Full wwPDB X-ray Structure Validation Report (i)

Oct 16, 2023 – 03:31 PM EDT

PDB ID	:	1T3Z
Title	:	Formyl-CoA Tranferase mutant Asp169 to Ser
Authors	:	Ricagno, S.; Jonsson, S.; Richards, N.G.; Lindqvist, Y.
Deposited on	:	2004-04-28
Resolution	:	2.30 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:

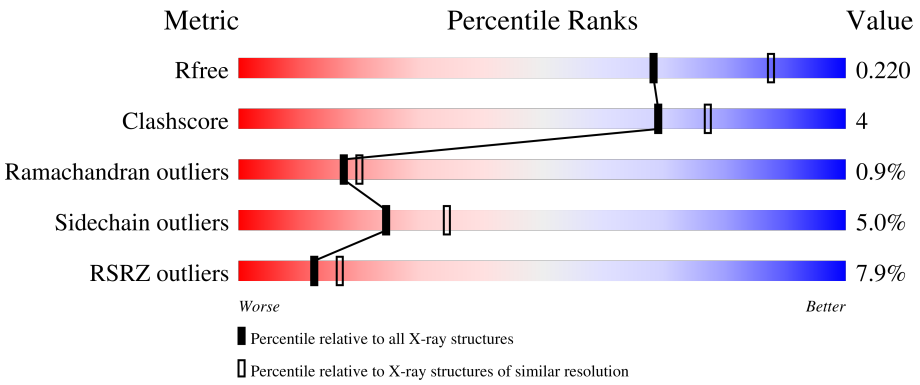
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	427	3% 88% 11%
1	B	427	13% 83% 15% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7159 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.

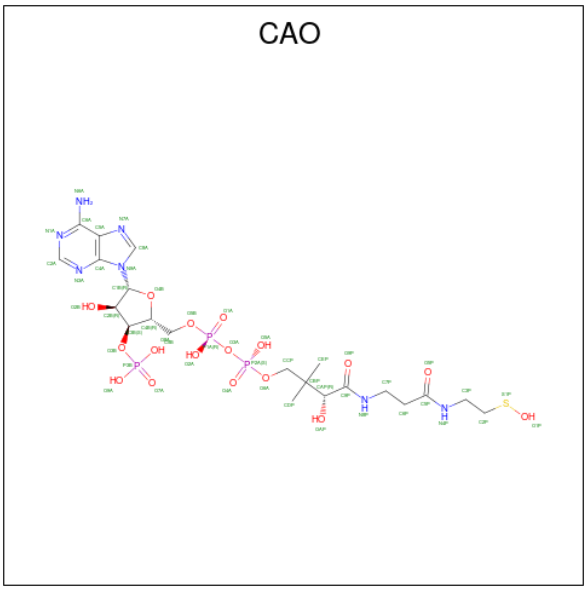
- Molecule 1 is a protein called Formyl-coenzyme A transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	427	3311	2095	568	625	23	0	0	0
1	B	427	3311	2095	568	625	23	4	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	SER	ASP	engineered mutation	UNP O06644
A	186	ILE	MET	SEE REMARK 999	UNP O06644
B	169	SER	ASP	engineered mutation	UNP O06644
B	186	ILE	MET	SEE REMARK 999	UNP O06644

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	49	21	7	17	3	1	0	0
			Total	C	N	O	P	S		
2	B	1	49	21	7	17	3	1	0	0

- Molecule 3 is water.

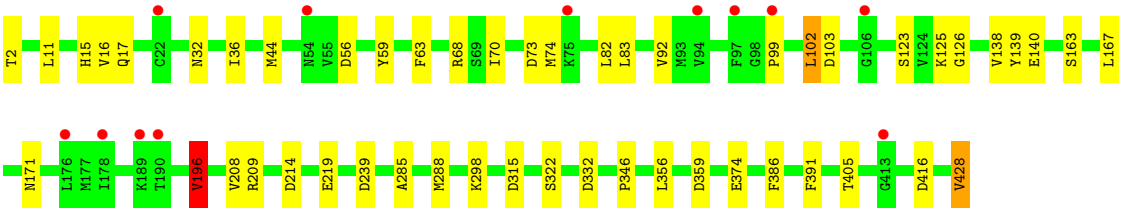
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	247	247	247	0	0
			Total	O		
3	B	192	192	192	0	0

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.

