



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2023 – 10:26 AM EDT

PDB ID : 1VGR
Title : Formyl-CoA transferase mutant Asp169 to Glu
Authors : Ricagno, S.; Jonsson, S.; Richards, N.G.; Lindqvist, Y.
Deposited on : 2004-04-28
Resolution : 2.10 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 : 4.02b-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

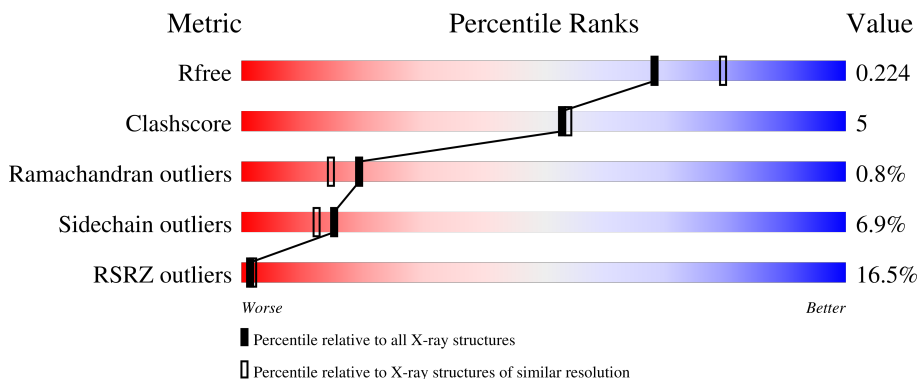
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	427	
1	B	427	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7177 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.

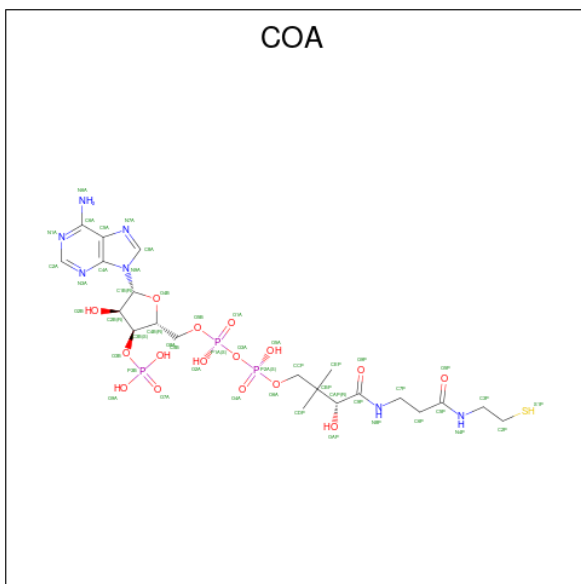
- Molecule 1 is a protein called Formyl-coenzyme A transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	427	3314	2097	568	626	23	0	0	0
1	B	427	3314	2097	568	626	23	4	0	0

There are 4 discrepancies between the modelled and reference sequences:

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

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



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

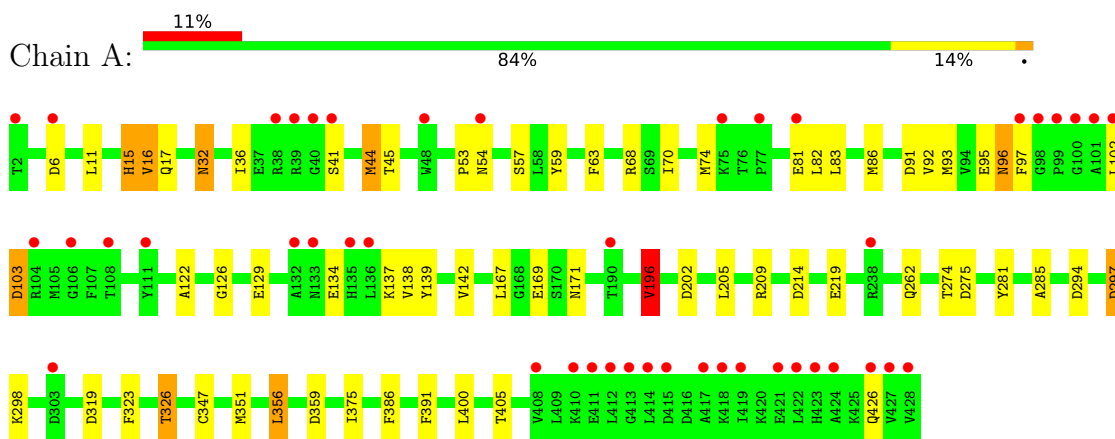
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	260	Total	O	0	0
			260	260		
3	B	193	Total	O	0	0
			193	193		

