



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 06:51 am BST

PDB ID : 2AHW
Title : Crystal Structure of Acyl-CoA transferase from E. coli O157:H7 (YdiF)-thioester complex with CoA- 2
Authors : Rangarajan, E.S.; Li, Y.; Ajamian, E.; Iannuzzi, P.; Kernaghan, S.D.; Fraser, M.E.; Cylger, M.; Matte, A.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on : 2005-07-28
Resolution : 2.15 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 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 : 2.11
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) : 2.11

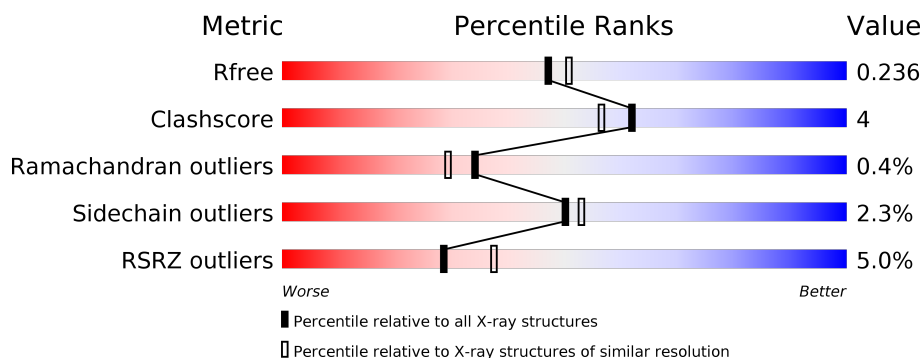
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 on 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	531	<div> <div>3%</div> <div>87%</div> <div>9%</div> <div>•</div> </div>
1	B	531	<div> <div>2%</div> <div>88%</div> <div>8%</div> <div>•</div> </div>
1	C	531	<div> <div>3%</div> <div>85%</div> <div>11%</div> <div>•</div> </div>
1	D	531	<div> <div>11%</div> <div>75%</div> <div>15%</div> <div>•</div> <div>8%</div> </div>

2 Entry composition [i](#)

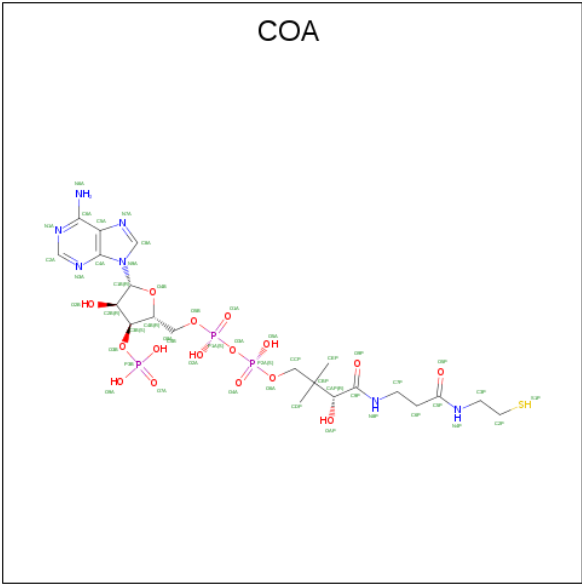
There are 3 unique types of molecules in this entry. The entry contains 16818 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 putative enzyme YdiF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			3905	2486	666	737	16			
1	B	512	Total	C	N	O	S	0	0	0
			3905	2486	666	737	16			
1	C	512	Total	C	N	O	S	0	0	0
			3905	2486	666	737	16			
1	D	487	Total	C	N	O	S	0	0	0
			3655	2323	625	692	15			

