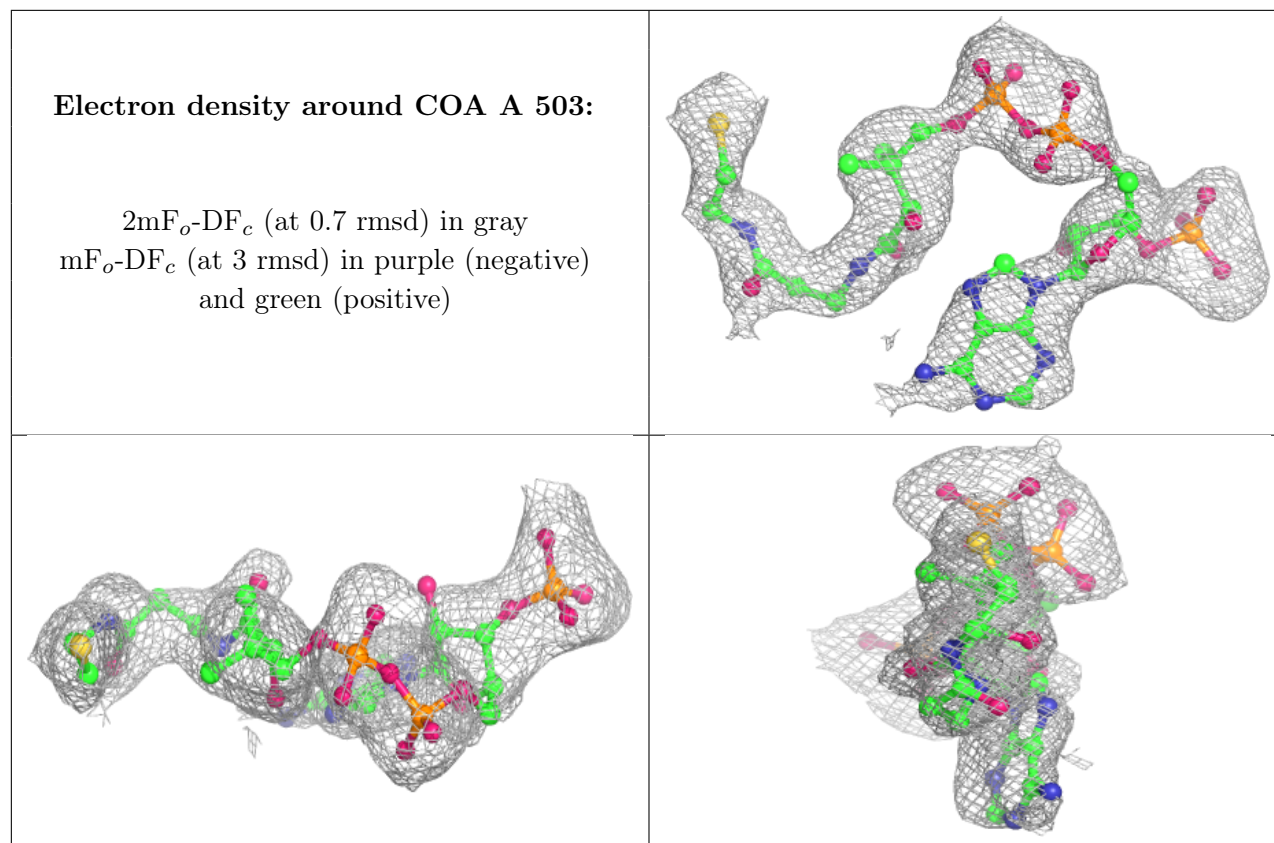
6.4 Ligands [i](#)

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, 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(Å ²)	Q<0.9
3	ACE	A	502	3/3	0.99	0.04	55,55,59,65	0
4	COA	A	503	48/48	0.99	0.02	44,72,81,82	0
2	OAA	A	501	9/9	1.00	0.01	34,39,42,43	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.