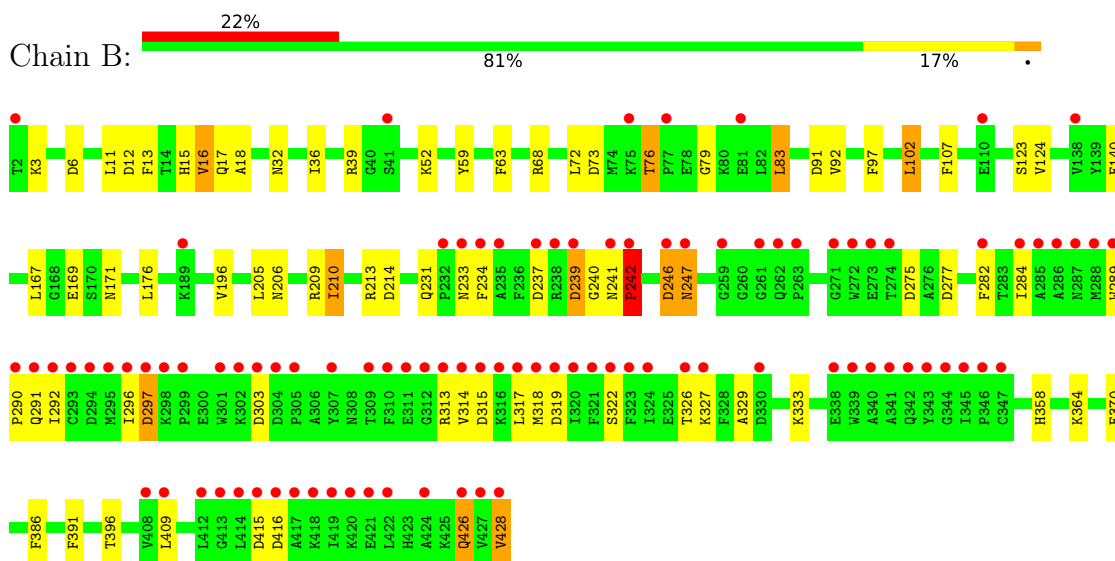
3 Residue-property plots [i](#)

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



- Molecule 1: Formyl-coenzyme A transferase



4 Data and refinement statistics i

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	150.04Å 150.04Å 99.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 2.10 19.76 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.80-2.10) 100.0 (19.76-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.09Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.182 , 0.220 0.188 , 0.224	Depositor DCC
R_{free} test set	3275 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtrriage
Anisotropy	0.025	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.022 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7177	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.61	0/3388	0.81	9/4581 (0.2%)
1	B	0.59	0/3388	0.84	15/4581 (0.3%)
All	All	0.60	0/6776	0.82	24/9162 (0.3%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ASP	CB-CG-OD2	7.31	124.88	118.30
1	A	275	ASP	CB-CG-OD1	7.11	124.70	118.30
1	B	214	ASP	CB-CG-OD2	6.97	124.57	118.30
1	B	242	PRO	CA-N-CD	-6.67	102.17	111.50
1	B	239	ASP	CB-CA-C	5.96	122.31	110.40
1	B	319	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	359	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	12	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	91	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	297	ASP	CB-CG-OD2	5.61	123.34	118.30
1	B	246	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	196	VAL	CB-CA-C	-5.56	100.84	111.40
1	B	416	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	202	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	73	ASP	CB-CG-OD2	5.28	123.06	118.30
1	B	275	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	103	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	315	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	214	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	6	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	91	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	303	ASP	CB-CG-OD2	5.08	122.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	415	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

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	3314	0	3254	34	0
1	B	3314	0	3254	41	0
2	A	48	0	32	4	0
2	B	48	0	32	3	0
3	A	260	0	0	6	0
3	B	193	0	0	6	0
All	All	7177	0	6572	72	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 5.

