



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 02:53 PM EDT

PDB ID : 2G2Z
Title : Structure of E.coli FabD complexed with malonyl-CoA
Authors : Oefner, Christian
Deposited on : 2006-02-17
Resolution : 2.80 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

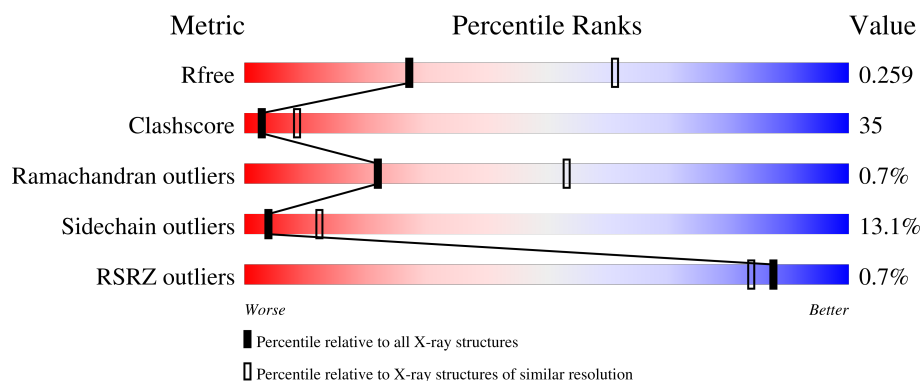
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

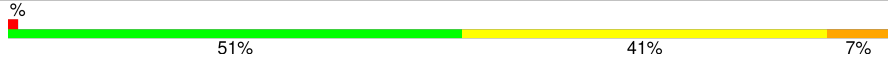
The reported resolution of this entry is 2.80 Å.

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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	308	

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
2	COZ	A	1001	X	-	-	-

2 Entry composition [i](#)

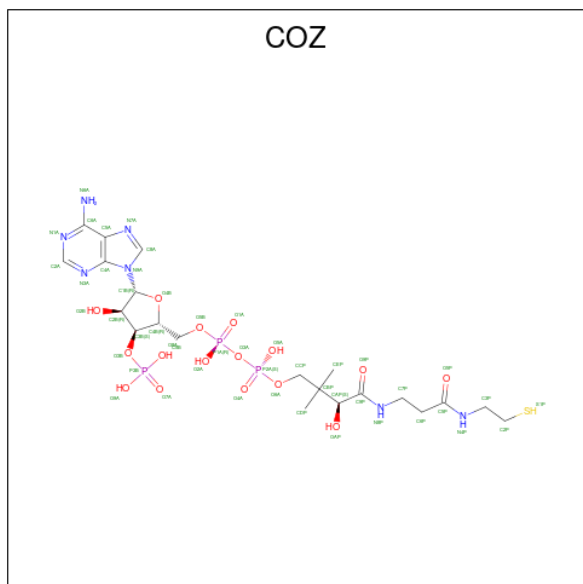
There are 4 unique types of molecules in this entry. The entry contains 2322 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Malonyl CoA-acyl carrier protein transacylase.

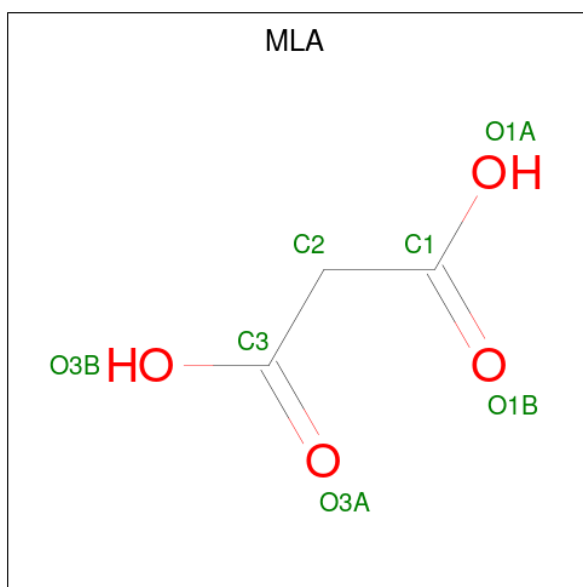
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2257	1427	382	433	15			

