



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:15 PM UTC

PDB ID : 1EAC / pdb_00001eac
Title : ATOMIC STRUCTURE OF THE CUBIC CORE OF THE PYRUVATE DE-HYDROGENASE MULTIENZYME COMPLEX
Authors : Mattevi, A.; Hol, W.G.J.
Deposited on : 1992-12-16
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

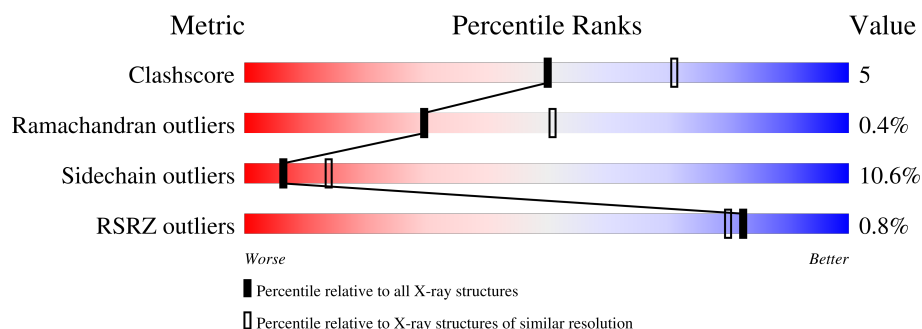
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	243	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1908 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.

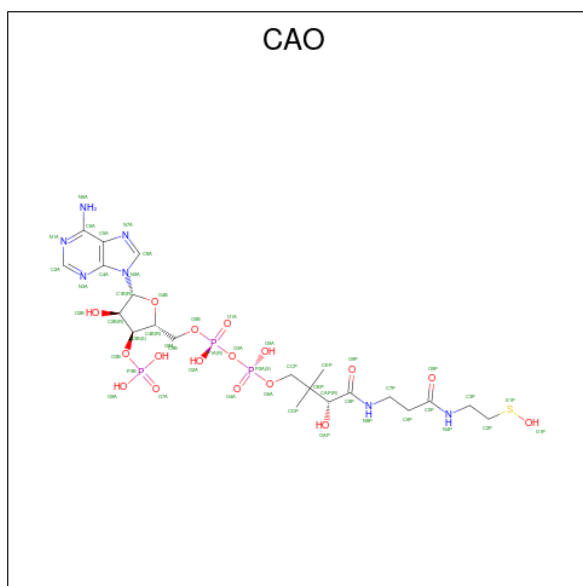
- Molecule 1 is a protein called DIHYDROLIPOYL-TRANSACETYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	0	0	0
			1816	1171	311	327	7			

There is a discrepancy between the modelled and reference sequences:

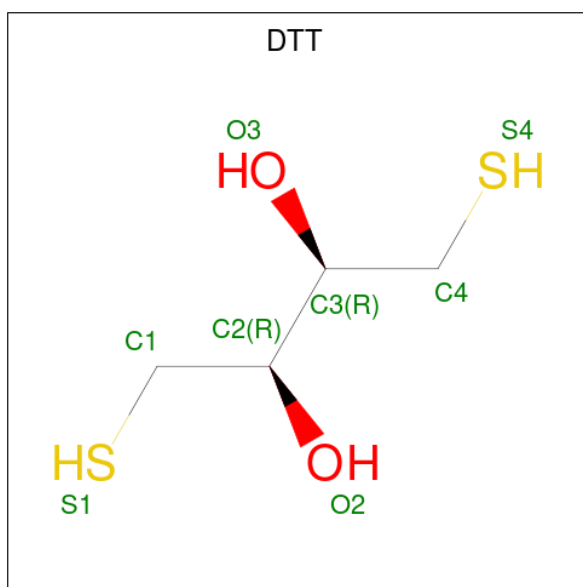
Chain	Residue	Modelled	Actual	Comment	Reference
A	458	LYS	GLU	conflict	UNP P10802

- Molecule 2 is OXIDIZED COENZYME A (CCD ID: CAO) (formula: $C_{21}H_{36}N_7O_{17}P_3S$).