All (72) 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:169:GLU:OE1	2:B:1429:COA:S1P	2.29	0.90
1:A:319:ASP:OD1	3:A:536:HOH:O	1.94	0.85
1:A:169:GLU:OE1	2:A:429:COA:S1P	2.36	0.82
1:B:11:LEU:HD11	1:B:36:ILE:HD11	1.61	0.81
1:B:329:ALA:O	3:B:1588:HOH:O	1.99	0.80
1:B:239:ASP:O	1:B:241:ASN:N	2.23	0.71
1:A:297:ASP:OD2	3:A:468:HOH:O	2.07	0.71
1:A:95:GLU:OE1	1:A:96:ASN:O	2.08	0.70
1:B:32:ASN:HD21	1:B:68:ARG:HH21	1.43	0.66
1:B:13:PHE:CZ	1:B:83:LEU:HD21	2.30	0.66
1:A:219:GLU:OE2	1:B:358:HIS:HE1	1.79	0.66
1:B:237:ASP:OD1	1:B:239:ASP:O	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HD11	1:A:86:MET:HB3	1.81	0.63
1:B:102:LEU:HD22	1:B:107:PHE:HB2	1.81	0.63
1:A:17:GLN:HG3	1:A:63:PHE:CE2	2.34	0.61
1:B:246:ASP:O	1:B:247:ASN:OD1	2.21	0.59
1:B:76:THR:HG22	1:B:79:GLY:H	1.67	0.58
1:A:32:ASN:HD21	1:A:68:ARG:HH21	1.52	0.58
1:B:233:ASN:ND2	1:B:242:PRO:HG3	2.20	0.57
1:A:167:LEU:HD21	1:B:167:LEU:HD21	1.86	0.57
1:A:351:MET:HB3	1:A:356:LEU:HD13	1.87	0.56
1:B:17:GLN:HG3	1:B:63:PHE:CE2	2.40	0.56
1:A:294:ASP:O	3:A:468:HOH:O	2.17	0.55
2:A:429:COA:H22	2:A:429:COA:CDP	2.36	0.55
1:B:284:ILE:HG23	1:B:292:ILE:HD13	1.90	0.54
1:A:139:TYR:HD1	3:A:472:HOH:O	1.91	0.52
1:B:233:ASN:HD22	1:B:242:PRO:HG3	1.75	0.52
1:B:231:GLN:OE1	1:B:314:VAL:O	2.28	0.52
1:A:326:THR:CG2	3:A:632:HOH:O	2.58	0.52
1:A:298:LYS:NZ	3:A:675:HOH:O	2.43	0.51
1:B:16:VAL:HB	2:B:1429:COA:S1P	2.51	0.51
1:A:375:ILE:HD13	1:A:400:LEU:HD11	1.93	0.51
1:B:3:LYS:HB2	1:B:6:ASP:OD1	2.13	0.49
2:A:429:COA:H22	2:A:429:COA:H131	1.94	0.48
1:B:39:ARG:NH2	1:B:426:GLN:HG3	2.29	0.48
1:A:53:PRO:O	1:A:54:ASN:HB3	2.14	0.47
1:B:18:ALA:H	2:B:1429:COA:HS1	1.61	0.47
1:A:262:GLN:HE21	1:A:285:ALA:HA	1.80	0.47
1:A:167:LEU:O	1:A:171:ASN:HB3	2.14	0.47
1:A:15:HIS:HD2	1:A:44:MET:SD	2.38	0.46
1:B:124:VAL:HG23	1:B:176:LEU:HD22	1.98	0.46
1:B:15:HIS:CE1	1:B:97:PHE:CD2	3.04	0.45
1:A:63:PHE:CZ	1:B:209:ARG:HD2	2.51	0.45
1:A:209:ARG:HD2	1:B:63:PHE:CZ	2.51	0.45
1:A:323:PHE:O	1:A:326:THR:HB	2.17	0.44
1:B:210:ILE:O	1:B:213:ARG:HB3	2.17	0.44
1:A:15:HIS:H	1:A:15:HIS:HD1	1.64	0.44
1:B:409:LEU:HD11	1:B:428:VAL:HG21	2.00	0.44
1:A:45:THR:O	1:A:57:SER:OG	2.30	0.44
1:A:142:VAL:HG23	3:B:1574:HOH:O	2.18	0.44
1:B:167:LEU:O	1:B:171:ASN:HB3	2.17	0.44
1:B:13:PHE:HZ	1:B:83:LEU:HD21	1.81	0.44
1:B:52:LYS:NZ	3:B:1554:HOH:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:PHE:CD2	1:B:318:MET:HG3	2.53	0.44
1:A:16:VAL:HB	2:A:429:COA:S1P	2.58	0.43
1:A:36:ILE:HG12	1:A:70:ILE:HD11	1.99	0.43
1:B:289:TRP:N	1:B:290:PRO:CD	2.81	0.43
1:B:52:LYS:NZ	3:B:1538:HOH:O	2.52	0.43
1:B:15:HIS:CD2	1:B:16:VAL:HG23	2.54	0.43
1:A:281:TYR:O	1:A:347:CYS:HA	2.19	0.42
1:A:70:ILE:HG22	1:A:405:THR:HA	2.00	0.42
1:B:3:LYS:HB2	1:B:6:ASP:CG	2.40	0.42
1:A:126:GLY:HA3	1:A:138:VAL:HG13	2.01	0.42
1:B:329:ALA:HA	3:B:1486:HOH:O	2.20	0.42
1:A:129:GLU:HG3	1:A:134:GLU:OE2	2.20	0.41
1:B:76:THR:HG22	1:B:79:GLY:N	2.34	0.41
1:A:209:ARG:HD2	1:B:63:PHE:CE2	2.55	0.41
1:B:32:ASN:ND2	3:B:1495:HOH:O	2.54	0.41
1:A:122:ALA:HA	1:A:196:VAL:O	2.20	0.40
1:B:72:LEU:CD2	1:B:83:LEU:HD12	2.51	0.40
1:A:83:LEU:HD23	1:A:83:LEU:HA	1.92	0.40
1:B:206:ASN:ND2	1:B:209:ARG:HH21	2.19	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%)	411 (97%)	12 (3%)	2 (0%)	29 26
1	B	425/427 (100%)	403 (95%)	17 (4%)	5 (1%)	13 8
All	All	850/854 (100%)	814 (96%)	29 (3%)	7 (1%)	19 15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	140	GLU
1	B	240	GLY
1	A	16	VAL
1	B	313	ARG
1	A	97	PHE
1	B	16	VAL
1	B	333	LYS