- Molecule 2 is COENZYME A (three-letter code: COZ) (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		

- Molecule 3 is MALONIC ACID (three-letter code: MLA) (formula: $C_3H_4O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		

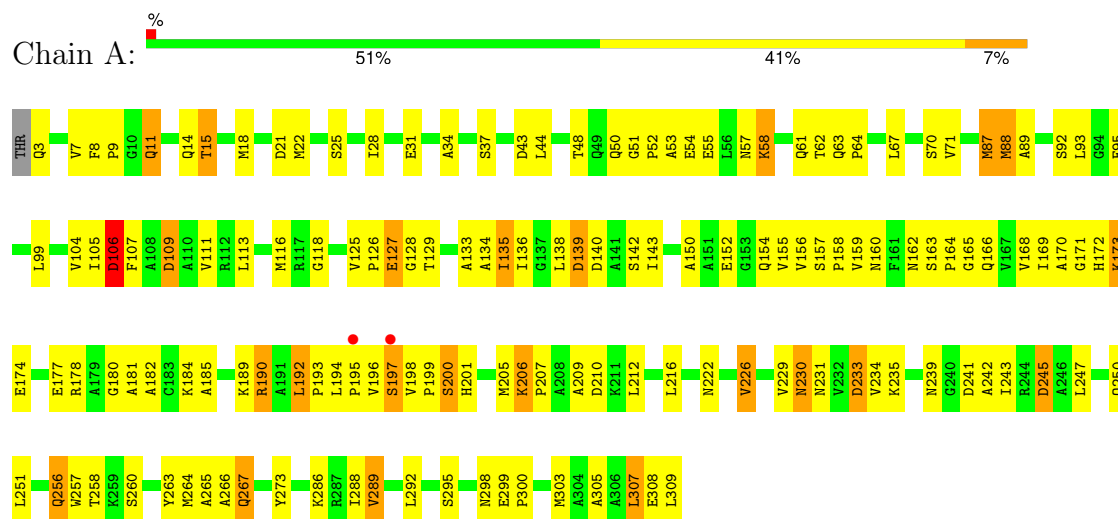
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total	O	0	0
			11	11		

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: Malonyl CoA-acyl carrier protein transacylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	83.34Å 83.34Å 164.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.87 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.00-2.80) 97.1 (19.87-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.238 , 0.284 0.223 , 0.259	Depositor DCC
R_{free} test set	731 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2322	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: MLA, COZ

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	0.66	0/2300	0.84	8/3132 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	233	ASP	CB-CG-OD2	6.35	124.01	118.30
1	A	21	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	245	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	140	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	106	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	43	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	139	ASP	CB-CG-OD2	5.64	123.38	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	GLY	Peptide
1	A	190	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	197	SER	Peptide

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	2257	0	2252	161	1
2	A	48	0	32	11	0
3	A	6	0	2	1	0
4	A	11	0	0	1	0
All	All	2322	0	2286	162	1

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 35.