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



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		

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

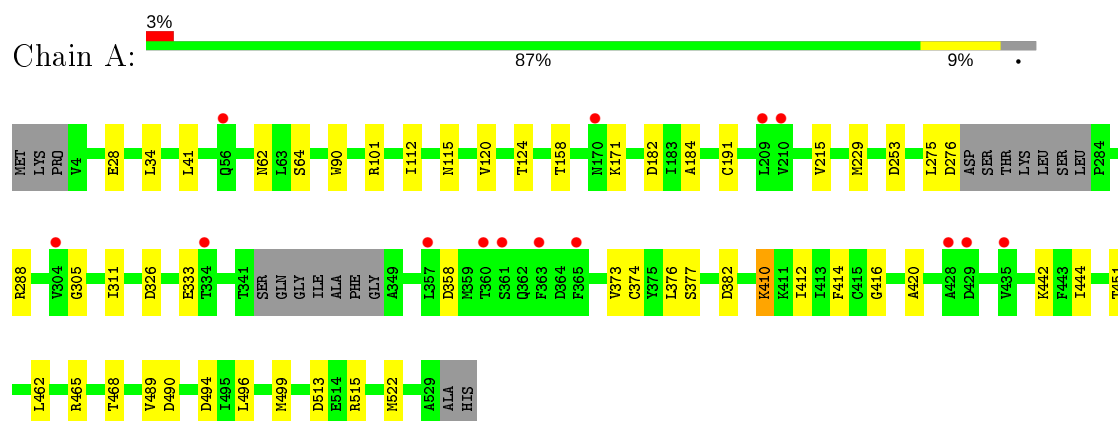
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	368	Total	O	0	0
			368	368		
3	B	341	Total	O	0	0
			341	341		
3	C	340	Total	O	0	0
			340	340		
3	D	255	Total	O	0	0
			255	255		

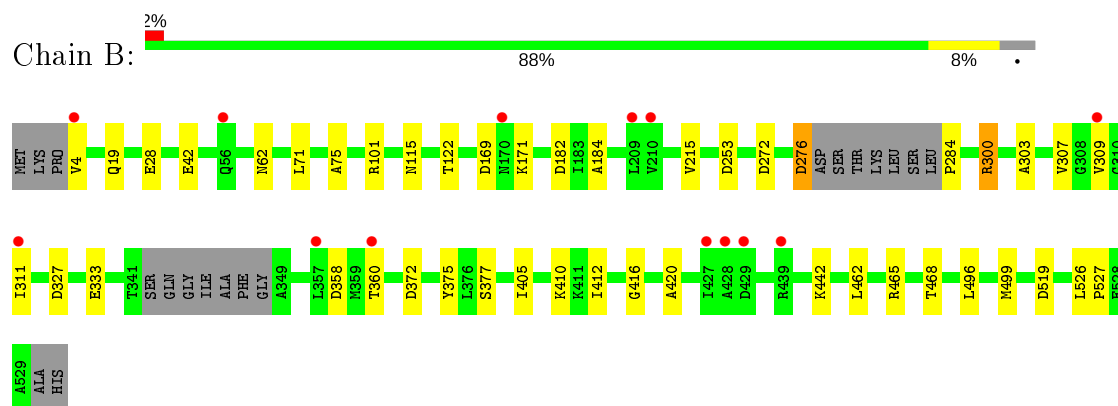
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