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%)	328 (94%)	22 (6%)	18 15
1	B	350/350 (100%)	324 (93%)	26 (7%)	13 10
All	All	700/700 (100%)	652 (93%)	48 (7%)	15 12

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	32	ASN
1	A	41	SER
1	A	44	MET
1	A	59	TYR
1	A	74	MET
1	A	81	GLU
1	A	82	LEU
1	A	92	VAL
1	A	93	MET
1	A	96	ASN
1	A	102	LEU
1	A	103	ASP
1	A	137	LYS
1	A	196	VAL
1	A	205	LEU
1	A	274	THR

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Mol	Chain	Res	Type
1	A	326	THR
1	A	356	LEU
1	A	386	PHE
1	A	391	PHE
1	A	426	GLN
1	B	59	TYR
1	B	76	THR
1	B	83	LEU
1	B	92	VAL
1	B	102	LEU
1	B	123	SER
1	B	196	VAL
1	B	205	LEU
1	B	210	ILE
1	B	242	PRO
1	B	247	ASN
1	B	282	PHE
1	B	291	GLN
1	B	296	ILE
1	B	297	ASP
1	B	317	LEU
1	B	322	SER
1	B	326	THR
1	B	327	LYS
1	B	364	LYS
1	B	370	GLU
1	B	386	PHE
1	B	391	PHE
1	B	396	THR
1	B	426	GLN
1	B	428	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	262	GLN
1	B	15	HIS
1	B	17	GLN
1	B	32	ASN
1	B	85	GLN
1	B	188	HIS

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Mol	Chain	Res	Type
1	B	206	ASN
1	B	233	ASN
1	B	247	ASN
1	B	262	GLN
1	B	358	HIS
1	B	378	ASN

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	COA	B	1429	-	41,50,50	1.72	4 (9%)	52,75,75	1.24	2 (3%)
2	COA	A	429	-	41,50,50	1.79	3 (7%)	52,75,75	1.15	4 (7%)

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	COA	B	1429	-	-	8/44/64/64	0/3/3/3
2	COA	A	429	-	-	9/44/64/64	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	429	COA	O9P-C9P	9.27	1.41	1.23
2	B	1429	COA	O9P-C9P	8.85	1.41	1.23
2	A	429	COA	C2A-N3A	4.76	1.39	1.32
2	B	1429	COA	C2A-N3A	3.82	1.38	1.32
2	A	429	COA	C2A-N1A	2.85	1.39	1.33
2	B	1429	COA	C2A-N1A	2.54	1.38	1.33
2	B	1429	COA	C3P-N4P	-2.17	1.41	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1429	COA	N3A-C2A-N1A	-5.65	119.84	128.68
2	A	429	COA	N3A-C2A-N1A	-5.45	120.16	128.68
2	A	429	COA	P2A-O3A-P1A	-3.04	122.41	132.83
2	B	1429	COA	C6P-C5P-N4P	-2.60	112.04	116.42
2	A	429	COA	O4B-C1B-C2B	-2.36	103.47	106.93
2	A	429	COA	CEP-CBP-CAP	2.17	112.58	108.82

