



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:31 AM UTC

PDB ID : 5WX6 / pdb_00005wx6
Title : Alkyldiketide-CoA synthase W332Q mutant from Evodia rutaecarpa
Authors : Matsui, T.; Kodama, T.; Tadakoshi, T.; Morita, H.
Deposited on : 2017-01-06
Resolution : 1.80 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	:	4-5-2 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

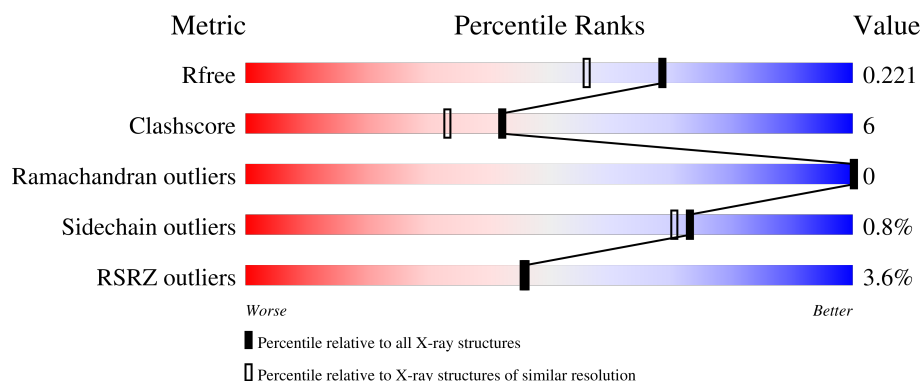
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	396	
1	B	396	
1	C	396	
1	D	396	

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	SO4	C	404	-	-	X	-

2 Entry composition [i](#)

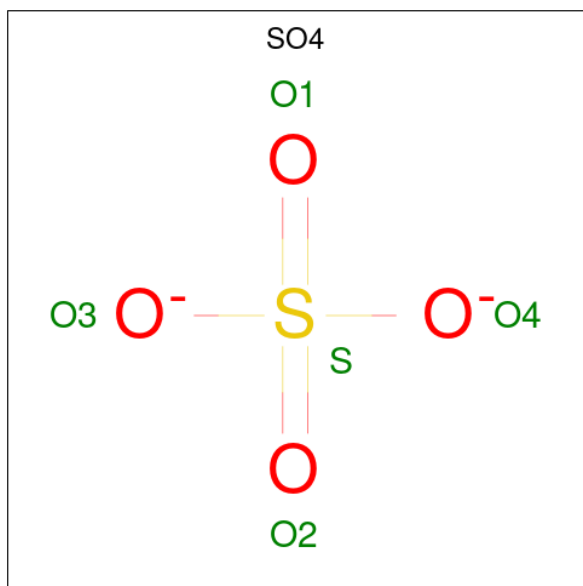
There are 4 unique types of molecules in this entry. The entry contains 12740 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alkyldiketide-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2824	1797	481	520	26			
1	B	376	Total	C	N	O	S	0	1	0
			2929	1861	498	543	27			
1	C	368	Total	C	N	O	S	0	0	0
			2865	1822	488	529	26			
1	D	375	Total	C	N	O	S	0	0	0
			2921	1854	499	542	26			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



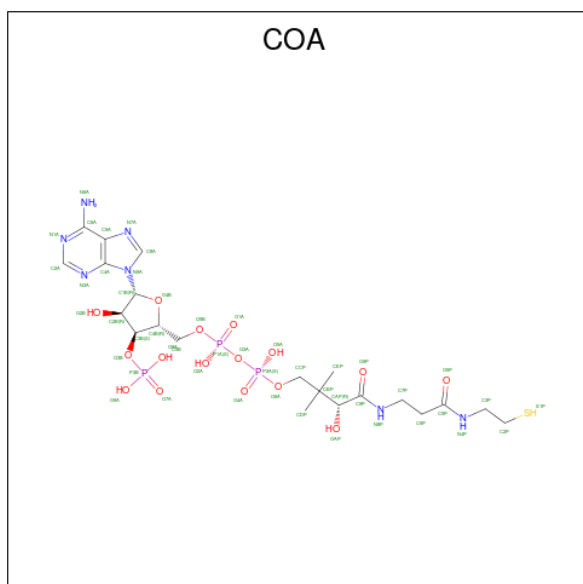
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



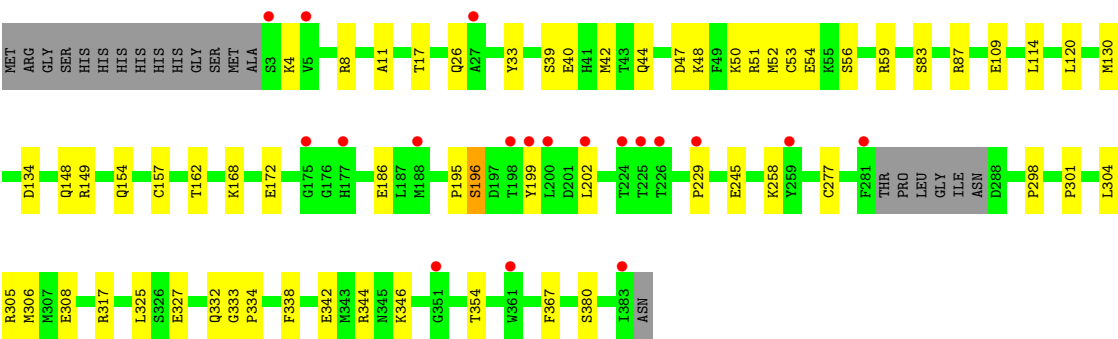
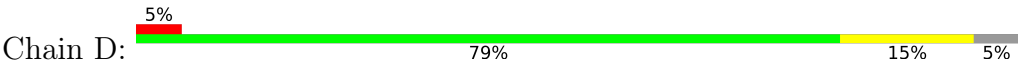
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	279	Total 279	O 279	0	0
4	B	315	Total 315	O 315	0	0
4	C	235	Total 235	O 235	0	0
4	D	140	Total 140	O 140	0	0



● Molecule 1: Alkyldiketide-CoA synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.08Å 84.66Å 137.86Å 90.00° 124.63° 90.00°	Depositor
Resolution (Å)	47.37 – 1.80 47.37 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.37-1.80) 98.4 (47.37-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.183 , 0.223 0.182 , 0.221	Depositor DCC
R_{free} test set	7083 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	29.8	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.020 for h,-k,-h-l	Depositor
Outliers	0 of 141647 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12740	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: SO4, 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	0.36	0/2882	0.53	0/3894
1	B	0.36	0/2993	0.55	0/4050
1	C	0.37	0/2924	0.54	0/3955
1	D	0.34	0/2980	0.51	0/4029
All	All	0.36	0/11779	0.53	0/15928

There are no bond length outliers.