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

- Molecule 3 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	S	
			8	4	2	2	
							0
							0

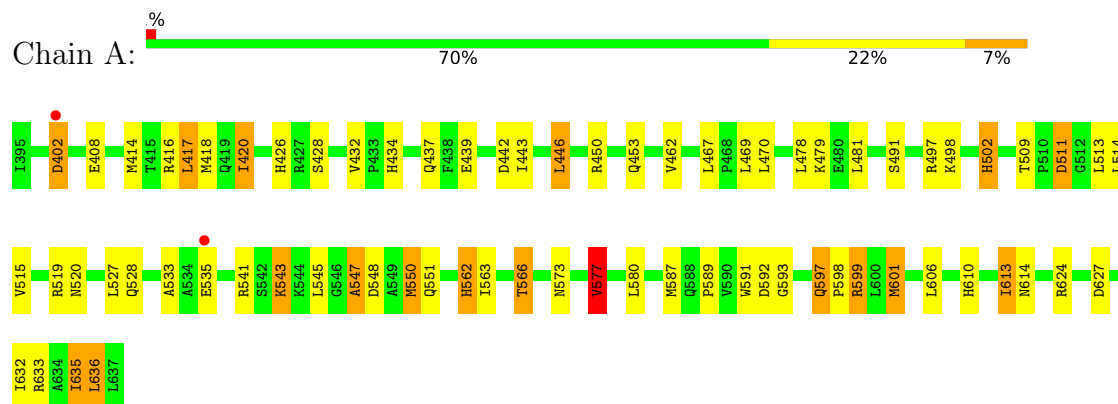
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total	O		
			36	36		
					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: DIHYDROLIPOYL-TRANSACETYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	F 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	225.54Å 225.54Å 225.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60 10.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.60) 89.7 (10.00-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.65Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.203 , (Not available) 0.184 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	1908	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% 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: CAO, DTT

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	1.27	8/1853 (0.4%)	1.89	42/2523 (1.7%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	502	HIS	CD2-NE2	-8.12	1.28	1.37
1	A	562	HIS	CD2-NE2	-5.93	1.31	1.37
1	A	426	HIS	CD2-NE2	-5.55	1.31	1.37
1	A	610	HIS	CD2-NE2	-5.38	1.31	1.37
1	A	434	HIS	CD2-NE2	-5.25	1.32	1.37
1	A	502	HIS	CG-ND1	-5.23	1.32	1.38
1	A	589	PRO	CA-CB	-5.22	1.47	1.53
1	A	515	VAL	CA-CB	5.06	1.60	1.54

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	577	VAL	N-CA-CB	-10.41	98.83	112.36
1	A	614	ASN	OD1-CG-ND2	-8.80	113.80	122.60
1	A	535	GLU	CA-CB-CG	8.51	131.12	114.10
1	A	566	THR	N-CA-CB	-8.50	98.85	110.67
1	A	627	ASP	CA-CB-CG	8.44	121.04	112.60
1	A	437	GLN	OE1-CD-NE2	-8.32	114.28	122.60
1	A	402	ASP	CA-CB-CG	8.09	120.69	112.60
1	A	577	VAL	CB-CA-C	7.45	119.12	110.93
1	A	497	ARG	CA-CB-CG	-6.96	100.18	114.10
1	A	437	GLN	CG-CD-NE2	6.95	126.82	116.40
1	A	420	ILE	N-CA-C	-6.87	103.82	110.42
1	A	614	ASN	CB-CG-ND2	6.77	126.55	116.40
1	A	548	ASP	CA-CB-CG	6.66	119.26	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	563	ILE	N-CA-C	-6.14	106.77	111.62
1	A	601	MET	CG-SD-CE	-6.07	87.54	100.90
1	A	566	THR	CA-CB-OG1	-6.01	100.58	109.60
1	A	573	ASN	N-CA-CB	-6.01	102.46	110.57
1	A	453	GLN	OE1-CD-NE2	-5.87	116.73	122.60
1	A	597	GLN	OE1-CD-NE2	-5.83	116.78	122.60
1	A	426	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	A	432	VAL	O-C-N	-5.64	117.82	121.37
1	A	592	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	610	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	A	541	ARG	CB-CG-CD	-5.55	98.53	111.30
1	A	593	GLY	N-CA-C	-5.45	107.42	113.79
1	A	432	VAL	N-CA-CB	-5.43	104.90	111.31
1	A	533	ALA	N-CA-C	-5.35	105.35	111.07
1	A	514	LEU	O-C-N	-5.23	116.80	123.24
1	A	439	GLU	CA-C-O	-5.19	115.67	121.23
1	A	479	LYS	CB-CG-CD	-5.17	99.40	111.30
1	A	566	THR	CB-CA-C	5.15	117.73	109.07
1	A	606	LEU	CA-C-O	-5.14	115.08	120.58
1	A	428	SER	CB-CA-C	-5.10	102.33	110.79
1	A	498	LYS	O-C-N	-5.10	117.41	123.22
1	A	591	TRP	CG-CD1-NE1	-5.09	103.58	110.20
1	A	513	LEU	N-CA-C	5.09	117.85	109.76
1	A	551	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	A	443	ILE	O-C-N	-5.07	116.88	122.05
1	A	481	LEU	CA-C-N	5.04	124.70	119.56
1	A	481	LEU	C-N-CA	5.04	124.70	119.56
1	A	528	GLN	CG-CD-NE2	5.04	123.96	116.40
1	A	566	THR	CA-CB-CG2	5.02	119.04	110.50