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	429	COA	C3B-O3B-P3B-O9A
2	A	429	COA	C5P-C6P-C7P-N8P
2	A	429	COA	S1P-C2P-C3P-N4P
2	B	1429	COA	P1A-O3A-P2A-O6A
2	B	1429	COA	CCP-O6A-P2A-O5A
2	B	1429	COA	S1P-C2P-C3P-N4P
2	B	1429	COA	C6P-C5P-N4P-C3P
2	B	1429	COA	O5P-C5P-N4P-C3P
2	A	429	COA	P1A-O3A-P2A-O6A
2	A	429	COA	O5P-C5P-N4P-C3P
2	B	1429	COA	CCP-O6A-P2A-O4A
2	A	429	COA	CAP-C9P-N8P-C7P
2	A	429	COA	O9P-C9P-N8P-C7P
2	A	429	COA	C6P-C5P-N4P-C3P

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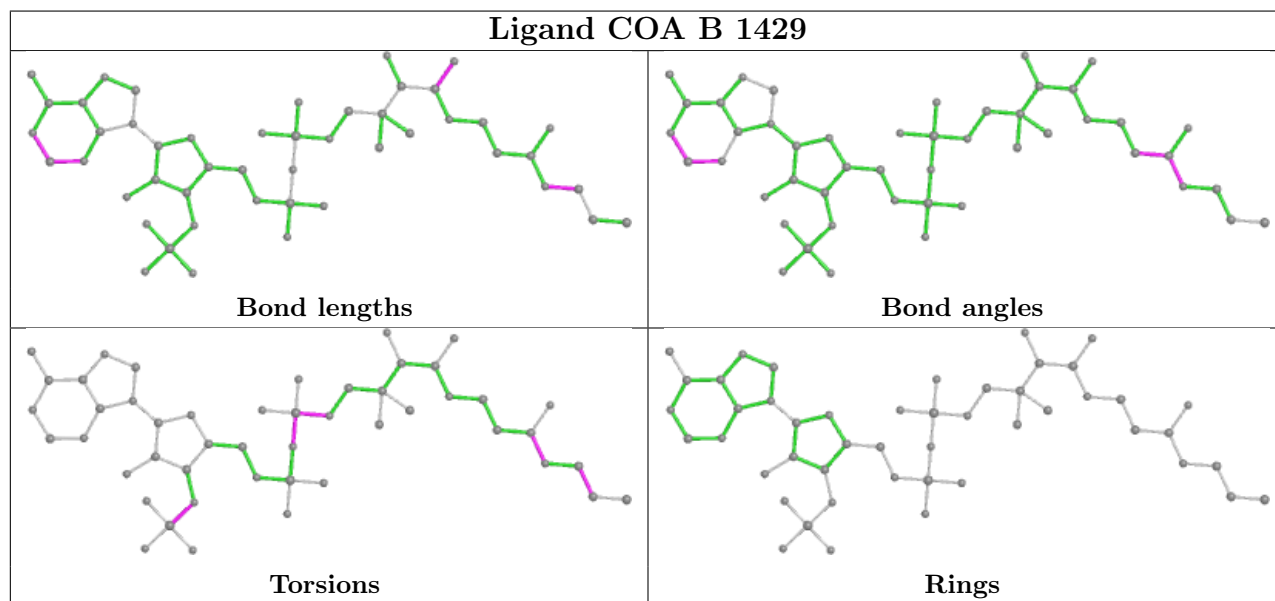
Mol	Chain	Res	Type	Atoms
2	B	1429	COA	C3B-O3B-P3B-O8A
2	B	1429	COA	CCP-O6A-P2A-O3A
2	A	429	COA	CCP-O6A-P2A-O4A