There are no bond angle outliers.

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	2824	0	2829	29	0
1	B	2929	0	2936	38	0
1	C	2865	0	2871	29	0
1	D	2921	0	2926	45	0
2	A	10	0	0	0	0
2	B	5	0	0	1	0
2	C	20	0	0	2	0
2	D	5	0	0	1	0
3	A	48	0	32	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	32	5	0
3	C	48	0	32	5	0
3	D	48	0	32	9	0
4	A	279	0	0	3	0
4	B	315	0	0	4	0
4	C	235	0	0	0	0
4	D	140	0	0	2	0
All	All	12740	0	11690	147	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 6.

All (147) 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)
3:A:403:COA:O4B	3:A:403:COA:C1B	1.66	1.28
3:C:405:COA:O4B	3:C:405:COA:C1B	1.67	1.26
3:B:402:COA:C1B	3:B:402:COA:O4B	1.66	1.25
3:D:402:COA:O4B	3:D:402:COA:C1B	1.67	1.22
1:D:51:ARG:NH2	3:D:402:COA:O8A	1.72	1.22
3:C:405:COA:H8A	3:C:405:COA:H51A	1.51	0.91
1:D:199:TYR:HB3	1:D:202:LEU:HD12	1.55	0.88
1:C:323:HIS:CD2	2:C:404:SO4:O3	2.29	0.86
1:A:255:MET:SD	1:A:258:LYS:HD2	2.24	0.77
1:C:290:ASN:HD21	1:C:313:LEU:HA	1.50	0.76
3:C:405:COA:H51A	3:C:405:COA:C8A	2.23	0.69
1:D:52:MET:O	3:D:402:COA:CDP	2.42	0.68
1:B:255:MET:SD	1:B:258:LYS:HD2	2.34	0.68
1:A:301:PRO:HD2	3:A:403:COA:OAP	1.94	0.67
1:B:205:GLY:HA3	1:B:259:TYR:CZ	2.30	0.66
1:B:258:LYS:NZ	2:B:401:SO4:O4	2.23	0.65
1:D:51:ARG:CZ	3:D:402:COA:O8A	2.45	0.64
1:C:323:HIS:HD2	2:C:404:SO4:O3	1.80	0.63
1:C:67:GLU:HG2	1:C:71:LYS:HE2	1.80	0.62
1:B:188[A]:MET:HG3	1:B:211:ASP:OD1	1.99	0.62
1:D:39:SER:HB3	1:D:42:MET:SD	2.41	0.61
1:D:50:LYS:O	1:D:54:GLU:HG3	1.99	0.60
1:D:56:SER:HA	3:D:402:COA:H143	1.83	0.60
1:D:47:ASP:O	1:D:51:ARG:HG3	2.01	0.60
1:D:11:ALA:HB1	1:D:229:PRO:HB3	1.83	0.60
1:D:304:LEU:O	1:D:308:GLU:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:VAL:HG11	1:C:310:LYS:HG2	1.85	0.59
1:C:318:MET:HE2	1:C:318:MET:HA	1.86	0.58
1:D:342:GLU:OE2	1:D:346:LYS:NZ	2.37	0.58
1:C:281:PHE:CD1	1:C:292:MET:HE1	2.39	0.57
1:A:176:GLY:O	1:A:179:ARG:NH1	2.38	0.57
1:D:59:ARG:NH2	4:D:505:HOH:O	2.38	0.57
1:D:4:LYS:O	1:D:8:ARG:HD3	2.03	0.56
1:A:238:GLN:H	1:D:148:GLN:NE2	2.03	0.56
1:D:120:LEU:HD23	1:D:149:ARG:HG2	1.86	0.56
4:B:774:HOH:O	1:C:255:MET:HE3	2.04	0.56
3:A:403:COA:O9P	3:A:403:COA:H133	2.05	0.55
1:B:202:LEU:O	1:B:259:TYR:OH	2.25	0.55
1:A:238:GLN:H	1:D:148:GLN:HE21	1.55	0.55
1:A:157:CYS:HB2	1:A:367:PHE:O	2.08	0.54
1:B:263:ARG:HG3	3:B:402:COA:C6A	2.37	0.54
1:D:59:ARG:NH1	1:D:327:GLU:OE1	2.41	0.54
1:D:40:GLU:H	1:D:40:GLU:CD	2.15	0.54
3:D:402:COA:H121	3:D:402:COA:O9P	2.09	0.53
1:D:186:GLU:HG3	1:D:332:GLN:HB2	1.91	0.53
1:B:188[B]:MET:SD	1:B:209:PHE:HB3	2.48	0.52
1:C:79:LEU:O	1:C:80:ASN:HB2	2.09	0.52
1:D:33:TYR:CZ	1:D:195:PRO:HD3	2.43	0.52
1:A:57:MET:HE1	1:B:42:MET:HG2	1.91	0.52
1:C:302:ALA:HB2	3:C:405:COA:H132	1.92	0.52
3:C:405:COA:O5A	3:C:405:COA:OAP	2.27	0.51
1:A:93:GLU:HG3	1:A:97:LYS:HE2	1.93	0.51
1:C:17:THR:HB	1:C:338:PHE:CZ	2.46	0.51
1:C:319:ARG:NH2	1:C:350:GLU:OE2	2.38	0.51
1:D:168:LYS:NZ	1:D:172:GLU:OE2	2.44	0.51
1:B:132:SER:HB2	1:B:134:ASP:OD1	2.11	0.50
1:D:301:PRO:HB2	1:D:305:ARG:NH1	2.27	0.50
1:B:65:LEU:H	1:B:188[A]:MET:HE1	1.75	0.50
1:C:308:GLU:HG3	1:C:318:MET:HG3	1.93	0.50
1:A:205:GLY:HA3	1:A:259:TYR:CE1	2.47	0.50
1:B:157:CYS:HB2	1:B:367:PHE:O	2.12	0.49
3:B:402:COA:O7A	3:B:402:COA:H4B	2.12	0.49
1:B:316:GLU:OE2	1:B:319:ARG:NH2	2.45	0.49
1:D:354:THR:HB	1:D:380:SER:HB2	1.94	0.49
1:A:186:GLU:HG3	1:A:332:GLN:HB2	1.95	0.49
3:D:402:COA:H52A	3:D:402:COA:H8A	1.95	0.49
1:A:346:LYS:NZ	4:A:512:HOH:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LYS:NZ	1:D:245:GLU:OE1	2.45	0.48
1:C:75:ASN:ND2	1:C:82:PRO:O	2.46	0.48
1:D:48:LYS:O	1:D:52:MET:HG3	2.14	0.48
1:D:317:ARG:HA	1:D:317:ARG:NE	2.27	0.48
1:B:159:ALA:O	1:B:162:THR:HG22	2.14	0.48
1:D:109:GLU:OE2	1:D:344:ARG:NH1	2.36	0.48