All (162) 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:134:ALA:CB	1:A:192:LEU:HD11	1.60	1.29
1:A:192:LEU:CD1	1:A:192:LEU:O	1.86	1.22
1:A:134:ALA:HB3	1:A:192:LEU:CD1	1.70	1.20
1:A:190:ARG:NH1	2:A:1001:COZ:H3B	1.58	1.14
1:A:192:LEU:O	1:A:192:LEU:HD13	1.45	1.13
1:A:163:SER:HB2	1:A:164:PRO:HD2	1.32	1.12
1:A:190:ARG:HH12	2:A:1001:COZ:H3B	0.96	1.09
1:A:154:GLN:HB3	1:A:172:HIS:ND1	1.74	1.02
1:A:192:LEU:O	1:A:192:LEU:HD12	1.59	1.00
1:A:264:MET:HA	1:A:267:GLN:HB2	1.48	0.94
1:A:128:GLY:O	1:A:173:LYS:HE2	1.66	0.94
1:A:160:ASN:HB2	1:A:168:VAL:HB	1.52	0.91
1:A:14:GLN:NE2	1:A:57:ASN:OD1	2.04	0.90
1:A:28:ILE:HA	1:A:31:GLU:HG3	1.52	0.90
1:A:163:SER:HB2	1:A:164:PRO:CD	2.05	0.87
1:A:61:GLN:C	1:A:64:PRO:HD2	1.95	0.86
1:A:92:SER:H	1:A:231:ASN:HD21	1.23	0.84
1:A:234:VAL:O	1:A:234:VAL:HG12	1.77	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLN:HE21	1:A:57:ASN:CG	1.84	0.81
1:A:136:ILE:HB	1:A:190:ARG:HB2	1.62	0.81
1:A:288:ILE:HG22	1:A:289:VAL:HG23	1.61	0.81
1:A:61:GLN:O	1:A:64:PRO:HD2	1.82	0.80
1:A:303:MET:O	1:A:307:LEU:HD12	1.83	0.79
1:A:157:SER:HB2	1:A:158:PRO:HD2	1.65	0.78
1:A:206:LYS:HB3	1:A:207:PRO:HD3	1.64	0.78
1:A:87:MET:HB3	1:A:264:MET:SD	2.22	0.77
1:A:155:VAL:N	1:A:172:HIS:ND1	2.31	0.77
1:A:67:LEU:O	1:A:71:VAL:HG23	1.85	0.76
2:A:1001:COZ:H71	4:A:2004:HOH:O	1.86	0.76
1:A:155:VAL:N	1:A:172:HIS:CE1	2.55	0.75
1:A:190:ARG:NH2	2:A:1001:COZ:O8A	2.18	0.75
1:A:162:ASN:HD21	2:A:1001:COZ:H61	1.49	0.75
1:A:134:ALA:HB2	1:A:194:LEU:HD11	1.69	0.75
1:A:107:PHE:O	1:A:111:VAL:HG23	1.86	0.74
1:A:190:ARG:HH12	2:A:1001:COZ:C3B	1.89	0.74
1:A:160:ASN:ND2	2:A:1001:COZ:O5P	2.21	0.72
1:A:263:TYR:O	1:A:267:GLN:HG2	1.89	0.72
1:A:196:VAL:HG12	1:A:198:VAL:H	1.53	0.72
1:A:126:PRO:O	1:A:129:THR:HB	1.90	0.72
1:A:192:LEU:CD1	1:A:192:LEU:C	2.51	0.71
1:A:92:SER:H	1:A:231:ASN:ND2	1.88	0.71
1:A:209:ALA:CB	1:A:251:LEU:HD23	2.20	0.70
1:A:264:MET:CA	1:A:267:GLN:HB2	2.21	0.70
1:A:150:ALA:O	1:A:178:ARG:NH1	2.24	0.70
1:A:209:ALA:HB2	1:A:251:LEU:HD23	1.71	0.70
1:A:209:ALA:CA	1:A:251:LEU:HD23	2.21	0.70
1:A:15:THR:O	1:A:18:MET:HG2	1.91	0.70
1:A:206:LYS:NZ	1:A:210:ASP:OD1	2.24	0.69
1:A:209:ALA:HA	1:A:251:LEU:HD23	1.74	0.68
1:A:265:ALA:C	1:A:267:GLN:H	1.93	0.68
1:A:135:ILE:HD13	1:A:135:ILE:N	2.08	0.68
1:A:155:VAL:H	1:A:172:HIS:CE1	2.09	0.68
1:A:92:SER:N	1:A:231:ASN:HD21	1.93	0.66