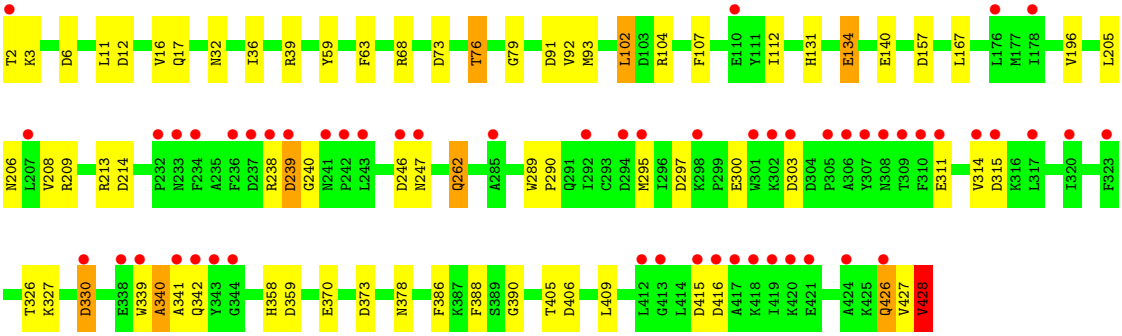
• Molecule 1: Formyl-coenzyme A transferase

Chain A:



• Molecule 1: Formyl-coenzyme A transferase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	151.82Å 151.82Å 100.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 30.26 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-2.30) 99.4 (30.26-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.76 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.177 , 0.216 0.184 , 0.220	Depositor DCC
R_{free} test set	2538 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	41.1	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7159	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CAO

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	0.59	0/3385	0.81	10/4577 (0.2%)
1	B	0.67	3/3385 (0.1%)	0.91	21/4577 (0.5%)
All	All	0.63	3/6770 (0.0%)	0.86	31/9154 (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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	239	ASP	C-N	17.31	1.64	1.33
1	B	240	GLY	C-N	11.52	1.60	1.34
1	B	428	VAL	C-OXT	-9.84	1.04	1.23

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	239	ASP	O-C-N	-21.37	86.87	123.20
1	B	239	ASP	CA-C-N	13.61	143.43	116.20
1	B	240	GLY	O-C-N	8.14	135.73	122.70
1	B	214	ASP	CB-CG-OD2	6.92	124.53	118.30
1	B	12	ASP	CB-CG-OD2	6.51	124.16	118.30
1	B	73	ASP	CB-CG-OD2	6.41	124.07	118.30
1	B	240	GLY	CA-C-N	-6.24	103.48	117.20
1	A	239	ASP	CB-CG-OD2	6.23	123.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	104	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	B	359	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	103	ASP	CB-CG-OD2	6.06	123.75	118.30
1	A	73	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	359	ASP	CB-CG-OD2	6.05	123.75	118.30
1	B	297	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	406	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	246	ASP	CB-CG-OD2	5.83	123.54	118.30
1	A	214	ASP	CB-CG-OD2	5.68	123.42	118.30
1	B	91	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	196	VAL	CB-CA-C	-5.67	100.64	111.40
1	B	6	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	330	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	415	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	416	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	239	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	416	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	157	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	56	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	303	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	315	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	332	ASP	CB-CG-OD2	5.07	122.87	118.30
1	B	315	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	239	ASP	Mainchain

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	3311	0	3253	24	0
1	B	3311	0	3253	32	0
2	A	49	0	32	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	49	0	32	0	0
3	A	247	0	0	2	0
3	B	192	0	0	6	0
All	All	7159	0	6570	49	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 4.