1:B:223:ASP:OD2	1:B:225:THR:HB	2.12	0.48
1:B:33:TYR:CZ	1:B:195:PRO:HD3	2.49	0.48
1:B:46:LYS:O	1:B:50:LYS:HG3	2.14	0.48
1:D:44:GLN:H	1:D:44:GLN:CD	2.17	0.47
1:D:83:SER:O	1:D:87:ARG:HG3	2.14	0.47
1:D:52:MET:HE2	3:D:402:COA:O4B	2.13	0.47
1:A:298:PRO:HD3	1:A:339:ILE:HD11	1.97	0.47
1:B:186:GLU:HG3	1:B:332:GLN:HB2	1.97	0.47
1:D:298:PRO:HB2	1:D:325:LEU:HD13	1.96	0.47
1:D:333:GLY:HA3	4:D:556:HOH:O	2.13	0.47
1:B:17:THR:HB	1:B:338:PHE:CZ	2.50	0.47
1:A:55:LYS:HD3	3:A:403:COA:O3A	2.14	0.47
3:B:402:COA:H141	3:B:402:COA:O9P	2.15	0.47
1:A:266:PRO:HG3	3:A:403:COA:H72	1.97	0.47
1:B:205:GLY:HA3	1:B:259:TYR:CE2	2.50	0.46
1:A:293:PHE:CE1	1:A:362:GLY:HA3	2.50	0.46
1:B:49:PHE:CD1	1:B:203:LEU:HD22	2.51	0.46
1:B:282:THR:OG1	4:B:501:HOH:O	2.20	0.46
1:D:17:THR:HB	1:D:338:PHE:CZ	2.51	0.46
1:D:157:CYS:HB2	1:D:367:PHE:O	2.15	0.46
1:B:65:LEU:CB	1:B:188[A]:MET:HE1	2.46	0.45
1:C:298:PRO:HB2	1:C:325:LEU:HD13	1.99	0.45
1:C:298:PRO:HD3	1:C:339:ILE:HD11	1.98	0.45
1:B:310:LYS:HB3	1:B:310:LYS:HE3	1.75	0.45
1:C:228:ARG:O	1:C:228:ARG:HD3	2.16	0.45
1:A:262:SER:HB3	1:A:265:VAL:HG23	1.99	0.45
1:A:17:THR:HB	1:A:338:PHE:CZ	2.52	0.45
1:B:176:GLY:HA2	1:B:221:ASP:HB2	1.98	0.45
1:B:151:MET:HE2	1:B:153:TYR:CE1	2.51	0.44
1:B:287:ASN:ND2	4:B:517:HOH:O	2.50	0.44
1:C:314:SER:OG	1:C:315:LYS:N	2.51	0.43
1:A:369:PRO:HG2	1:D:130:MET:HE2	1.99	0.43
1:C:186:GLU:HG3	1:C:332:GLN:HB2	1.99	0.43
1:D:26:GLN:HG3	1:D:53:CYS:HB3	2.00	0.43
1:B:306:MET:O	1:B:310:LYS:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ARG:NE	1:A:317:ARG:HA	2.33	0.43
1:C:199:TYR:HB3	1:C:202:LEU:HD13	1.98	0.43
1:B:159:ALA:HA	1:B:162:THR:HG22	2.00	0.43
1:C:203:LEU:HD12	1:C:203:LEU:HA	1.84	0.43
1:D:42:MET:HE1	1:D:196:SER:HA	1.99	0.43
1:A:202:LEU:HA	1:A:259:TYR:CE1	2.54	0.43
1:D:134:ASP:OD2	1:D:149:ARG:HB3	2.19	0.43
1:A:134:ASP:OD2	1:A:149:ARG:HB3	2.19	0.42
1:C:157:CYS:HB3	1:C:297:HIS:CE1	2.55	0.42
1:D:44:GLN:OE1	1:D:44:GLN:N	2.47	0.42
1:A:130:MET:HE3	1:D:154:GLN:O	2.20	0.42
1:C:317:ARG:NE	1:C:317:ARG:HA	2.34	0.42
1:A:384:ASN:ND2	4:A:518:HOH:O	2.49	0.42
1:B:100:LYS:NZ	4:B:505:HOH:O	2.41	0.42
1:D:51:ARG:NE	3:D:402:COA:O8A	2.53	0.42
1:D:258:LYS:NZ	2:D:401:SO4:O3	2.39	0.42
1:B:157:CYS:HB3	1:B:297:HIS:CE1	2.54	0.42
1:B:201:ASP:O	1:B:259:TYR:HE2	2.03	0.42
1:A:89:GLU:OE2	4:A:501:HOH:O	2.22	0.42
1:C:205:GLY:HA3	1:C:259:TYR:CE1	2.56	0.41
1:C:306:MET:HE2	1:C:306:MET:HB3	1.77	0.41
1:A:157:CYS:HB3	1:A:297:HIS:CE1	2.55	0.41
1:B:202:LEU:O	1:B:206:ASN:ND2	2.52	0.41
1:B:364:MET:HB3	1:B:376:VAL:HB	2.01	0.41
1:A:281:PHE:CZ	1:A:363:VAL:HB	2.55	0.41
1:B:293:PHE:CE1	1:B:362:GLY:HA3	2.55	0.41
1:B:281:PHE:CZ	1:B:363:VAL:HB	2.56	0.41
1:C:182:ILE:O	1:C:215:ALA:HA	2.21	0.41
1:C:344:ARG:HG3	1:C:345:ASN:N	2.35	0.41
1:D:186:GLU:HG2	1:D:334:PRO:HD2	2.02	0.41
1:D:306:MET:HB3	1:D:306:MET:HE2	1.76	0.41
1:A:62:HIS:O	1:A:63:MET:HG3	2.21	0.41
1:B:20:PRO:HD3	1:B:98:LEU:HD21	2.02	0.41
1:D:114:LEU:HA	1:D:114:LEU:HD23	1.85	0.41
1:C:278:ARG:HG2	1:C:289:TRP:CZ2	2.57	0.40
1:C:296:VAL:HG23	1:C:318:MET:HE1	2.04	0.40
1:A:159:ALA:O	1:A:162:THR:HG22	2.20	0.40
1:B:55:LYS:HD3	3:B:402:COA:O3A	2.21	0.40
1:B:262:SER:HB3	1:B:265:VAL:HG23	2.02	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	357/396 (90%)	347 (97%)	10 (3%)	0	100	100
1	B	375/396 (95%)	363 (97%)	12 (3%)	0	100	100
1	C	364/396 (92%)	353 (97%)	11 (3%)	0	100	100
1	D	371/396 (94%)	364 (98%)	7 (2%)	0	100	100
All	All	1467/1584 (93%)	1427 (97%)	40 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	306/335 (91%)	304 (99%)	2 (1%)	76	73
1	B	319/335 (95%)	317 (99%)	2 (1%)	78	77
1	C	311/335 (93%)	307 (99%)	4 (1%)	61	54
1	D	318/335 (95%)	315 (99%)	3 (1%)	70	67
All	All	1254/1340 (94%)	1243 (99%)	11 (1%)	73	67