1:A:206:LYS:CB	1:A:207:PRO:HD3	2.24	0.65
1:A:134:ALA:HB3	1:A:192:LEU:HD11	0.74	0.65
1:A:162:ASN:ND2	2:A:1001:COZ:H61	2.12	0.64
1:A:95:GLU:O	1:A:99:LEU:HG	1.99	0.63
1:A:196:VAL:CG1	1:A:198:VAL:H	2.12	0.63
1:A:265:ALA:C	1:A:267:GLN:N	2.50	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLU:O	1:A:177:GLU:HB2	1.99	0.62
1:A:163:SER:HA	1:A:258:THR:OG1	1.99	0.61
1:A:196:VAL:HG12	1:A:198:VAL:N	2.15	0.61
1:A:230:ASN:HD22	1:A:230:ASN:C	2.04	0.61
1:A:230:ASN:ND2	1:A:233:ASP:H	1.97	0.61
1:A:22:MET:HE1	1:A:299:GLU:CA	2.30	0.61
1:A:134:ALA:CA	1:A:192:LEU:HD11	2.29	0.61
1:A:22:MET:HE1	1:A:299:GLU:C	2.22	0.60
1:A:212:LEU:HG	1:A:216:LEU:HD11	1.83	0.60
1:A:44:LEU:O	1:A:48:THR:HG23	2.02	0.59
1:A:212:LEU:HG	1:A:216:LEU:CD1	2.33	0.59
1:A:150:ALA:O	1:A:178:ARG:HD2	2.03	0.59
1:A:14:GLN:HG2	1:A:14:GLN:O	2.03	0.58
1:A:162:ASN:HB2	1:A:166:GLN:HG2	1.85	0.58
1:A:155:VAL:O	1:A:171:GLY:HA3	2.03	0.58
1:A:192:LEU:HD12	1:A:192:LEU:N	2.15	0.58
1:A:63:GLN:N	1:A:64:PRO:CD	2.65	0.58
1:A:158:PRO:HA	1:A:169:ILE:HG22	1.87	0.57
1:A:258:THR:HA	1:A:288:ILE:HD13	1.87	0.57
1:A:192:LEU:HD12	1:A:192:LEU:H	1.69	0.57
1:A:53:ALA:O	1:A:54:GLU:C	2.44	0.56
1:A:135:ILE:N	1:A:135:ILE:CD1	2.68	0.56
1:A:206:LYS:HB3	1:A:207:PRO:CD	2.35	0.56
1:A:182:ALA:O	1:A:185:ALA:HB3	2.06	0.56
1:A:93:LEU:C	1:A:93:LEU:HD13	2.26	0.56
1:A:134:ALA:H	1:A:192:LEU:CD1	2.18	0.56
1:A:155:VAL:HB	1:A:172:HIS:CE1	2.41	0.55
1:A:192:LEU:HD13	1:A:192:LEU:C	2.23	0.55
1:A:104:VAL:HG12	1:A:105:ILE:HG13	1.89	0.55
1:A:265:ALA:O	1:A:267:GLN:N	2.41	0.54
1:A:11:GLN:OE1	1:A:62:THR:HG21	2.09	0.53
1:A:309:LEU:HD12	1:A:309:LEU:N	2.24	0.53
1:A:263:TYR:O	1:A:267:GLN:CG	2.57	0.53
1:A:201:HIS:NE2	3:A:2001:MLA:O1A	2.42	0.52
1:A:264:MET:HA	1:A:267:GLN:CB	2.32	0.52
1:A:22:MET:CE	1:A:299:GLU:HA	2.40	0.51
1:A:106:ASP:OD2	1:A:109:ASP:CG	2.48	0.51
1:A:181:ALA:O	1:A:182:ALA:C	2.45	0.51
1:A:22:MET:CE	1:A:299:GLU:CA	2.88	0.51
1:A:190:ARG:NH1	2:A:1001:COZ:C3B	2.52	0.50
1:A:138:LEU:HD22	1:A:142:SER:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:VAL:HG23	1:A:172:HIS:HE1	1.76	0.50
1:A:14:GLN:NE2	1:A:57:ASN:CG	2.57	0.49
1:A:125:VAL:HG21	1:A:199:PRO:HD2	1.93	0.49
1:A:127:GLU:OE2	1:A:197:SER:OG	2.30	0.49
1:A:11:GLN:O	2:A:1001:COZ:H22	2.12	0.49
1:A:273:TYR:HA	1:A:295:SER:O	2.13	0.49
1:A:88:MET:HG2	1:A:226:VAL:HG21	1.94	0.49