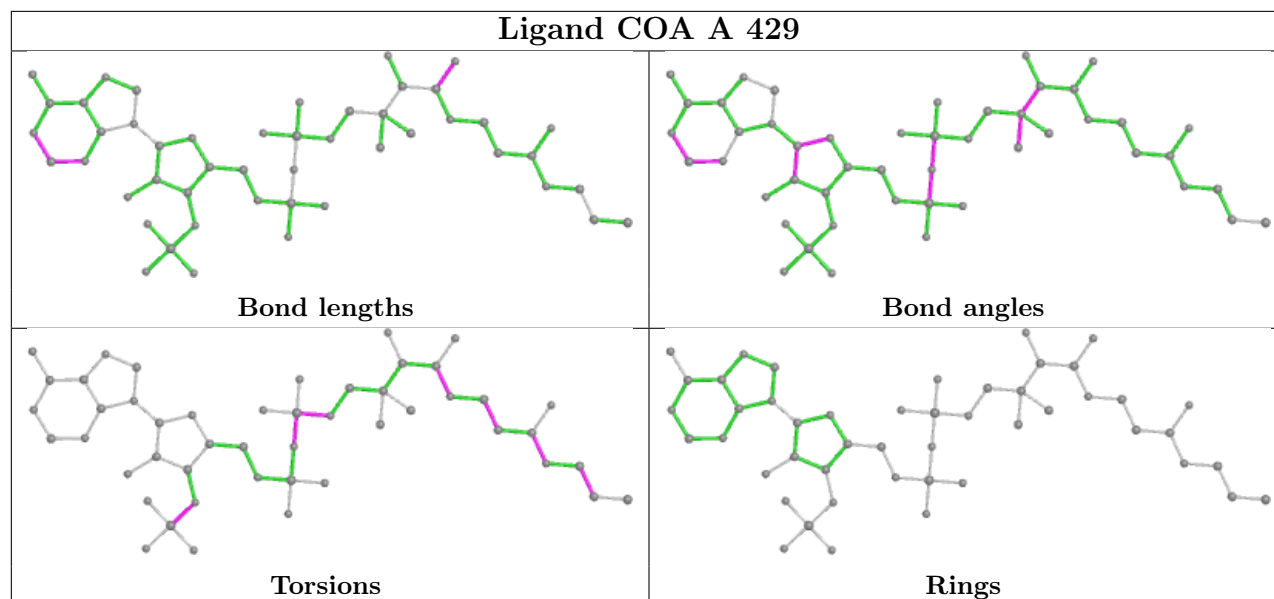
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1429	COA	3	0
2	A	429	COA	4	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, 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%)	0.56	45 (10%) 6 8	23, 34, 70, 74	16 (3%)
1	B	426/427 (99%)	1.29	96 (22%) 0 0	26, 38, 97, 111	33 (7%)
All	All	853/854 (99%)	0.93	141 (16%) 1 2	23, 36, 77, 111	49 (5%)

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	302	LYS	17.0
1	B	303	ASP	13.9
1	B	309	THR	13.3
1	B	296	ILE	12.0
1	B	320	ILE	10.7
1	B	286	ALA	10.6
1	B	295	MET	10.4
1	B	301	TRP	10.2
1	B	323	PHE	9.9
1	A	413	GLY	9.9
1	A	428	VAL	9.7
1	B	292	ILE	9.5
1	B	317	LEU	9.4
1	B	305	PRO	8.9
1	A	427	VAL	8.3
1	B	297	ASP	8.2
1	B	293	CYS	8.0
1	B	330	ASP	7.8
1	B	343	TYR	6.9
1	A	99	PRO	6.8
1	B	314	VAL	6.7
1	B	234	PHE	6.6
1	B	233	ASN	6.2
1	B	310	PHE	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	97	PHE	6.1
1	B	345	ILE	5.9
1	B	284	ILE	5.8
1	A	2	THR	5.8
1	B	339	TRP	5.8
1	B	341	ALA	5.8
1	B	285	ALA	5.7
1	B	311	GLU	5.5
1	B	307	TYR	5.5
1	B	344	GLY	5.5
1	A	101	ALA	5.4
1	A	422	LEU	5.4
1	B	315	ASP	5.4
1	B	239	ASP	5.3
1	A	106	GLY	5.3
1	B	289	TRP	5.2
1	B	415	ASP	5.2
1	B	2	THR	5.1
1	B	417	ALA	5.0
1	A	412	LEU	5.0
1	B	298	LYS	4.9
1	B	338	GLU	4.9
1	B	282	PHE	4.9
1	B	241	ASN	4.9
1	A	423	HIS	4.8
1	A	77	PRO	4.8
1	A	108	THR	4.5
1	B	110	GLU	4.4
1	B	321	PHE	4.3
1	B	261	GLY	4.3
1	B	342	GLN	4.2
1	A	100	GLY	4.2
1	B	290	PRO	4.2
1	B	316	LYS	4.2
1	B	189	LYS	4.1
1	A	135	HIS	4.1
1	A	38	ARG	4.1
1	B	313	ARG	4.1
1	B	326	THR	4.0
1	B	288	MET	4.0
1	B	322	SER	3.9
1	B	287	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	238	ARG	3.8
1	B	312	GLY	3.8
1	B	263	PRO	3.8
1	B	347	CYS	3.7
1	A	48	TRP	3.7
1	B	346	PRO	3.6
1	B	77	PRO	3.6
1	B	242	PRO	3.6
1	B	422	LEU	3.6
1	B	413	GLY	3.5
1	A	132	ALA	3.5
1	A	111	TYR	3.5
1	A	419	ILE	3.4
1	B	424	ALA	3.4
1	B	409	LEU	3.4
1	A	418	LYS	3.3
1	A	40	GLY	3.3
1	A	410	LYS	3.3
1	A	424	ALA	3.3
1	A	414	LEU	3.2
1	B	324	ILE	3.2
1	A	75	LYS	3.1
1	A	411	GLU	3.1
1	A	417	ALA	3.1
1	B	294	ASP	3.1
1	B	247	ASN	3.1
1	B	274	THR	3.1
1	A	190	THR	3.0
1	B	340	ALA	3.0
1	A	104	ARG	3.0
1	B	418	LYS	3.0
1	A	421	GLU	3.0
1	B	419	ILE	2.9
1	B	416	ASP	2.9
1	B	319	ASP	2.9
1	B	428	VAL	2.9
1	A	41	SER	2.9
1	B	304	ASP	2.9
1	B	237	ASP	2.9
1	B	412	LEU	2.9
1	B	232	PRO	2.8
1	A	426	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	136	LEU	2.7
1	B	291	GLN	2.7
1	A	54	ASN	2.7
1	B	41	SER	2.6
1	A	408	VAL	2.6
1	B	318	MET	2.6
1	B	420	LYS	2.6
1	B	235	ALA	2.5
1	B	273	GLU	2.5
1	B	426	GLN	2.4
1	B	272	TRP	2.4
1	B	262	GLN	2.4
1	B	421	GLU	2.4
1	B	271	GLY	2.4
1	A	39	ARG	2.4
1	B	327	LYS	2.4
1	B	75	LYS	2.4
1	A	415	ASP	2.3
1	B	81	GLU	2.3
1	A	102	LEU	2.3
1	A	238	ARG	2.3
1	A	303	ASP	2.3
1	B	259	GLY	2.3
1	B	414	LEU	2.2
1	A	6	ASP	2.2
1	B	427	VAL	2.2
1	A	98	GLY	2.2
1	B	246	ASP	2.2
1	A	81	GLU	2.0
1	B	299	PRO	2.0
1	B	138	VAL	2.0
1	A	133	ASN	2.0
1	B	408	VAL	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](#)