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	THR
1	A	203	LEU

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Mol	Chain	Res	Type
1	B	188[A]	MET
1	B	188[B]	MET
1	C	162	THR
1	C	272	ASN
1	C	277	CYS
1	C	353	SER
1	D	162	THR
1	D	196	SER
1	D	277	CYS

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	154	GLN
1	A	177	HIS
1	A	206	ASN
1	A	323	HIS
1	B	9	GLN
1	B	267	GLN
1	B	271	ASN
1	C	73	ASN
1	C	323	HIS
1	D	41	HIS
1	D	148	GLN
1	D	154	GLN
1	D	275	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

12 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	SO4	A	402	-	4,4,4	0.33	0	6,6,6	0.33	0
2	SO4	C	404	-	4,4,4	0.42	0	6,6,6	0.08	0
3	COA	D	402	-	47,50,50	3.77	16 (34%)	69,75,75	1.74	12 (17%)
2	SO4	C	401	-	4,4,4	0.27	0	6,6,6	0.28	0
2	SO4	C	402	-	4,4,4	0.22	0	6,6,6	0.34	0
3	COA	C	405	-	47,50,50	3.71	16 (34%)	69,75,75	1.89	17 (24%)
2	SO4	C	403	-	4,4,4	0.25	0	6,6,6	0.10	0
2	SO4	D	401	-	4,4,4	0.41	0	6,6,6	0.07	0
3	COA	B	402	-	47,50,50	3.76	16 (34%)	69,75,75	1.74	12 (17%)
3	COA	A	403	-	47,50,50	3.75	16 (34%)	69,75,75	1.73	11 (15%)
2	SO4	B	401	-	4,4,4	0.41	0	6,6,6	0.07	0
2	SO4	A	401	-	4,4,4	0.30	0	6,6,6	0.14	0

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	COA	A	403	-	-	9/48/64/64	0/3/3/3
3	COA	D	402	-	-	12/48/64/64	0/3/3/3
3	COA	C	405	-	-	19/48/64/64	0/3/3/3
3	COA	B	402	-	-	12/48/64/64	0/3/3/3