1:A:139:ASP:O	1:A:143:ILE:HG13	2.13	0.48
1:A:230:ASN:HD21	1:A:233:ASP:H	1.61	0.48
1:A:134:ALA:H	1:A:192:LEU:HD12	1.78	0.48
1:A:239:ASN:O	1:A:243:ILE:HG13	2.14	0.47
1:A:205:MET:O	1:A:206:LYS:C	2.52	0.47
1:A:109:ASP:O	1:A:113:LEU:HB2	2.15	0.47
1:A:256:GLN:HE21	1:A:256:GLN:HA	1.80	0.47
1:A:150:ALA:HB1	1:A:178:ARG:CB	2.44	0.47
1:A:234:VAL:O	1:A:234:VAL:CG1	2.50	0.47
1:A:288:ILE:C	1:A:289:VAL:HG23	2.35	0.47
1:A:7:VAL:HA	1:A:89:ALA:O	2.15	0.46
1:A:159:VAL:CG2	1:A:168:VAL:HG12	2.45	0.46
1:A:31:GLU:O	1:A:34:ALA:HB3	2.15	0.46
1:A:177:GLU:O	1:A:178:ARG:C	2.52	0.46
1:A:192:LEU:HA	1:A:193:PRO:HD3	1.78	0.46
1:A:239:ASN:O	1:A:242:ALA:N	2.49	0.45
1:A:289:VAL:O	1:A:292:LEU:HB2	2.17	0.45
1:A:299:GLU:HB3	1:A:300:PRO:HD2	1.98	0.45
1:A:206:LYS:N	1:A:207:PRO:CD	2.79	0.45
1:A:104:VAL:HG22	1:A:222:ASN:O	2.17	0.44
1:A:7:VAL:O	1:A:7:VAL:HG23	2.18	0.44
1:A:200:SER:HB2	1:A:201:HIS:ND1	2.32	0.44
1:A:206:LYS:CB	1:A:207:PRO:CD	2.94	0.44
1:A:155:VAL:CB	1:A:172:HIS:CE1	3.01	0.43
1:A:305:ALA:O	1:A:309:LEU:CD1	2.65	0.43
1:A:184:LYS:O	1:A:185:ALA:C	2.55	0.43
1:A:201:HIS:HD2	1:A:250:GLN:O	2.00	0.43
1:A:265:ALA:O	1:A:266:ALA:C	2.55	0.43
1:A:51:GLY:HA3	1:A:52:PRO:HA	1.90	0.43
1:A:99:LEU:HD23	1:A:99:LEU:HA	1.84	0.43
1:A:87:MET:CE	1:A:229:VAL:HG21	2.48	0.43
1:A:133:ALA:C	1:A:194:LEU:HD12	2.40	0.42
1:A:309:LEU:N	1:A:309:LEU:CD1	2.82	0.42
1:A:22:MET:HE2	1:A:299:GLU:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LEU:HA	1:A:195:PRO:HD3	1.93	0.42
1:A:209:ALA:HA	1:A:251:LEU:CD2	2.46	0.42
1:A:154:GLN:CB	1:A:172:HIS:ND1	2.65	0.42
1:A:55:GLU:OE2	1:A:58:LYS:CE	2.68	0.42
1:A:180:GLY:O	1:A:181:ALA:C	2.57	0.42
1:A:209:ALA:O	1:A:210:ASP:C	2.57	0.42
1:A:126:PRO:O	1:A:129:THR:CB	2.63	0.42
1:A:257:TRP:O	1:A:260:SER:N	2.48	0.42
1:A:136:ILE:HG21	2:A:1001:COZ:H1B	2.01	0.42
1:A:134:ALA:C	1:A:135:ILE:HD13	2.40	0.42
1:A:264:MET:C	1:A:267:GLN:HB2	2.40	0.41
1:A:156:VAL:HA	1:A:170:ALA:O	2.21	0.41
1:A:163:SER:CB	1:A:164:PRO:CD	2.76	0.41
1:A:8:PHE:HA	1:A:9:PRO:HD3	1.93	0.41
1:A:157:SER:HB2	1:A:158:PRO:CD	2.45	0.41
1:A:55:GLU:CD	1:A:58:LYS:HE2	2.41	0.40
1:A:247:LEU:HD23	1:A:247:LEU:HA	1.93	0.40
1:A:125:VAL:O	1:A:125:VAL:HG23	2.20	0.40
1:A:135:ILE:HD12	1:A:135:ILE:HA	1.83	0.40
1:A:150:ALA:HB1	1:A:178:ARG:HB2	2.04	0.40
1:A:288:ILE:C	1:A:289:VAL:CG2	2.89	0.40