All (49) 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:213:ARG:CZ	3:B:1466:HOH:O	2.19	0.89
1:A:167:LEU:HD21	1:B:167:LEU:CD2	2.19	0.72
1:B:11:LEU:HD11	1:B:36:ILE:HD11	1.71	0.72
1:A:219:GLU:OE2	1:B:358:HIS:HE1	1.75	0.69
1:A:167:LEU:HD21	1:B:167:LEU:HD21	1.76	0.67
1:A:285:ALA:HB3	1:A:288:MET:HE2	1.77	0.67
1:B:340:ALA:O	1:B:342:GLN:N	2.29	0.65
1:B:32:ASN:HD21	1:B:68:ARG:HH21	1.43	0.65
1:B:208:VAL:O	1:B:208:VAL:HG12	2.03	0.59
1:A:11:LEU:HD11	1:A:36:ILE:HD11	1.85	0.58
1:A:139:TYR:CZ	1:B:262:GLN:NE2	2.73	0.56
1:A:32:ASN:HD21	1:A:68:ARG:HH21	1.52	0.56
1:A:208:VAL:HG12	1:A:208:VAL:O	2.08	0.53
1:B:2:THR:N	1:B:390:GLY:O	2.42	0.53
1:A:163:SER:HB2	3:B:1545:HOH:O	2.09	0.52
1:A:126:GLY:HA3	1:A:138:VAL:HG13	1.92	0.51
1:B:373:ASP:H	1:B:378:ASN:ND2	2.09	0.51
1:A:405:THR:HG21	1:A:428:VAL:HG13	1.93	0.51
2:A:429:CAO:H4B	2:A:429:CAO:O8A	2.10	0.51
1:B:32:ASN:ND2	3:B:1492:HOH:O	2.44	0.50
1:A:298:LYS:NZ	3:A:667:HOH:O	2.45	0.50
1:B:93:MET:HE1	1:B:112:ILE:HG23	1.93	0.49
1:B:39:ARG:NH2	1:B:426:GLN:HE21	2.10	0.49
1:B:17:GLN:HG3	1:B:63:PHE:CE2	2.48	0.49
1:B:11:LEU:CD1	1:B:36:ILE:HD11	2.41	0.49
1:A:70:ILE:HG22	1:A:405:THR:HA	1.96	0.48
1:A:2:THR:HA	3:A:658:HOH:O	2.14	0.47
1:B:238:ARG:NH2	3:B:1531:HOH:O	2.47	0.47
1:A:209:ARG:HD2	1:B:63:PHE:CZ	2.49	0.46
1:B:131:HIS:O	1:B:134:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:MET:HE1	1:B:112:ILE:CG2	2.46	0.46
1:A:167:LEU:O	1:A:171:ASN:HB3	2.16	0.46
1:B:213:ARG:NH1	3:B:1466:HOH:O	2.44	0.45
1:A:288:MET:HE1	1:A:346:PRO:HD3	1.99	0.45
1:A:196:VAL:HG13	1:B:388:PHE:CE2	2.53	0.44
1:A:63:PHE:CZ	1:B:209:ARG:HD2	2.53	0.44
1:B:289:TRP:N	1:B:290:PRO:CD	2.81	0.44
1:A:17:GLN:HG3	1:A:63:PHE:CE2	2.53	0.43
1:B:102:LEU:HD22	1:B:107:PHE:HB2	2.00	0.43
1:B:409:LEU:HD11	1:B:428:VAL:HG21	2.01	0.43
1:B:93:MET:CE	1:B:112:ILE:HG21	2.49	0.43
1:B:206:ASN:ND2	1:B:209:ARG:HH21	2.17	0.42
1:A:83:LEU:HD23	1:A:83:LEU:HA	1.89	0.42
1:B:405:THR:HG21	1:B:428:VAL:HG13	2.02	0.41
1:A:196:VAL:HG13	1:B:388:PHE:CD2	2.55	0.41
1:B:314:VAL:HG12	3:B:1518:HOH:O	2.20	0.41
1:B:76:THR:CG2	1:B:79:GLY:H	2.34	0.41
1:A:99:PRO:HA	1:A:125:LYS:HD2	2.02	0.40
1:A:102:LEU:HD23	1:A:102:LEU:HA	2.00	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	425/427 (100%)	412 (97%)	11 (3%)	2 (0%)	29 35
1	B	425/427 (100%)	409 (96%)	10 (2%)	6 (1%)	11 11
All	All	850/854 (100%)	821 (97%)	21 (2%)	8 (1%)	17 20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	LYS
1	B	140	GLU
1	B	341	ALA
1	A	16	VAL
1	A	140	GLU
1	B	16	VAL
1	B	340	ALA
1	B	134	GLU