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	COA	P2A-O3A	11.85	1.72	1.59
3	B	402	COA	P2A-O3A	11.70	1.72	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	COA	P2A-O3A	11.69	1.72	1.59
3	C	405	COA	P2A-O3A	11.24	1.71	1.59
3	C	405	COA	O4B-C1B	11.22	1.67	1.42
3	D	402	COA	O4B-C1B	10.81	1.67	1.42
3	B	402	COA	O4B-C1B	10.77	1.66	1.42
3	A	403	COA	O4B-C1B	10.65	1.66	1.42
3	D	402	COA	P1A-O3A	10.11	1.70	1.59
3	B	402	COA	P1A-O3A	10.05	1.70	1.59
3	A	403	COA	P1A-O3A	9.98	1.70	1.59
3	C	405	COA	P1A-O3A	9.65	1.69	1.59
3	C	405	COA	C6A-N6A	6.86	1.51	1.34
3	D	402	COA	C6A-N6A	6.83	1.51	1.34
3	A	403	COA	C6A-N6A	6.82	1.51	1.34
3	B	402	COA	C6A-N6A	6.79	1.51	1.34
3	C	405	COA	O4B-C4B	-6.73	1.30	1.45
3	A	403	COA	C2B-C1B	-6.60	1.32	1.53
3	D	402	COA	C2B-C1B	-6.53	1.33	1.53
3	B	402	COA	C2B-C1B	-6.46	1.33	1.53
3	B	402	COA	O4B-C4B	-6.34	1.30	1.45
3	B	402	COA	C9P-N8P	6.33	1.48	1.33
3	D	402	COA	O4B-C4B	-6.31	1.31	1.45
3	D	402	COA	C9P-N8P	6.29	1.48	1.33
3	A	403	COA	O4B-C4B	-6.27	1.31	1.45
3	A	403	COA	C9P-N8P	6.27	1.48	1.33
3	A	403	COA	C5P-N4P	6.24	1.48	1.33
3	C	405	COA	C9P-N8P	6.24	1.48	1.33
3	D	402	COA	C5P-N4P	6.22	1.48	1.33
3	B	402	COA	C5P-N4P	6.22	1.48	1.33
3	C	405	COA	C5P-N4P	6.06	1.47	1.33
3	C	405	COA	C2B-C1B	-6.03	1.34	1.53
3	A	403	COA	P3B-O3B	4.64	1.67	1.59
3	B	402	COA	P3B-O3B	4.64	1.67	1.59
3	D	402	COA	P3B-O3B	4.56	1.67	1.59
3	C	405	COA	P3B-O3B	4.04	1.66	1.59
3	C	405	COA	O3B-C3B	-3.09	1.33	1.44
3	D	402	COA	O3B-C3B	-2.82	1.34	1.44
3	B	402	COA	O3B-C3B	-2.78	1.34	1.44
3	A	403	COA	O3B-C3B	-2.78	1.34	1.44
3	D	402	COA	O9P-C9P	-2.67	1.18	1.23
3	B	402	COA	O9P-C9P	-2.66	1.18	1.23
3	A	403	COA	O9P-C9P	-2.65	1.18	1.23
3	C	405	COA	CCP-CBP	2.56	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	COA	C8A-N7A	2.51	1.36	1.31
3	A	403	COA	C3B-C4B	2.48	1.59	1.52
3	D	402	COA	C8A-N7A	2.46	1.36	1.31
3	B	402	COA	C8A-N7A	2.46	1.36	1.31
3	C	405	COA	O9P-C9P	-2.41	1.18	1.23
3	C	405	COA	C2A-N1A	2.40	1.38	1.33
3	D	402	COA	P2A-O6A	2.35	1.68	1.59
3	A	403	COA	P2A-O6A	2.33	1.68	1.59
3	B	402	COA	P2A-O6A	2.32	1.68	1.59
3	D	402	COA	C3B-C4B	2.29	1.58	1.52
3	C	405	COA	P2A-O6A	2.29	1.68	1.59
3	C	405	COA	C8A-N7A	2.24	1.36	1.31
3	B	402	COA	C3B-C4B	2.23	1.58	1.52
3	C	405	COA	C5A-N7A	-2.19	1.35	1.39
3	D	402	COA	CCP-CBP	2.11	1.56	1.52
3	A	403	COA	CCP-CBP	2.10	1.56	1.52
3	A	403	COA	C5A-N7A	-2.10	1.35	1.39
3	D	402	COA	C5A-N7A	-2.08	1.35	1.39
3	B	402	COA	C5A-N7A	-2.08	1.35	1.39
3	B	402	COA	CCP-CBP	2.01	1.55	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	COA	N3A-C2A-N1A	-5.60	120.10	128.58
3	A	403	COA	N3A-C2A-N1A	-5.59	120.11	128.58
3	D	402	COA	N3A-C2A-N1A	-5.58	120.13	128.58
3	C	405	COA	N3A-C2A-N1A	-5.57	120.15	128.58
3	B	402	COA	N6A-C6A-N1A	-5.17	106.86	118.38
3	A	403	COA	N6A-C6A-N1A	-5.16	106.88	118.38
3	D	402	COA	N6A-C6A-N1A	-5.15	106.90	118.38
3	D	402	COA	C5A-C4A-N3A	-4.92	119.94	126.72
3	C	405	COA	C5A-C4A-N3A	-4.90	119.96	126.72
3	B	402	COA	C5A-C4A-N3A	-4.88	120.00	126.72
3	A	403	COA	C5A-C4A-N3A	-4.86	120.03	126.72
3	A	403	COA	N9A-C8A-N7A	-4.18	108.00	113.94
3	B	402	COA	N9A-C8A-N7A	-4.17	108.02	113.94
3	D	402	COA	N9A-C8A-N7A	-4.16	108.03	113.94
3	C	405	COA	N6A-C6A-N1A	-4.08	109.28	118.38
3	A	403	COA	C5A-C6A-N6A	4.01	133.21	123.29
3	B	402	COA	C5A-C6A-N6A	4.00	133.20	123.29
3	D	402	COA	C5A-C6A-N6A	4.00	133.18	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	405	COA	C5B-C4B-C3B	-3.88	101.46	114.38
3	C	405	COA	N9A-C8A-N7A	-3.66	108.74	113.94
3	C	405	COA	P3B-O3B-C3B	-3.59	113.83	123.43
3	B	402	COA	C2A-N3A-C4A	3.39	120.10	111.83
3	D	402	COA	C2A-N3A-C4A	3.38	120.08	111.83
3	A	403	COA	C2A-N3A-C4A	3.37	120.05	111.83
3	C	405	COA	N3A-C4A-N9A	3.27	132.73	127.17
3	C	405	COA	CDP-CBP-CAP	3.23	114.28	108.77
3	C	405	COA	C7P-C6P-C5P	-3.22	107.03	112.39
3	C	405	COA	C2A-N3A-C4A	3.19	119.62	111.83
3	C	405	COA	C5A-C6A-N6A	3.18	131.16	123.29
3	B	402	COA	C5A-N7A-C8A	2.92	108.05	103.45
3	D	402	COA	N3A-C4A-N9A	2.92	132.14	127.17
3	D	402	COA	C5A-N7A-C8A	2.92	108.04	103.45
3	A	403	COA	C5A-N7A-C8A	2.89	108.00	103.45
3	B	402	COA	N3A-C4A-N9A	2.86	132.04	127.17
3	A	403	COA	N3A-C4A-N9A	2.85	132.02	127.17
3	C	405	COA	C5A-N7A-C8A	2.65	107.61	103.45
3	C	405	COA	C7P-N8P-C9P	-2.47	118.11	122.55
3	C	405	COA	C6A-C5A-C4A	2.39	120.44	117.18
3	B	402	COA	C4A-C5A-N7A	-2.35	107.89	110.58
3	D	402	COA	C4A-C5A-N7A	-2.34	107.91	110.58
3	A	403	COA	C4A-C5A-N7A	-2.30	107.95	110.58
3	C	405	COA	C3P-N4P-C5P	-2.28	118.59	122.82
3	A	403	COA	C4A-N9A-C8A	2.25	108.10	105.74
3	D	402	COA	C4A-N9A-C8A	2.24	108.09	105.74
3	B	402	COA	C4A-N9A-C8A	2.23	108.08	105.74
3	B	402	COA	C3B-C2B-C1B	2.22	104.78	99.89
3	C	405	COA	C6P-C5P-N4P	2.19	120.33	116.34
3	C	405	COA	C3B-C2B-C1B	2.16	104.63	99.89
3	B	402	COA	C6P-C5P-N4P	2.13	120.23	116.34
3	D	402	COA	C6P-C5P-N4P	2.06	120.09	116.34
3	A	403	COA	C6P-C5P-N4P	2.05	120.08	116.34
3	D	402	COA	C3B-C2B-C1B	2.01	104.30	99.89

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	COA	CAP-CBP-CCP-O6A
3	A	403	COA	C5P-C6P-C7P-N8P
3	A	403	COA	S1P-C2P-C3P-N4P

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Mol	Chain	Res	Type	Atoms
3	B	402	COA	C5B-O5B-P1A-O3A
3	B	402	COA	S1P-C2P-C3P-N4P
3	C	405	COA	C5B-O5B-P1A-O2A
3	C	405	COA	C5B-O5B-P1A-O3A
3	C	405	COA	CCP-O6A-P2A-O3A
3	C	405	COA	CCP-O6A-P2A-O4A
3	C	405	COA	CCP-O6A-P2A-O5A
3	C	405	COA	CBP-CCP-O6A-P2A
3	C	405	COA	CDP-CBP-CCP-O6A
3	C	405	COA	CEP-CBP-CCP-O6A
3	C	405	COA	CAP-CBP-CCP-O6A
3	C	405	COA	C5P-C6P-C7P-N8P
3	C	405	COA	S1P-C2P-C3P-N4P
3	D	402	COA	C5B-O5B-P1A-O1A
3	D	402	COA	C5B-O5B-P1A-O2A
3	D	402	COA	C5B-O5B-P1A-O3A
3	D	402	COA	CCP-O6A-P2A-O3A
3	D	402	COA	CCP-O6A-P2A-O4A
3	D	402	COA	C5P-C6P-C7P-N8P
3	D	402	COA	S1P-C2P-C3P-N4P
3	B	402	COA	C6P-C7P-N8P-C9P
3	C	405	COA	C3B-C4B-C5B-O5B
3	B	402	COA	C4B-C3B-O3B-P3B
3	B	402	COA	C2B-C3B-O3B-P3B
3	C	405	COA	O4B-C4B-C5B-O5B
3	C	405	COA	P1A-O3A-P2A-O4A
3	A	403	COA	O9P-C9P-CAP-CBP
3	A	403	COA	N8P-C9P-CAP-CBP
3	C	405	COA	N8P-C9P-CAP-CBP
3	C	405	COA	P1A-O3A-P2A-O6A
3	B	402	COA	C5P-C6P-C7P-N8P
3	A	403	COA	P1A-O3A-P2A-O5A
3	B	402	COA	P1A-O3A-P2A-O5A
3	C	405	COA	O9P-C9P-CAP-OAP
3	A	403	COA	CDP-CBP-CCP-O6A
3	A	403	COA	CEP-CBP-CCP-O6A
3	D	402	COA	O4B-C4B-C5B-O5B
3	A	403	COA	CCP-O6A-P2A-O4A
3	B	402	COA	CCP-O6A-P2A-O3A
3	B	402	COA	CCP-O6A-P2A-O4A
3	D	402	COA	P2A-O3A-P1A-O1A
3	D	402	COA	O9P-C9P-CAP-CBP