There are no chirality outliers.

There are no planarity outliers.

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	1816	0	1866	20	2
2	A	48	0	31	0	0
3	A	8	0	8	0	0
4	A	36	0	0	1	1
All	All	1908	0	1905	20	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 5.

All (20) 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:502:HIS:HD2	1:A:520:ASN:H	1.40	0.69
1:A:417:LEU:HD12	1:A:511:ASP:HB3	1.77	0.67
1:A:416:ARG:O	1:A:420:ILE:HG12	2.03	0.58
1:A:547:ALA:HA	1:A:550:MET:HE2	1.84	0.58
1:A:502:HIS:CG	1:A:519:ARG:HD3	2.42	0.55
1:A:633:ARG:O	1:A:636:LEU:HB2	2.09	0.53
1:A:587:MET:HE2	1:A:598:PRO:HB2	1.92	0.51
1:A:414:MET:HE2	1:A:418:MET:HB3	1.94	0.50
1:A:562:HIS:CD2	4:A:652:HOH:O	2.64	0.49
1:A:599:ARG:HB2	1:A:601:MET:HE3	1.93	0.49
1:A:462:VAL:HG21	1:A:527:LEU:HD22	1.92	0.49
1:A:446:LEU:HD21	1:A:469:LEU:HD22	1.94	0.48
1:A:442:ASP:OD2	1:A:599:ARG:HD3	2.14	0.47
1:A:624:ARG:HD2	1:A:624:ARG:HA	1.80	0.46
1:A:511:ASP:HB2	1:A:543:LYS:NZ	2.32	0.45
1:A:599:ARG:CB	1:A:601:MET:HE3	2.50	0.41
1:A:547:ALA:HA	1:A:550:MET:CE	2.48	0.41
1:A:632:ILE:HD11	1:A:635:ILE:HD12	2.03	0.40
1:A:577:VAL:HG13	1:A:613:ILE:HD12	2.01	0.40
1:A:545:LEU:HD23	1:A:550:MET:SD	2.61	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:A:402:ASP:OD1	1:A:402:ASP:OD1[28_555]	1.52	0.68
1:A:402:ASP:OD2	4:A:674:HOH:O[28_555]	1.84	0.36

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	241/243 (99%)	231 (96%)	9 (4%)	1 (0%)	30	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	547	ALA

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	188/195 (96%)	168 (89%)	20 (11%)	6	14

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	408	GLU
1	A	417	LEU
1	A	446	LEU
1	A	450	ARG
1	A	467	LEU
1	A	470	LEU
1	A	478	LEU
1	A	491	SER
1	A	509	THR
1	A	511	ASP

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Mol	Chain	Res	Type
1	A	543	LYS
1	A	550	MET
1	A	566	THR
1	A	577	VAL
1	A	580	LEU
1	A	597	GLN
1	A	599	ARG
1	A	613	ILE
1	A	635	ILE
1	A	636	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	424	ASN
1	A	426	HIS
1	A	431	ASN
1	A	502	HIS
1	A	562	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](#)

2 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	DTT	A	639	-	7,7,7	1.19	0	4,8,8	2.19	1 (25%)
2	CAO	A	638	-	47,50,51	0.99	1 (2%)	69,75,76	1.91	14 (20%)