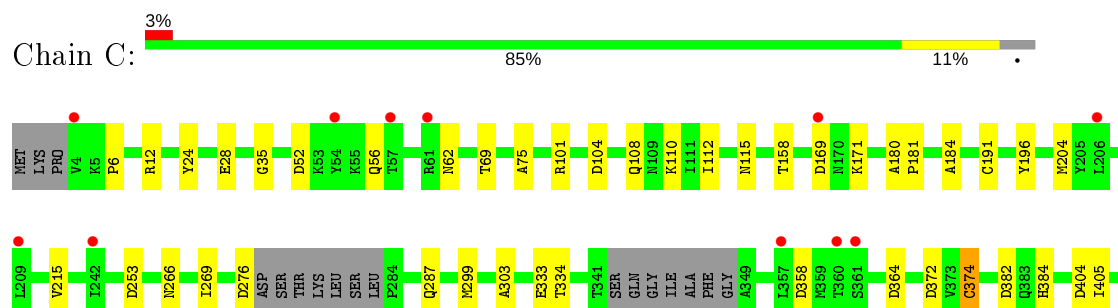
- Molecule 1: putative enzyme YdiF



- Molecule 1: putative enzyme YdiF

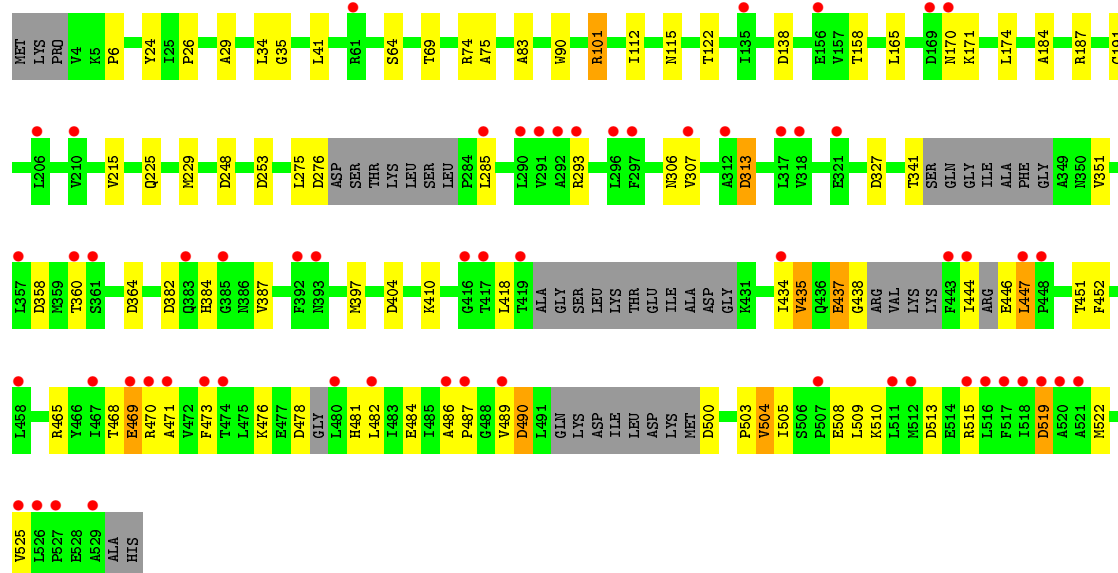
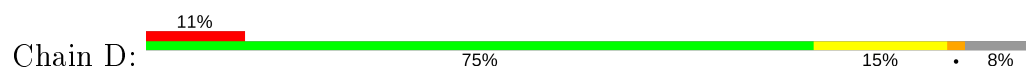