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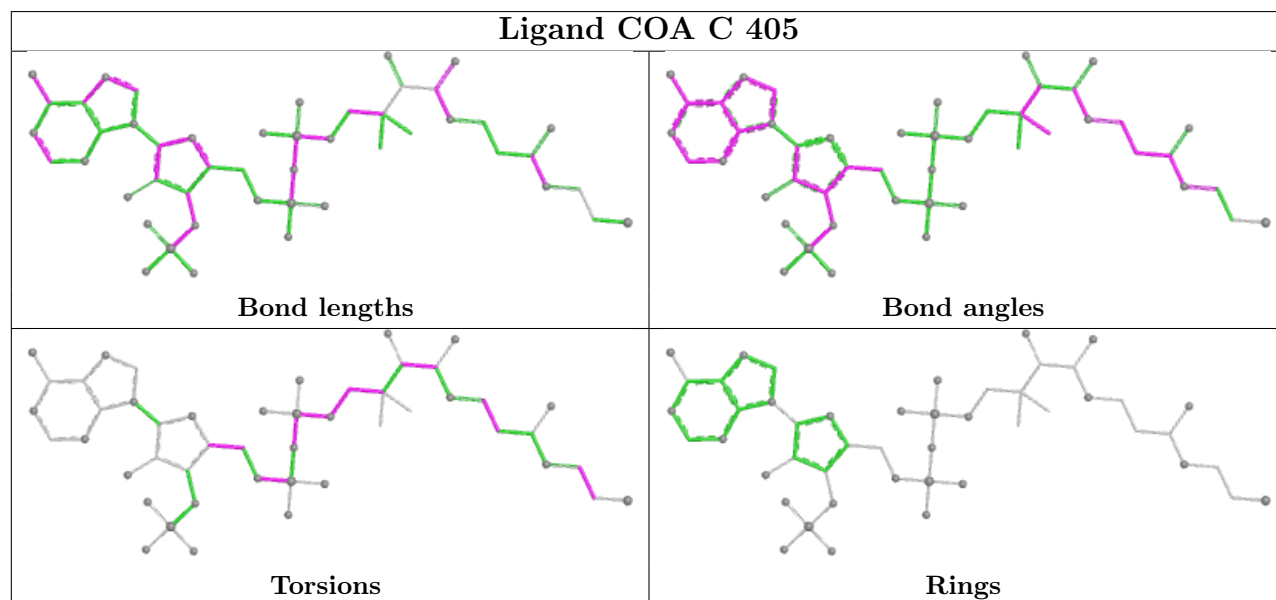
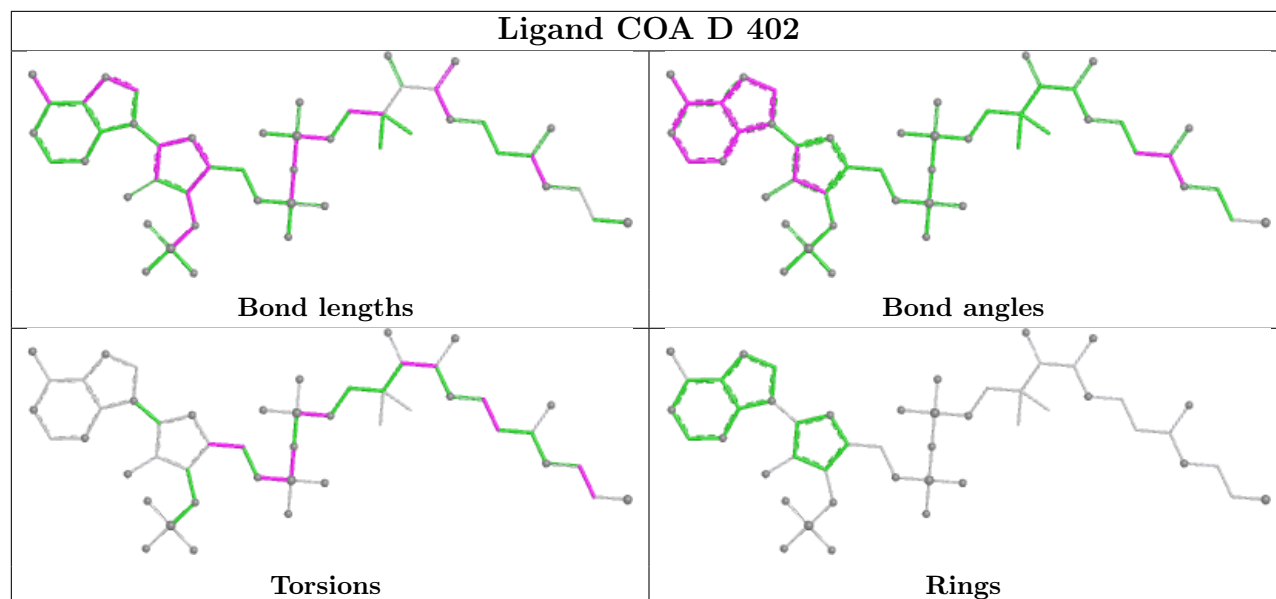
Mol	Chain	Res	Type	Atoms
3	D	402	COA	N8P-C9P-CAP-CBP
3	C	405	COA	N8P-C9P-CAP-OAP
3	B	402	COA	O5P-C5P-C6P-C7P
3	D	402	COA	P2A-O3A-P1A-O2A
3	C	405	COA	O9P-C9P-CAP-CBP
3	B	402	COA	CBP-CCP-O6A-P2A
3	B	402	COA	N4P-C5P-C6P-C7P