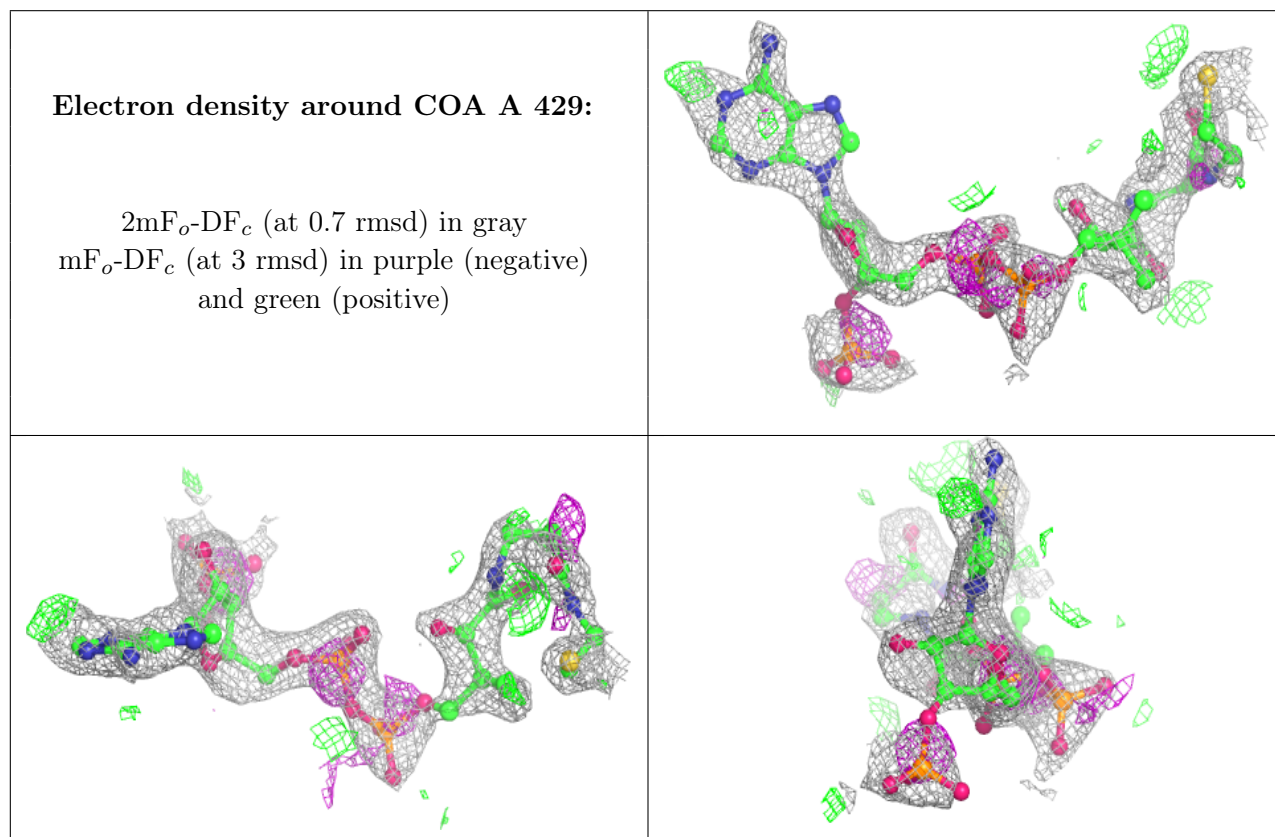
There are no monosaccharides in this entry.