- Molecule 1: putative enzyme YdiF





- Molecule 1: putative enzyme YdiF



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.88Å 137.09Å 110.42Å 90.00° 105.83° 90.00°	Depositor
Resolution (Å)	50.00 – 2.15 43.33 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.15) 98.6 (43.33-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.186 , 0.235 0.186 , 0.236	Depositor DCC
R_{free} test set	11494 reflections (8.66%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16818	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: 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	0.54	0/3971	0.77	8/5375 (0.1%)
1	B	0.53	0/3971	0.78	8/5375 (0.1%)
1	C	0.49	0/3971	0.77	13/5375 (0.2%)
1	D	0.46	0/3715	0.75	10/5034 (0.2%)
All	All	0.51	0/15628	0.77	39/21159 (0.2%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	276	ASP	CB-CG-OD2	7.98	125.48	118.30
1	D	276	ASP	CB-CG-OD2	6.70	124.33	118.30
1	A	276	ASP	CB-CG-OD2	6.67	124.30	118.30
1	B	276	ASP	CB-CG-OD2	6.18	123.86	118.30
1	C	372	ASP	CB-CG-OD2	6.05	123.75	118.30
1	D	248	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	182	ASP	CB-CG-OD2	5.95	123.65	118.30
1	A	326	ASP	CB-CG-OD2	5.94	123.64	118.30
1	C	253	ASP	CB-CG-OD2	5.70	123.43	118.30
1	B	519	ASP	CB-CG-OD2	5.67	123.40	118.30
1	C	169	ASP	CB-CG-OD2	5.65	123.39	118.30
1	C	429	ASP	CB-CG-OD2	5.64	123.38	118.30
1	D	404	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	358	ASP	CB-CG-OD2	5.61	123.35	118.30
1	D	138	ASP	CB-CG-OD2	5.61	123.35	118.30
1	D	358	ASP	CB-CG-OD2	5.57	123.32	118.30
1	B	358	ASP	CB-CG-OD2	5.55	123.30	118.30
1	D	364	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	494	ASP	CB-CG-OD2	5.46	123.21	118.30
1	C	404	ASP	CB-CG-OD2	5.45	123.20	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	182	ASP	CB-CG-OD2	5.44	123.19	118.30
1	C	364	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	358	ASP	CB-CG-OD2	5.37	123.14	118.30
1	B	169	ASP	CB-CG-OD2	5.35	123.12	118.30
1	B	253	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	478	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	494	ASP	CB-CG-OD2	5.27	123.05	118.30
1	D	490	ASP	CB-CG-OD2	5.26	123.03	118.30
1	C	52	ASP	CB-CG-OD2	5.24	123.02	118.30
1	C	104	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	490	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	272	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	490	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	327	ASP	CB-CG-OD2	5.10	122.89	118.30
1	D	253	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	253	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	519	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	513	ASP	CB-CG-OD2	5.04	122.83	118.30
1	B	327	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3905	0	3963	20	0
1	B	3905	0	3963	22	0
1	C	3905	0	3963	27	0
1	D	3655	0	3623	70	0
2	A	48	0	31	1	0
2	B	48	0	31	2	0
2	C	48	0	31	0	0
3	A	368	0	0	1	0
3	B	341	0	0	2	0
3	C	340	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	255	0	0	1	0
All	All	16818	0	15605	138	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 (138) 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:D:476:LYS:HG3	1:D:481:HIS:CD2	1.58	1.39