All (1) 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:245:ASP:OD1	1:A:245:ASP:OD1[8_665]	1.90	0.30

5.3 Torsion angles

5.3.1 Protein backbone

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	305/308 (99%)	286 (94%)	17 (6%)	2 (1%)	22 53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	VAL
1	A	118	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	229/230 (100%)	199 (87%)	30 (13%)	4 12

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	11	GLN
1	A	15	THR
1	A	25	SER
1	A	37	SER
1	A	50	GLN
1	A	58	LYS
1	A	70	SER
1	A	87	MET
1	A	88	MET
1	A	106	ASP
1	A	116	MET
1	A	127	GLU
1	A	135	ILE
1	A	152	GLU
1	A	173	LYS
1	A	189	LYS
1	A	192	LEU
1	A	200	SER

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Mol	Chain	Res	Type
1	A	206	LYS
1	A	226	VAL
1	A	230	ASN
1	A	235	LYS
1	A	241	ASP
1	A	256	GLN
1	A	267	GLN
1	A	286	LYS
1	A	298	ASN
1	A	307	LEU
1	A	308	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	230	ASN
1	A	231	ASN
1	A	250	GLN
1	A	256	GLN
1	A	298	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
3	MLA	A	2001	1	4,5,6	1.14	1 (25%)	5,5,7	2.14	2 (40%)
2	COZ	A	1001	-	43,50,50	2.68	11 (25%)	56,75,75	1.37	5 (8%)

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	MLA	A	2001	1	-	0/2/3/4	-
2	COZ	A	1001	-	3/3/11/13	8/44/64/64	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	COZ	C4A-N3A	8.93	1.47	1.35
2	A	1001	COZ	P1A-O3A	7.42	1.67	1.59
2	A	1001	COZ	P2A-O3A	7.25	1.67	1.59
2	A	1001	COZ	C2A-N3A	7.12	1.43	1.32
2	A	1001	COZ	C8A-N7A	3.46	1.41	1.34
2	A	1001	COZ	P3B-O3B	3.18	1.65	1.59
2	A	1001	COZ	C5P-N4P	2.43	1.39	1.33
2	A	1001	COZ	C6A-N6A	2.38	1.42	1.34
2	A	1001	COZ	C9P-N8P	2.27	1.39	1.33
2	A	1001	COZ	C2A-N1A	2.22	1.37	1.33
2	A	1001	COZ	O4B-C1B	2.16	1.43	1.40
3	A	2001	MLA	O1A-C1	-2.16	1.23	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	COZ	N3A-C2A-N1A	-6.90	119.30	128.67
3	A	2001	MLA	O3A-C3-C2	-3.25	116.27	126.34
2	A	1001	COZ	C5A-C6A-N6A	3.01	124.89	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	MLA	C3-C2-C1	-2.92	107.96	113.68
2	A	1001	COZ	C6A-C5A-C4A	2.92	123.57	117.90
2	A	1001	COZ	C7P-C6P-C5P	-2.10	108.90	112.39
2	A	1001	COZ	P3B-O3B-C3B	-2.07	117.90	123.43