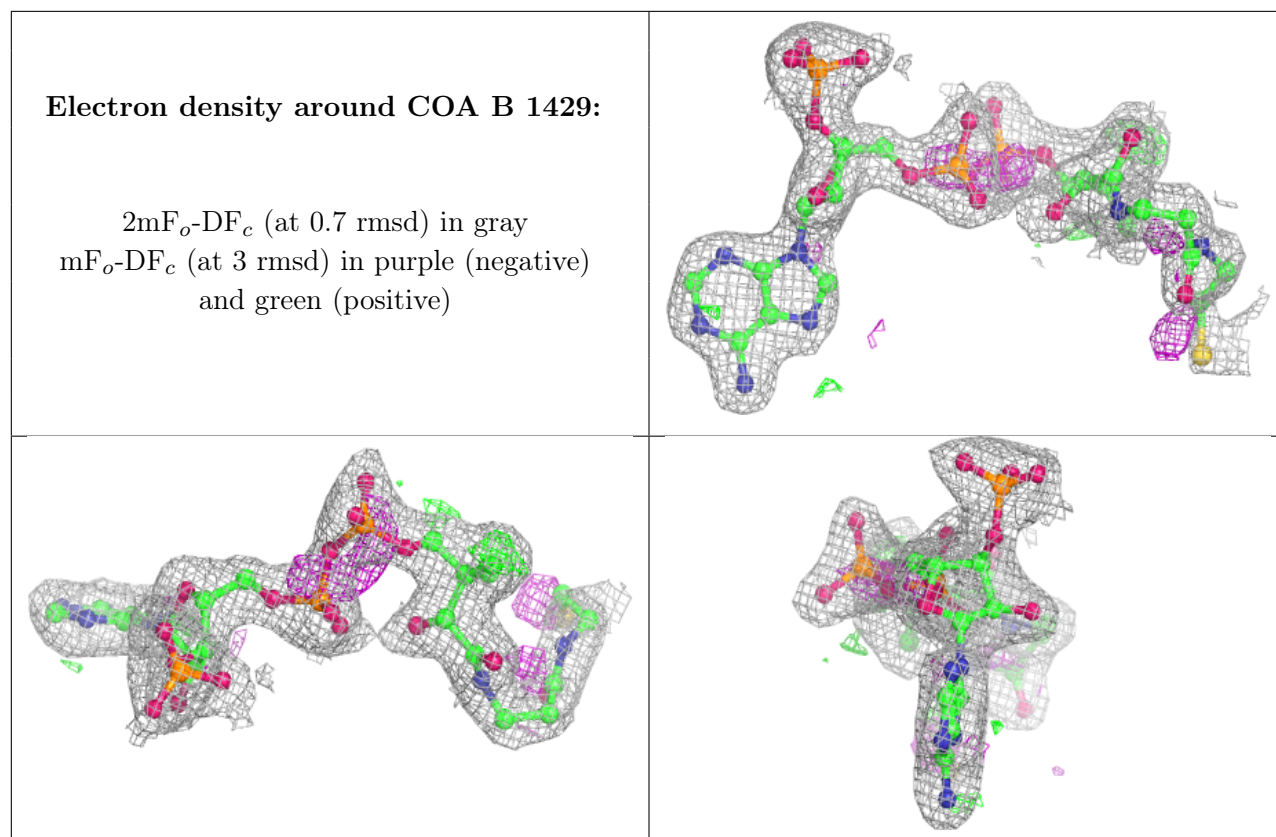
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
2	COA	A	429	48/48	0.67	0.40	60,79,85,86	1
2	COA	B	1429	48/48	0.86	0.20	44,50,55,56	1

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 [i](#)

There are no such residues in this entry.