1:D:418:LEU:HD13	1:D:470:ARG:HD2	1.39	1.03
1:C:495:ILE:HG22	1:C:499:MET:CE	1.91	1.00
1:D:444:ILE:HD11	1:D:447:LEU:HD12	1.46	0.98
1:D:437:GLU:HG3	1:D:438:GLY:H	1.27	0.96
1:D:476:LYS:CG	1:D:481:HIS:CD2	2.49	0.93
1:C:495:ILE:HG22	1:C:499:MET:HE2	1.49	0.92
1:D:285:LEU:CD1	1:D:293:ARG:NH1	2.38	0.86
1:D:437:GLU:HG3	1:D:438:GLY:N	1.91	0.84
1:D:504:VAL:HG12	1:D:505:ILE:N	1.91	0.83
1:D:470:ARG:O	1:D:486:ALA:N	2.13	0.81
1:A:410:LYS:N	1:A:410:LYS:HD2	1.93	0.80
1:C:495:ILE:CG2	1:C:499:MET:HE2	2.13	0.77
1:D:503:PRO:O	1:D:504:VAL:O	2.03	0.75
1:D:473:PHE:CE1	1:D:482:LEU:HD12	2.23	0.74
1:C:28:GLU:HA	1:C:62:ASN:O	1.87	0.74
1:D:468:THR:HG22	1:D:469:GLU:HG3	1.72	0.70
1:D:470:ARG:HA	1:D:486:ALA:HB2	1.73	0.70
1:C:416:GLY:O	1:C:468:THR:HA	1.92	0.70
1:D:184:ALA:HB2	1:D:215:VAL:HG21	1.72	0.70
1:D:504:VAL:HG12	1:D:505:ILE:H	1.55	0.69
1:D:285:LEU:HD13	1:D:293:ARG:NH1	2.07	0.69
1:D:285:LEU:HB2	1:D:519:ASP:OD1	1.92	0.69
1:D:293:ARG:HG2	1:D:522:MET:HE1	1.75	0.69
1:D:504:VAL:CG1	1:D:505:ILE:N	2.56	0.68
1:D:418:LEU:HD13	1:D:470:ARG:CD	2.22	0.66
1:C:495:ILE:CG2	1:C:499:MET:CE	2.70	0.65
1:D:293:ARG:NE	1:D:522:MET:HE2	2.12	0.65
1:D:504:VAL:CG1	1:D:505:ILE:H	2.08	0.65
1:C:108:GLN:HB3	1:C:110:LYS:HE3	1.79	0.64
1:D:418:LEU:HB2	1:D:468:THR:HG21	1.80	0.64
1:B:300:ARG:HD3	3:B:2822:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:476:LYS:HG3	1:D:481:HIS:CG	2.28	0.64
1:C:184:ALA:HB2	1:C:215:VAL:HG21	1.78	0.64
1:B:284:PRO:HD3	3:B:2878:HOH:O	1.97	0.63
1:D:478:ASP:OD2	1:D:504:VAL:HG21	2.00	0.62
1:D:382:ASP:HB3	1:D:447:LEU:HD13	1.81	0.61
1:D:285:LEU:HD13	1:D:293:ARG:HH12	1.66	0.60
1:D:293:ARG:HG2	1:D:522:MET:CE	2.31	0.60
1:A:416:GLY:O	1:A:468:THR:HA	2.01	0.59
1:D:285:LEU:HD11	1:D:293:ARG:NH1	2.16	0.59
1:B:496:LEU:HA	1:B:499:MET:HE2	1.86	0.58
1:B:300:ARG:HG3	1:B:303:ALA:HB2	1.86	0.57
1:D:508:GLU:O	1:D:509:LEU:C	2.42	0.57
1:B:412:ILE:HD11	1:B:462:LEU:HD13	1.85	0.56
1:D:437:GLU:CG	1:D:438:GLY:H	2.10	0.56
1:A:112:ILE:HG23	1:A:158:THR:HG23	1.88	0.55
1:D:285:LEU:CB	1:D:519:ASP:OD1	2.54	0.55
1:B:372:ASP:HA	1:B:410:LYS:HD3	1.89	0.55
1:B:496:LEU:HD23	1:B:499:MET:HE1	1.87	0.55
1:C:374:CYS:SG	1:C:405:ILE:HG22	2.47	0.54
1:D:503:PRO:C	1:D:504:VAL:O	2.43	0.54
1:D:470:ARG:HA	1:D:486:ALA:CB	2.37	0.54
1:C:495:ILE:HG22	1:C:499:MET:HE1	1.87	0.54
1:D:476:LYS:HG3	1:D:481:HIS:NE2	2.18	0.54
1:D:74:ARG:HH22	1:D:397:MET:HE1	1.72	0.53
1:A:34:LEU:HD21	1:A:41:LEU:HD13	1.90	0.53
1:A:377:SER:HB3	2:A:2600:COA:H122	1.92	0.52
1:D:444:ILE:HD12	1:D:446:GLU:O	2.10	0.52
1:A:120:VAL:O	1:A:124:THR:HG23	2.11	0.51
1:D:503:PRO:O	1:D:504:VAL:C	2.49	0.51
1:D:468:THR:HG22	1:D:469:GLU:N	2.27	0.50
1:C:444:ILE:HA	1:C:500:ASP:HB2	1.94	0.50
1:D:112:ILE:HG23	1:D:158:THR:HG23	1.94	0.50
1:A:496:LEU:HA	1:A:499:MET:HE2	1.93	0.49
1:D:473:PHE:CE1	1:D:482:LEU:CD1	2.95	0.49
1:D:515:ARG:HD2	1:D:522:MET:O	2.12	0.49
1:D:478:ASP:OD2	1:D:481:HIS:NE2	2.45	0.49
1:A:28:GLU:HA	1:A:62:ASN:O	2.13	0.48
1:D:490:ASP:HA	3:D:661:HOH:O	2.12	0.48
1:D:26:PRO:HD2	1:D:29:ALA:HB2	1.94	0.48
1:D:74:ARG:HH22	1:D:397:MET:CE	2.26	0.48