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	DTT	A	639	-	-	3/8/8/8	-
2	CAO	A	638	-	-	10/48/64/65	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	638	CAO	C5A-N7A	-3.32	1.33	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	638	CAO	C5A-C4A-N3A	-6.99	117.09	126.72
2	A	638	CAO	N3A-C4A-N9A	5.95	137.29	127.17
2	A	638	CAO	C6A-C5A-C4A	5.38	124.53	117.18
2	A	638	CAO	C6A-C5A-N7A	-4.57	123.29	132.09
3	A	639	DTT	O3-C3-C2	-3.43	102.38	109.57
2	A	638	CAO	CEP-CBP-CAP	3.23	114.27	108.77
2	A	638	CAO	C6P-C5P-N4P	3.04	121.88	116.34
2	A	638	CAO	N3A-C2A-N1A	-2.90	124.19	128.58
2	A	638	CAO	C2A-N3A-C4A	2.86	118.82	111.83
2	A	638	CAO	O2B-C2B-C1B	2.60	119.07	110.10
2	A	638	CAO	O5P-C5P-C6P	-2.23	117.99	122.02
2	A	638	CAO	CAP-C9P-N8P	-2.21	112.29	116.48
2	A	638	CAO	O2B-C2B-C3B	2.14	117.17	111.19
2	A	638	CAO	N6A-C6A-N1A	2.10	123.06	118.38
2	A	638	CAO	O9A-P3B-O8A	2.05	115.48	107.80

There are no chirality outliers.

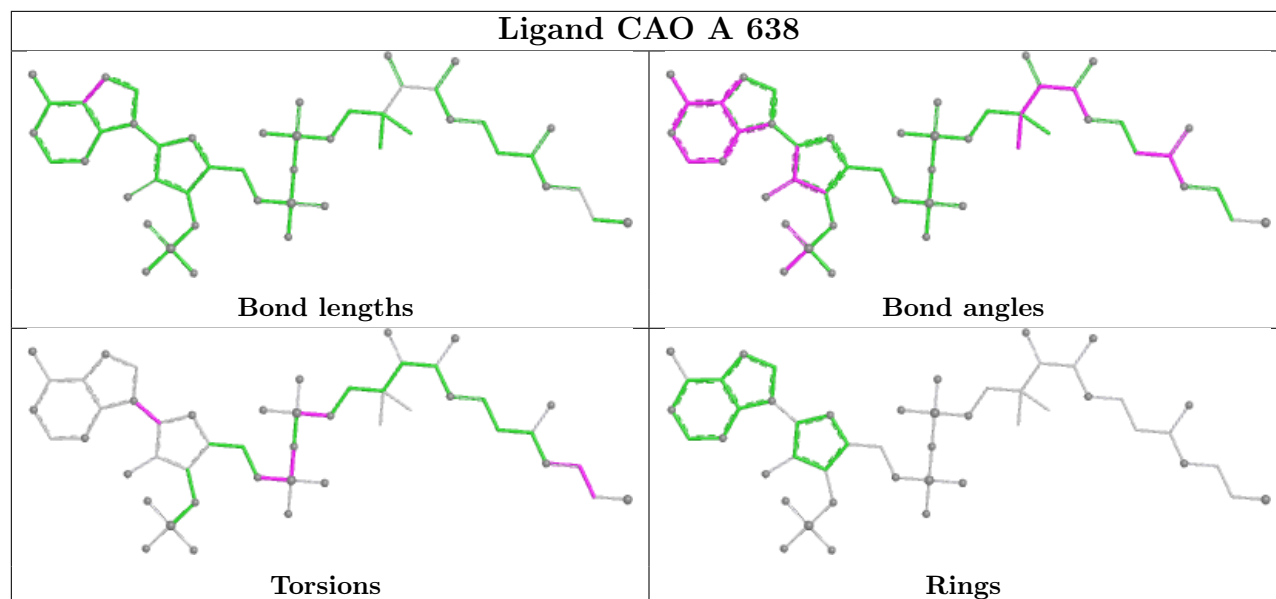
All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	638	CAO	C5B-O5B-P1A-O1A
2	A	638	CAO	C5B-O5B-P1A-O3A
2	A	638	CAO	CCP-O6A-P2A-O3A
2	A	638	CAO	CCP-O6A-P2A-O4A
3	A	639	DTT	C2-C3-C4-S4
2	A	638	CAO	C2B-C1B-N9A-C8A
2	A	638	CAO	S1P-C2P-C3P-N4P
3	A	639	DTT	O3-C3-C4-S4
2	A	638	CAO	C2P-C3P-N4P-C5P
2	A	638	CAO	P2A-O3A-P1A-O1A
2	A	638	CAO	O4B-C1B-N9A-C8A
2	A	638	CAO	P2A-O3A-P1A-O2A
3	A	639	DTT	C1-C2-C3-C4

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 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	243/243 (100%)	-0.70	2 (0%) 82 80	2, 15, 42, 49	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	402	ASP	2.4
1	A	535	GLU	2.1

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.