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	350/350 (100%)	335 (96%)	15 (4%)	29	40
1	B	350/350 (100%)	330 (94%)	20 (6%)	20	28
All	All	700/700 (100%)	665 (95%)	35 (5%)	24	34

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	44	MET
1	A	59	TYR
1	A	74	MET
1	A	82	LEU
1	A	92	VAL
1	A	102	LEU
1	A	123	SER
1	A	196	VAL
1	A	322	SER
1	A	356	LEU
1	A	374	GLU
1	A	386	PHE
1	A	391	PHE
1	A	428	VAL
1	B	59	TYR

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Mol	Chain	Res	Type
1	B	76	THR
1	B	92	VAL
1	B	102	LEU
1	B	196	VAL
1	B	205	LEU
1	B	247	ASN
1	B	262	GLN
1	B	295	MET
1	B	300	GLU
1	B	311	GLU
1	B	326	THR
1	B	327	LYS
1	B	330	ASP
1	B	339	TRP
1	B	370	GLU
1	B	386	PHE
1	B	426	GLN
1	B	427	VAL
1	B	428	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	32	ASN
1	A	188	HIS
1	A	262	GLN
1	B	9	ASN
1	B	32	ASN
1	B	85	GLN
1	B	206	ASN
1	B	262	GLN
1	B	358	HIS
1	B	378	ASN
1	B	426	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 monosaccharides 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	$\#\|Z\| > 2$
2	CAO	B	1429	-	41,51,51	1.08	4 (9%)	53,76,76	1.64	7 (13%)
2	CAO	A	429	-	41,51,51	1.18	6 (14%)	53,76,76	1.62	10 (18%)

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	CAO	B	1429	-	-	2/44/65/65	0/3/3/3
2	CAO	A	429	-	-	8/44/65/65	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1429	CAO	P3B-O7A	2.99	1.60	1.50
2	A	429	CAO	C8A-N7A	2.84	1.39	1.34
2	A	429	CAO	P3B-O7A	2.73	1.59	1.50
2	B	1429	CAO	C2A-N3A	2.42	1.36	1.32
2	A	429	CAO	P2A-O4A	2.37	1.59	1.50
2	A	429	CAO	O4B-C1B	2.34	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	429	CAO	P1A-O1A	2.26	1.58	1.50
2	B	1429	CAO	P2A-O4A	2.20	1.58	1.50
2	A	429	CAO	C2A-N3A	2.16	1.35	1.32
2	B	1429	CAO	C8A-N7A	2.09	1.38	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1429	CAO	C3P-C2P-S1P	-5.09	100.62	113.12
2	B	1429	CAO	C1B-N9A-C4A	-5.02	117.82	126.64
2	A	429	CAO	C1B-N9A-C4A	-4.61	118.54	126.64
2	A	429	CAO	N3A-C2A-N1A	-4.00	122.43	128.68
2	A	429	CAO	P2A-O3A-P1A	-4.00	119.11	132.83
2	B	1429	CAO	N3A-C2A-N1A	-3.71	122.88	128.68
2	A	429	CAO	C2P-C3P-N4P	3.69	120.16	112.42
2	B	1429	CAO	C3P-N4P-C5P	-3.52	116.31	122.84
2	B	1429	CAO	C2B-C3B-C4B	3.37	109.19	103.22
2	B	1429	CAO	O3B-C3B-C2B	-3.11	100.41	111.68
2	A	429	CAO	CEP-CBP-CAP	2.89	113.83	108.82
2	A	429	CAO	O5P-C5P-C6P	-2.60	117.27	122.02
2	B	1429	CAO	N6A-C6A-N1A	2.59	123.96	118.57
2	A	429	CAO	C3B-C2B-C1B	2.58	105.61	99.89
2	A	429	CAO	CDP-CBP-CCP	2.29	111.97	108.23
2	A	429	CAO	C6P-C5P-N4P	2.22	120.15	116.42
2	A	429	CAO	C2B-C3B-C4B	2.11	106.96	103.22