1:B:416:GLY:O	1:B:468:THR:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:ALA:HB2	1:B:442:LYS:HD2	1.96	0.47
1:D:122:THR:HG23	1:D:360:THR:HG23	1.96	0.47
1:D:165:LEU:HD12	1:D:174:LEU:HD23	1.97	0.47
1:C:112:ILE:HG23	1:C:158:THR:HG23	1.97	0.46
1:A:382:ASP:HA	1:A:444:ILE:O	2.16	0.46
1:C:489:VAL:HG13	1:C:494:ASP:HB2	1.97	0.46
1:C:424:LYS:HB2	1:C:436:GLN:HB3	1.97	0.46
1:C:204:MET:SD	1:C:334:THR:HB	2.56	0.45
1:C:384:HIS:NE2	1:C:446:GLU:OE2	2.49	0.45
1:D:484:GLU:HA	1:D:510:LYS:O	2.16	0.45
1:B:333:GLU:HG2	1:B:405:ILE:HD11	1.98	0.45
1:B:276:ASP:OD1	1:C:12:ARG:NH2	2.45	0.45
1:B:122:THR:HG23	1:B:360:THR:HG23	1.98	0.45
1:D:468:THR:HB	1:D:471:ALA:O	2.16	0.45
1:A:305:GLY:HA2	1:A:373:VAL:O	2.16	0.44
1:A:288:ARG:HG2	1:A:311:ILE:HG13	1.99	0.44
1:D:285:LEU:HD11	1:D:293:ARG:HH11	1.81	0.44
1:C:432:LEU:HD23	1:C:489:VAL:HG21	1.99	0.44
1:D:293:ARG:CG	1:D:522:MET:HE1	2.45	0.44
1:D:444:ILE:HA	1:D:500:ASP:HB2	1.99	0.44
1:B:377:SER:HB3	2:B:2600:COA:H122	2.00	0.44
1:B:307:VAL:HG12	1:B:375:TYR:CD2	2.53	0.43
1:D:191:CYS:O	1:D:229:MET:HA	2.17	0.43
1:A:412:ILE:HD11	1:A:462:LEU:HD13	1.99	0.43
1:A:420:ALA:HB2	1:A:442:LYS:HD2	1.99	0.43
1:C:382:ASP:HA	1:C:444:ILE:O	2.18	0.43
1:A:64:SER:HB3	1:A:90:TRP:CE3	2.53	0.43
1:D:275:LEU:HD22	1:D:351:VAL:HG21	2.00	0.43
1:D:486:ALA:HB3	1:D:489:VAL:HG21	2.01	0.43
1:D:187:ARG:HA	1:D:225:GLN:O	2.18	0.43
1:A:184:ALA:HB2	1:A:215:VAL:HG21	2.01	0.43
1:C:266:ASN:HB3	1:C:269:ILE:HD12	2.00	0.43
1:D:83:ALA:HB3	1:D:101:ARG:HB3	2.01	0.42
1:C:299:MET:SD	1:C:303:ALA:HB3	2.59	0.42
1:D:486:ALA:HA	1:D:487:PRO:HD3	1.81	0.42
1:D:387:VAL:HB	1:D:452:PHE:HB3	2.01	0.42
1:B:19:GLN:H	1:B:19:GLN:CD	2.23	0.42
1:B:184:ALA:HB2	1:B:215:VAL:HG21	2.00	0.42
1:B:333:GLU:HG3	1:B:333:GLU:H	1.47	0.42
1:B:405:ILE:CD1	2:B:2600:COA:S1P	3.08	0.42
1:D:34:LEU:HD21	1:D:41:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ALA:HA	1:C:181:PRO:HD3	1.81	0.42
1:D:307:VAL:CG1	1:D:313:ASP:HA	2.49	0.42
1:B:42:GLU:HG3	1:B:71:LEU:HD23	2.02	0.42
1:C:6:PRO:HD3	1:C:24:TYR:CE1	2.55	0.42
1:D:83:ALA:CB	1:D:101:ARG:HB3	2.50	0.42
1:D:35:GLY:O	1:D:69:THR:CG2	2.67	0.41
1:D:293:ARG:HE	1:D:522:MET:HE2	1.80	0.41
1:D:384:HIS:NE2	1:D:446:GLU:OE2	2.53	0.41
1:D:434:ILE:O	1:D:435:VAL:O	2.39	0.41
1:A:191:CYS:O	1:A:229:MET:HA	2.20	0.41
1:A:410:LYS:HE3	3:A:2785:HOH:O	2.20	0.41
1:A:515:ARG:HD2	1:A:522:MET:O	2.20	0.41
1:D:64:SER:HB3	1:D:90:TRP:CE3	2.56	0.41
1:B:311:ILE:HG21	1:B:416:GLY:HA2	2.01	0.41
1:C:333:GLU:HG3	3:C:2673:HOH:O	2.20	0.41
1:C:287:GLN:HE21	1:C:287:GLN:HB3	1.66	0.41
1:D:6:PRO:HD3	1:D:24:TYR:CE1	2.56	0.41
1:D:35:GLY:O	1:D:69:THR:HG23	2.20	0.41
1:B:28:GLU:HA	1:B:62:ASN:O	2.20	0.41
1:C:35:GLY:O	1:C:69:THR:HG22	2.21	0.41
1:B:526:LEU:HA	1:B:527:PRO:HD3	1.95	0.40
1:C:191:CYS:HA	1:C:196:TYR:O	2.21	0.40
1:A:376:LEU:O	1:A:414:PHE:HA	2.21	0.40
1:A:333:GLU:HG3	1:A:333:GLU:H	1.61	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	506/531 (95%)	487 (96%)	19 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	506/531 (95%)	491 (97%)	14 (3%)	1 (0%)	47	46
1	C	506/531 (95%)	491 (97%)	14 (3%)	1 (0%)	47	46
1	D	471/531 (89%)	446 (95%)	20 (4%)	5 (1%)	14	8
All	All	1989/2124 (94%)	1915 (96%)	67 (3%)	7 (0%)	34	29