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1001	COZ	CAP
2	A	1001	COZ	C2B
2	A	1001	COZ	C3B

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	COZ	C5B-O5B-P1A-O2A
2	A	1001	COZ	C5B-O5B-P1A-O3A
2	A	1001	COZ	C3B-C4B-C5B-O5B
2	A	1001	COZ	O4B-C4B-C5B-O5B
2	A	1001	COZ	C4B-C5B-O5B-P1A
2	A	1001	COZ	O5P-C5P-C6P-C7P
2	A	1001	COZ	N4P-C5P-C6P-C7P
2	A	1001	COZ	C5B-O5B-P1A-O1A

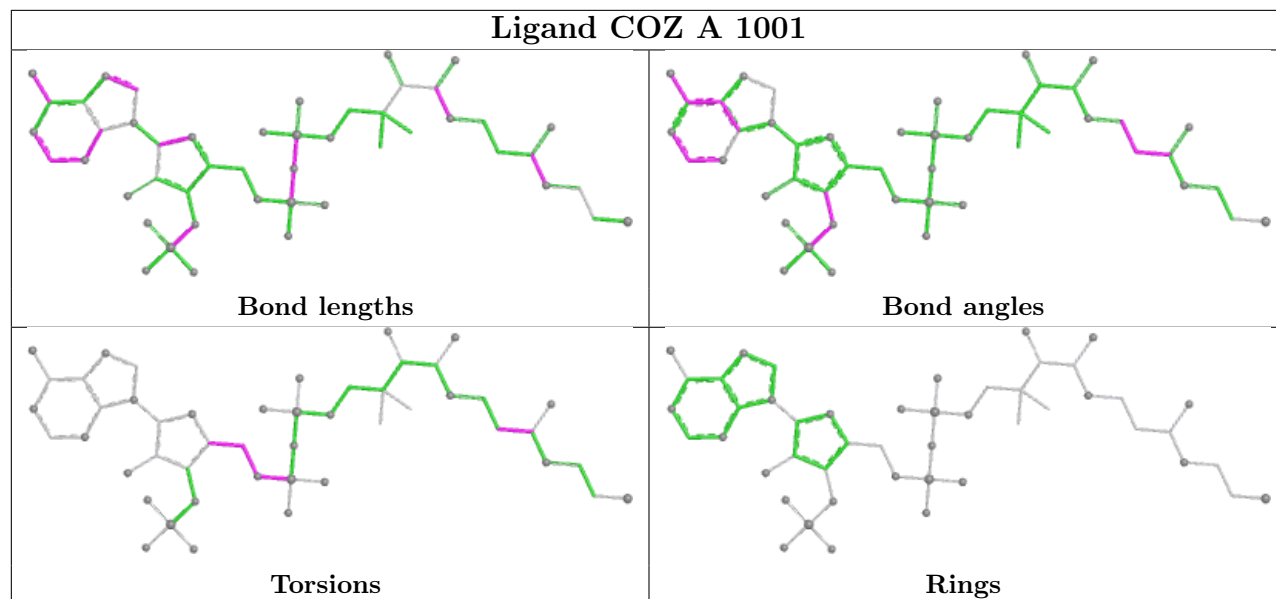
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	MLA	1	0
2	A	1001	COZ	11	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	307/308 (99%)	-0.52	2 (0%) 87 84	23, 39, 63, 97	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	SER	3.2
1	A	195	PRO	2.6

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.