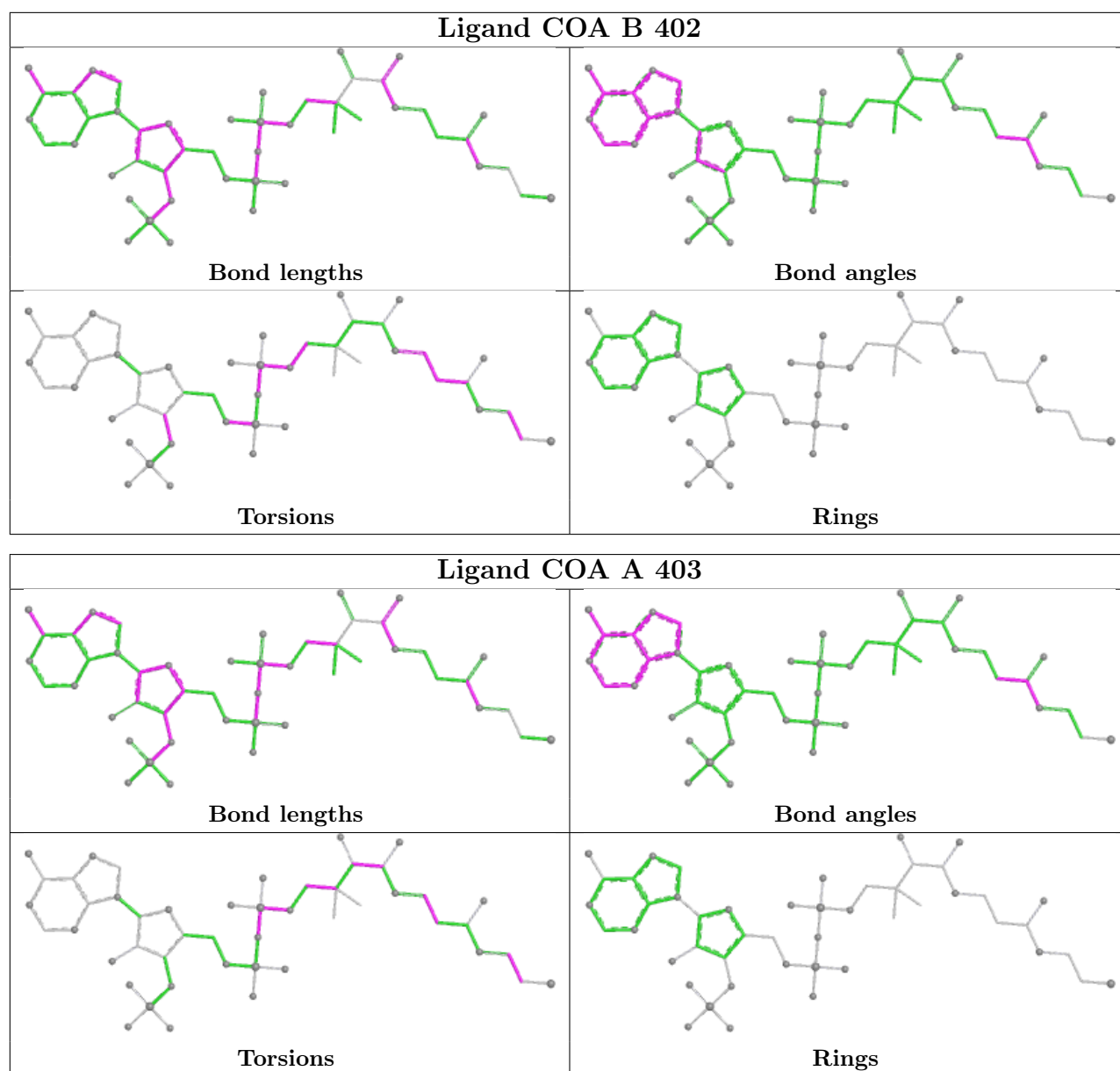
There are no ring outliers.

7 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	404	SO4	2	0
3	D	402	COA	9	0
3	C	405	COA	5	0
2	D	401	SO4	1	0
3	B	402	COA	5	0
3	A	403	COA	5	0
2	B	401	SO4	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 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	363/396 (91%)	0.05	13 (3%) 46 46	19, 29, 51, 84	0
1	B	376/396 (94%)	-0.12	9 (2%) 59 60	16, 28, 48, 78	1 (0%)
1	C	368/396 (92%)	0.09	13 (3%) 47 47	21, 31, 59, 92	0
1	D	375/396 (94%)	0.61	19 (5%) 33 32	25, 42, 72, 114	0
All	All	1482/1584 (93%)	0.16	54 (3%) 46 46	16, 32, 63, 114	1 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	199	TYR	6.4
1	D	259	TYR	5.7
1	B	259	TYR	5.5
1	D	199	TYR	5.3
1	C	259	TYR	5.0
1	B	199	TYR	5.0
1	B	202	LEU	4.8
1	A	282	THR	4.7
1	C	202	LEU	4.5
1	A	259	TYR	4.3
1	A	202	LEU	3.9
1	D	383	ILE	3.8
1	C	176	GLY	3.6
1	D	202	LEU	3.4
1	D	5	VAL	3.4
1	B	203	LEU	3.3
1	C	199	TYR	3.1
1	D	281	PHE	3.1
1	D	224	THR	3.0
1	D	225	THR	3.0
1	A	175	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	281	PHE	2.9
1	B	175	GLY	2.9
1	D	361	TRP	2.9
1	D	177	HIS	2.8
1	A	272	ASN	2.8
1	A	176	GLY	2.8
1	D	200	LEU	2.7
1	C	300	GLY	2.7
1	B	224	THR	2.6
1	D	198	THR	2.6
1	C	203	LEU	2.6
1	A	316	GLU	2.5
1	A	315	LYS	2.4
1	C	222	LEU	2.4
1	A	220	ALA	2.3
1	C	311	LEU	2.3
1	D	3	SER	2.3
1	D	175	GLY	2.3
1	C	224	THR	2.3
1	B	176	GLY	2.3
1	C	228	ARG	2.2
1	A	201	ASP	2.2
1	B	384	ASN	2.2
1	A	263	ARG	2.1
1	A	278	ARG	2.1
1	D	351	GLY	2.1
1	D	188	MET	2.1
1	C	175	GLY	2.1
1	C	261	LEU	2.1
1	D	226	THR	2.1
1	D	229	PRO	2.1
1	B	316	GLU	2.0
1	D	27	ALA	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 oligosaccharides in this entry.