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	435	VAL
1	D	504	VAL
1	D	437	GLU
1	D	75	ALA
1	D	313	ASP
1	B	75	ALA
1	C	75	ALA

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	416/431 (96%)	407 (98%)	9 (2%)	52	55
1	B	416/431 (96%)	409 (98%)	7 (2%)	60	65
1	C	416/431 (96%)	407 (98%)	9 (2%)	52	55
1	D	379/431 (88%)	366 (97%)	13 (3%)	37	35
All	All	1627/1724 (94%)	1589 (98%)	38 (2%)	50	53

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	ARG
1	A	115	ASN
1	A	171	LYS
1	A	275	LEU

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Mol	Chain	Res	Type
1	A	374	CYS
1	A	410	LYS
1	A	451	THR
1	A	465	ARG
1	A	489	VAL
1	B	4	VAL
1	B	101	ARG
1	B	115	ASN
1	B	171	LYS
1	B	300	ARG
1	B	309	VAL
1	B	465	ARG
1	C	56	GLN
1	C	101	ARG
1	C	115	ASN
1	C	171	LYS
1	C	374	CYS
1	C	410	LYS
1	C	451	THR
1	C	465	ARG
1	C	525	VAL
1	D	101	ARG
1	D	115	ASN
1	D	170	ASN
1	D	171	LYS
1	D	306	ASN
1	D	341	THR
1	D	410	LYS
1	D	447	LEU
1	D	451	THR
1	D	465	ARG
1	D	469	GLU
1	D	513	ASP
1	D	525	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	GLN
1	A	350	ASN
1	B	287	GLN
1	B	306	ASN

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Mol	Chain	Res	Type
1	B	350	ASN
1	C	287	GLN
1	C	350	ASN
1	C	436	GLN
1	D	287	GLN
1	D	350	ASN
1	D	383	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