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	429	CAO	C4B-C3B-O3B-P3B
2	A	429	CAO	C3B-O3B-P3B-O9A
2	A	429	CAO	C9P-CAP-CBP-CCP
2	A	429	CAO	C9P-CAP-CBP-CEP
2	A	429	CAO	OAP-CAP-CBP-CCP
2	B	1429	CAO	C6P-C5P-N4P-C3P
2	A	429	CAO	CDP-CBP-CCP-O6A
2	A	429	CAO	C9P-CAP-CBP-CDP
2	A	429	CAO	OAP-CAP-CBP-CDP
2	B	1429	CAO	CCP-O6A-P2A-O4A

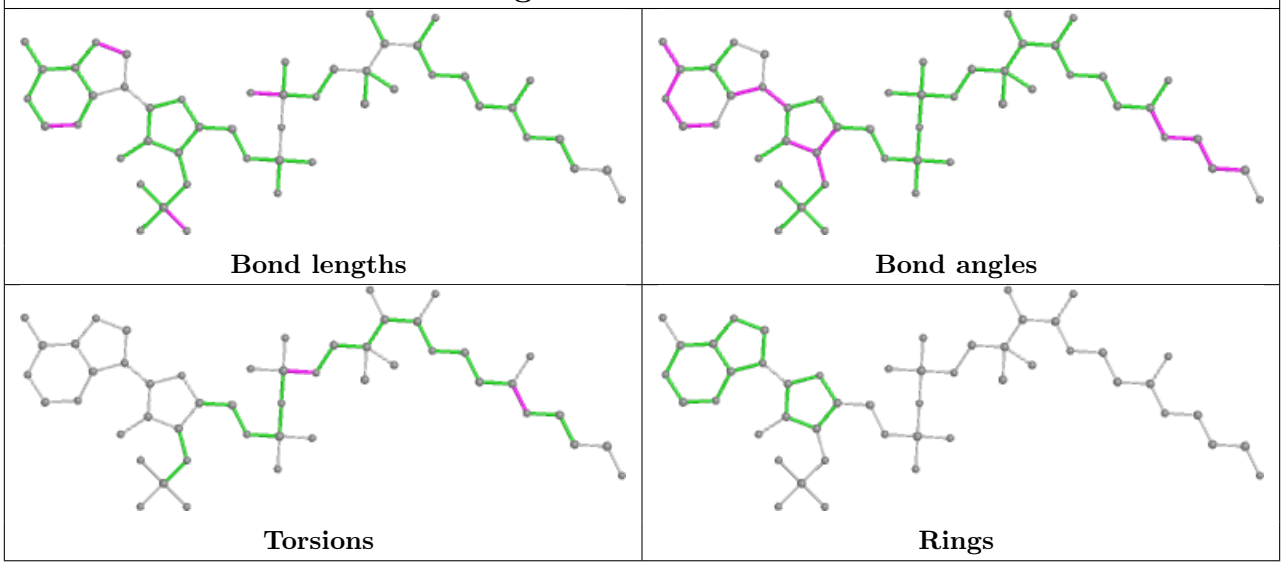
There are no ring outliers.

1 monomer is involved in 1 short contact:

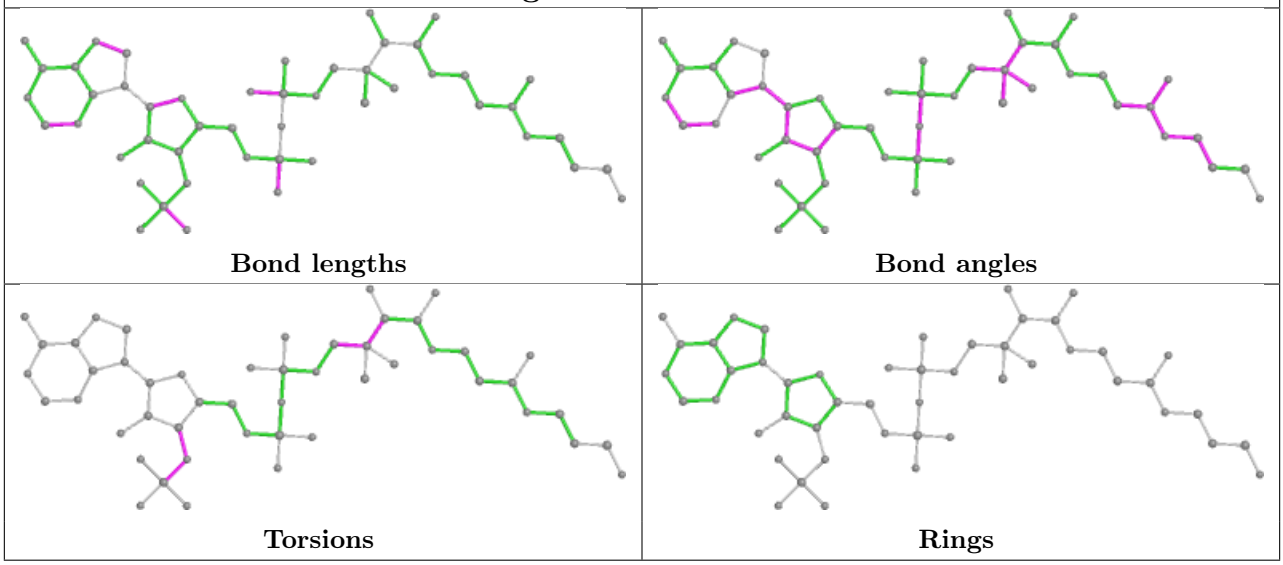
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	429	CAO	1	0

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 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 CAO B 1429



Ligand CAO A 429



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	239:ASP	C	240:GLY	N	1.64
1	B	240:GLY	C	241:ASN	N	1.60

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	427/427 (100%)	0.08	12 (2%) 53 60	26, 37, 62, 70	16 (3%)
1	B	426/427 (99%)	0.39	55 (12%) 3 5	29, 40, 80, 92	33 (7%)
All	All	853/854 (99%)	0.24	67 (7%) 12 17	26, 39, 73, 92	49 (5%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	314	VAL	8.5
1	B	417	ALA	6.3
1	B	303	ASP	6.1
1	B	238	ARG	5.1
1	B	305	PRO	5.0
1	B	416	ASP	4.8
1	B	302	LYS	4.6
1	B	421	GLU	4.4
1	B	233	ASN	4.4
1	B	311	GLU	4.4
1	B	339	TRP	4.4
1	B	415	ASP	4.2
1	B	243	LEU	4.1
1	B	294	ASP	4.1
1	B	307	TYR	4.1
1	B	241	ASN	4.0
1	B	301	TRP	3.8
1	B	315	ASP	3.8
1	B	342	GLN	3.7
1	B	242	PRO	3.6
1	A	99	PRO	3.5
1	B	309	THR	3.4
1	B	418	LYS	3.4
1	B	310	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	247	ASN	3.4
1	B	426	GLN	3.4
1	A	190	THR	3.3
1	B	178	ILE	3.3
1	B	343	TYR	3.3
1	B	317	LEU	3.2
1	A	413	GLY	3.2
1	B	298	LYS	3.1
1	B	323	PHE	3.1
1	B	424	ALA	3.1
1	B	2	THR	3.1
1	B	207	LEU	3.0
1	B	344	GLY	3.0
1	A	178	ILE	3.0
1	B	295	MET	2.9
1	B	413	GLY	2.7
1	B	246	ASP	2.7
1	B	308	ASN	2.6
1	B	338	GLU	2.6
1	B	341	ALA	2.6
1	B	176	LEU	2.6
1	B	234	PHE	2.6
1	B	419	ILE	2.5
1	A	75	LYS	2.5
1	B	412	LEU	2.5
1	A	54	ASN	2.5
1	B	232	PRO	2.5
1	B	239	ASP	2.5
1	B	330	ASP	2.5
1	A	189	LYS	2.4
1	B	285	ALA	2.4
1	B	237	ASP	2.4
1	A	22	CYS	2.4
1	B	292	ILE	2.3
1	A	106	GLY	2.3
1	B	236	PHE	2.3
1	B	420	LYS	2.2
1	B	110	GLU	2.2
1	B	306	ALA	2.2
1	A	97	PHE	2.1
1	A	94	VAL	2.1
1	A	176	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	320	ILE	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)