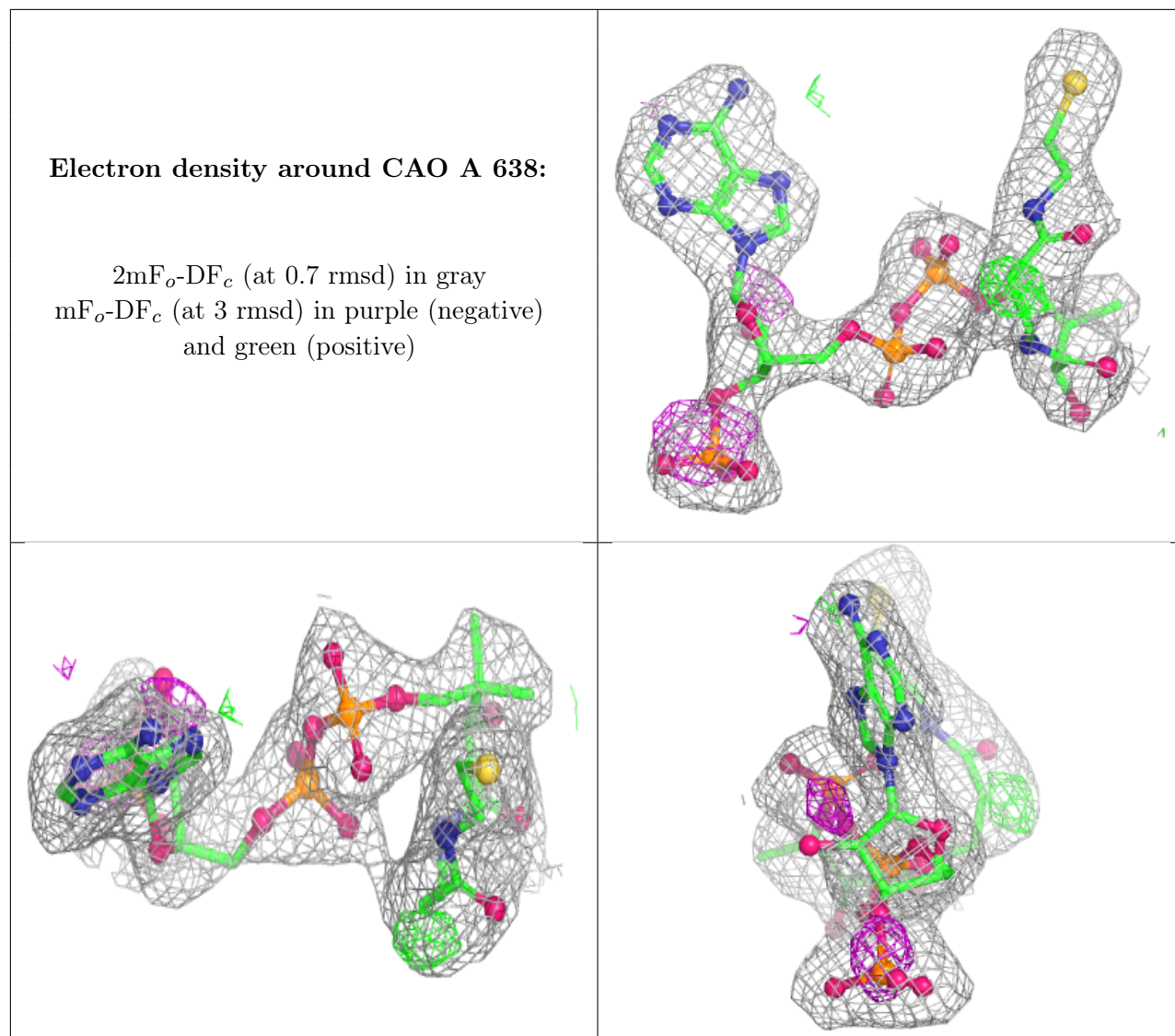
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
3	DTT	A	639	8/8	0.72	0.15	63,65,66,67	0
2	CAO	A	638	48/49	0.92	0.10	37,40,52,53	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.