6.4 Ligands

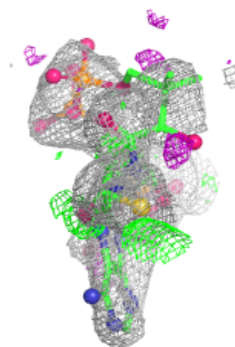
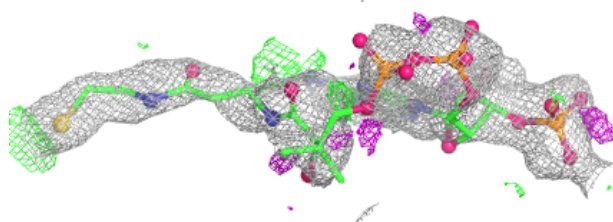
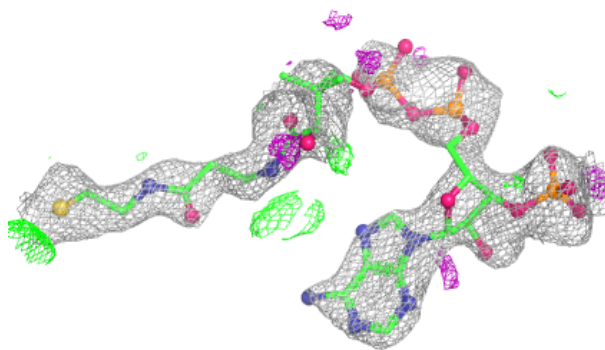
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	C	403	5/5	0.74	0.12	100,100,105,106	0
2	SO4	C	404	5/5	0.74	0.12	119,120,122,123	0
3	COA	D	402	48/48	0.78	0.16	72,105,116,116	0
2	SO4	C	402	5/5	0.80	0.16	70,73,77,79	0
3	COA	B	402	48/48	0.81	0.15	38,70,85,88	0
3	COA	C	405	48/48	0.83	0.16	44,71,91,97	0
3	COA	A	403	48/48	0.84	0.14	54,73,87,101	0
2	SO4	C	401	5/5	0.90	0.10	50,61,64,74	0
2	SO4	A	402	5/5	0.90	0.10	47,51,53,63	0
2	SO4	A	401	5/5	0.91	0.09	61,63,66,66	0
2	SO4	D	401	5/5	0.93	0.11	68,69,74,76	0
2	SO4	B	401	5/5	0.95	0.09	60,61,62,65	0

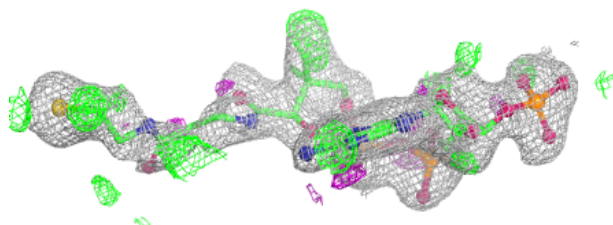
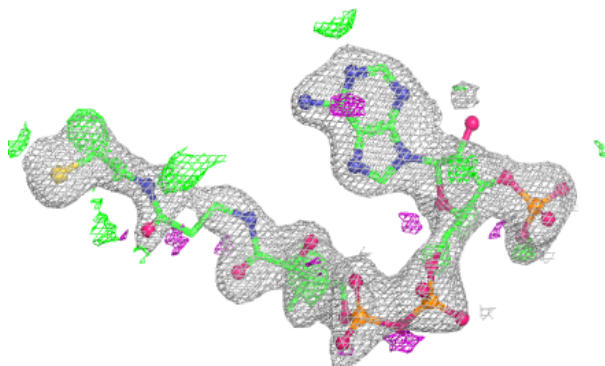
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around COA D 402:

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

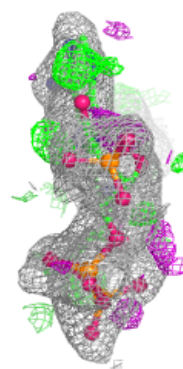
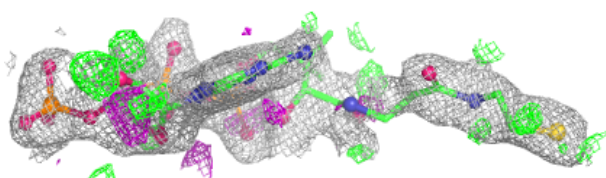
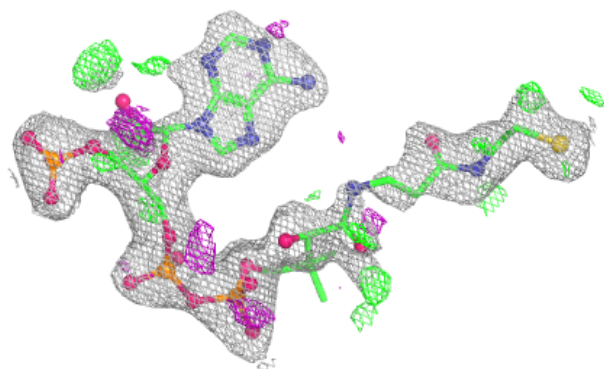
**Electron density around COA B 402:**

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

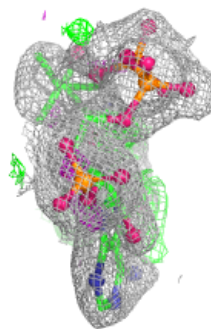
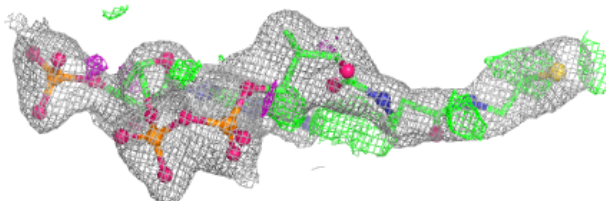
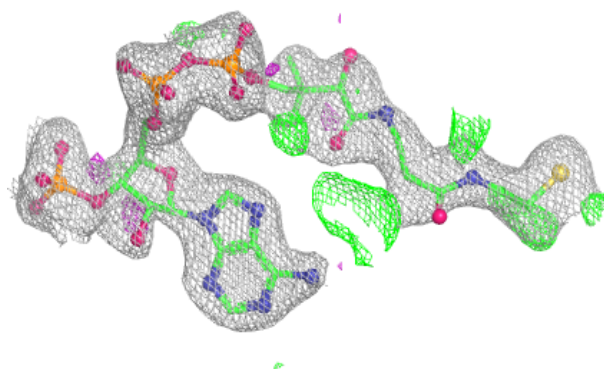


Electron density around COA C 405:

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

**Electron density around COA A 403:**

$2mF_o-DF_c$ (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.