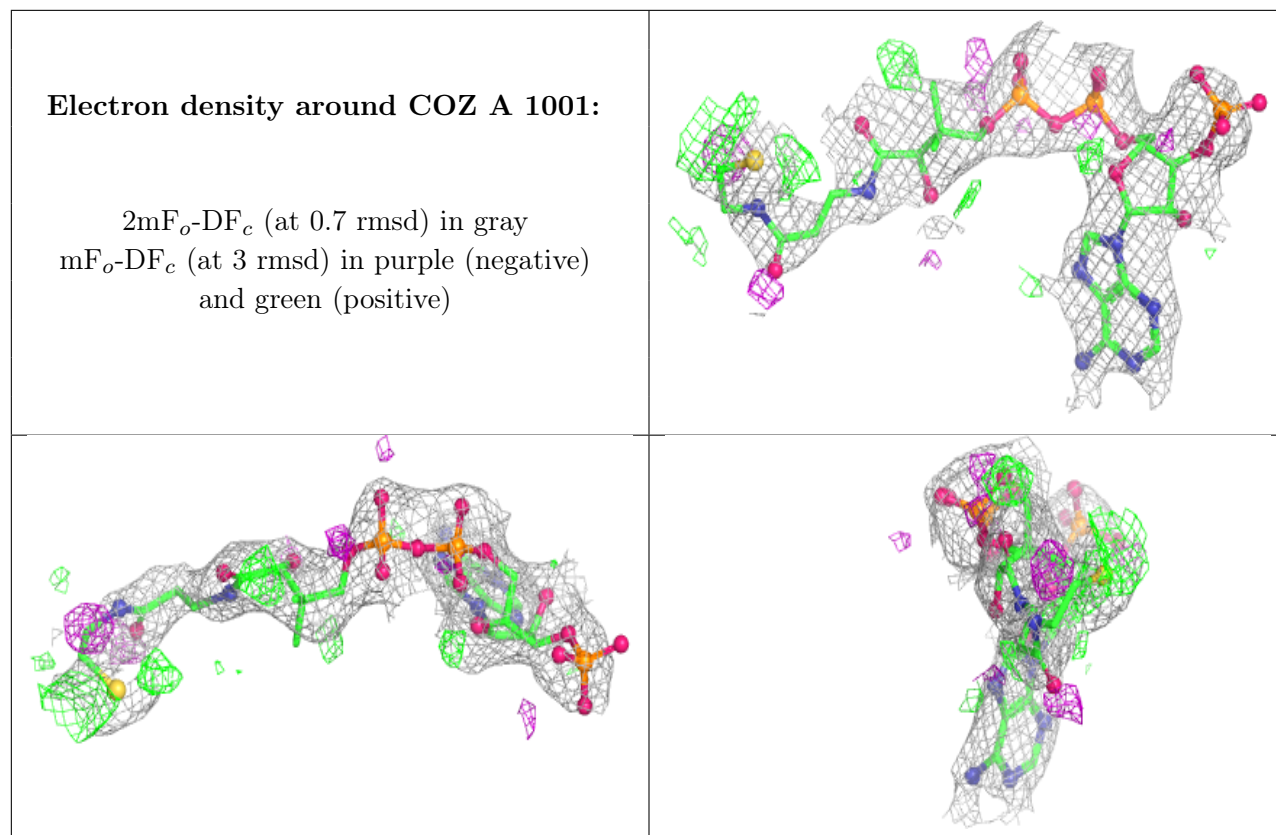
6.4 Ligands [i](#)

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	COZ	A	1001	48/48	0.83	0.27	38,56,88,92	48
3	MLA	A	2001	6/7	0.85	0.24	48,56,61,61	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.