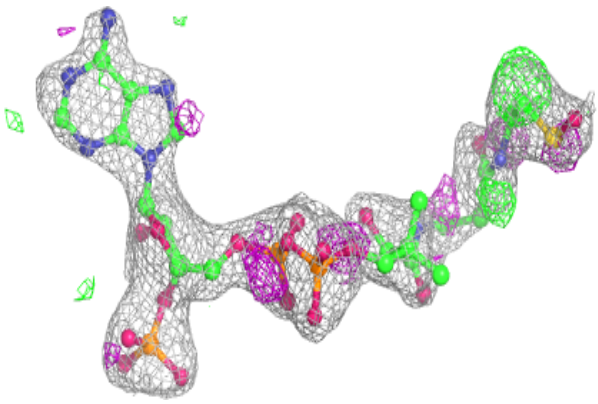
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

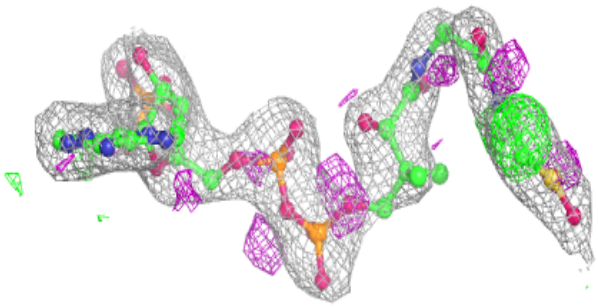
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CAO	A	429	49/49	0.81	0.23	58,77,84,85	0
2	CAO	B	1429	49/49	0.94	0.12	41,53,61,62	0

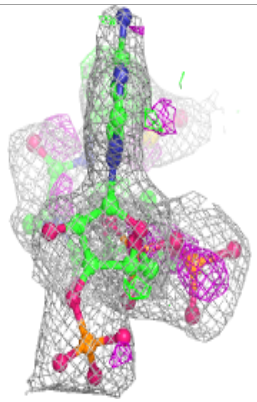
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CAO A 429:

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

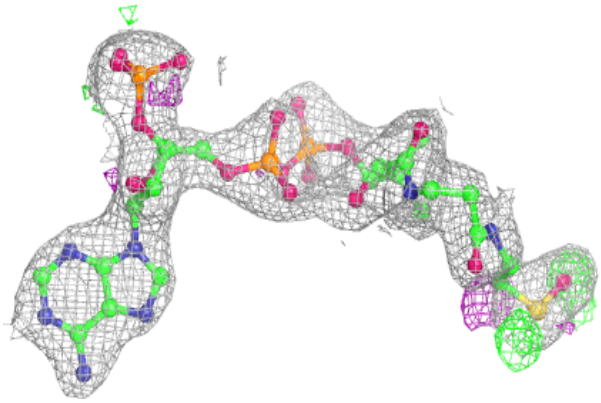


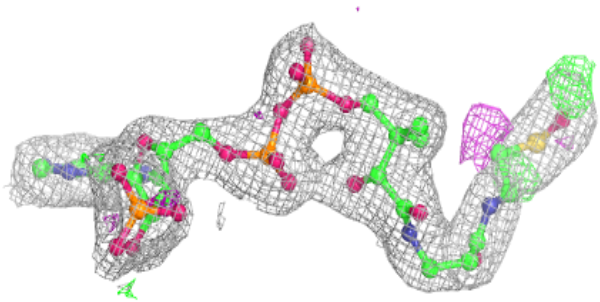


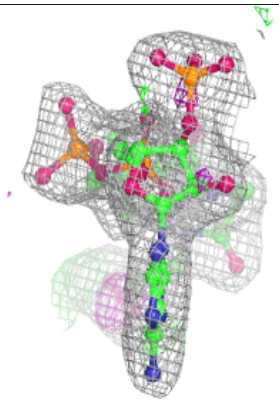


Electron density around CAO B 1429:

$2mF_o$-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.