3 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	A	2600	1	41,50,50	0.90	2 (4%)	52,75,75	1.18	4 (7%)
2	COA	B	2600	1	41,50,50	0.90	2 (4%)	52,75,75	1.09	3 (5%)
2	COA	C	2600	1	41,50,50	0.84	1 (2%)	52,75,75	1.18	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	A	2600	1	-	5/44/64/64	0/3/3/3
2	COA	B	2600	1	-	10/44/64/64	0/3/3/3
2	COA	C	2600	1	-	7/44/64/64	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2600	COA	C5A-C4A	2.65	1.47	1.40
2	B	2600	COA	C5A-C4A	2.58	1.47	1.40
2	C	2600	COA	C5A-C4A	2.50	1.47	1.40
2	A	2600	COA	O4B-C1B	2.23	1.44	1.41
2	B	2600	COA	O4B-C1B	2.02	1.43	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2600	COA	N3A-C2A-N1A	-3.96	122.49	128.68
2	B	2600	COA	N3A-C2A-N1A	-3.54	123.14	128.68
2	A	2600	COA	N3A-C2A-N1A	-3.30	123.52	128.68
2	A	2600	COA	O6A-CCP-CBP	3.27	115.80	110.55
2	A	2600	COA	P2A-O3A-P1A	-3.15	122.01	132.83
2	A	2600	COA	C4A-C5A-N7A	-2.79	106.49	109.40
2	C	2600	COA	C4A-C5A-N7A	-2.66	106.63	109.40
2	B	2600	COA	C4A-C5A-N7A	-2.58	106.71	109.40
2	C	2600	COA	C2A-N1A-C6A	2.31	122.71	118.75
2	C	2600	COA	O6A-CCP-CBP	2.23	114.14	110.55
2	B	2600	COA	P2A-O3A-P1A	-2.08	125.68	132.83

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2600	COA	C5B-O5B-P1A-O1A
2	B	2600	COA	C5B-O5B-P1A-O1A
2	B	2600	COA	OAP-CAP-CBP-CCP
2	B	2600	COA	C9P-CAP-CBP-CCP
2	B	2600	COA	OAP-CAP-CBP-CDP
2	B	2600	COA	C9P-CAP-CBP-CDP
2	C	2600	COA	C5B-O5B-P1A-O1A

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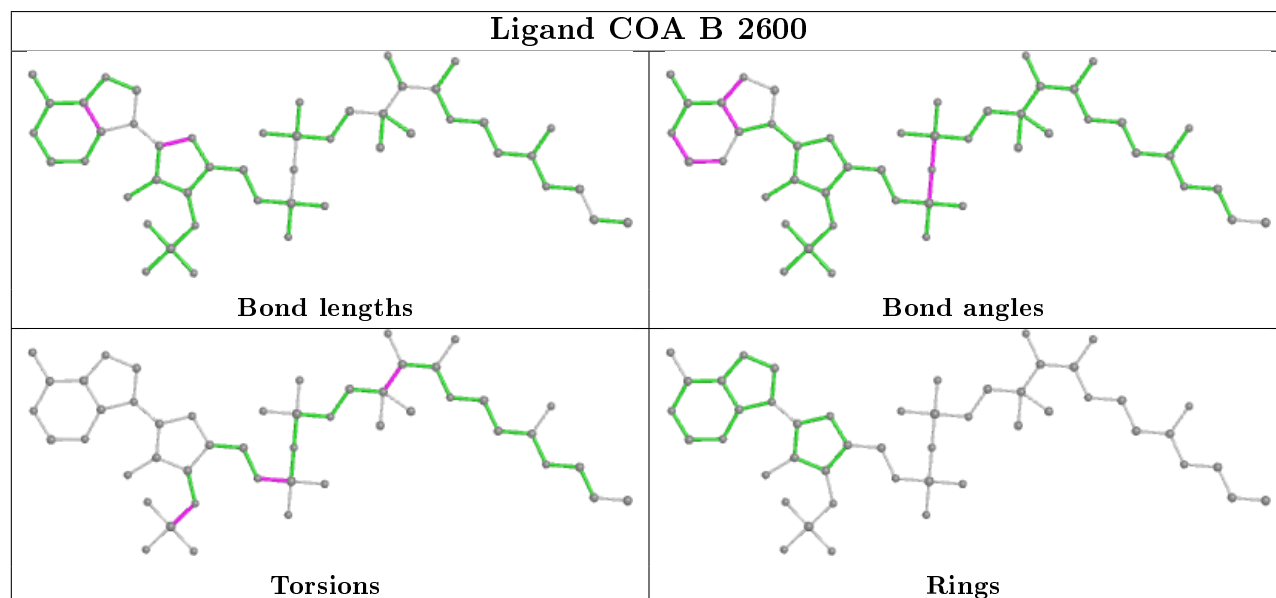
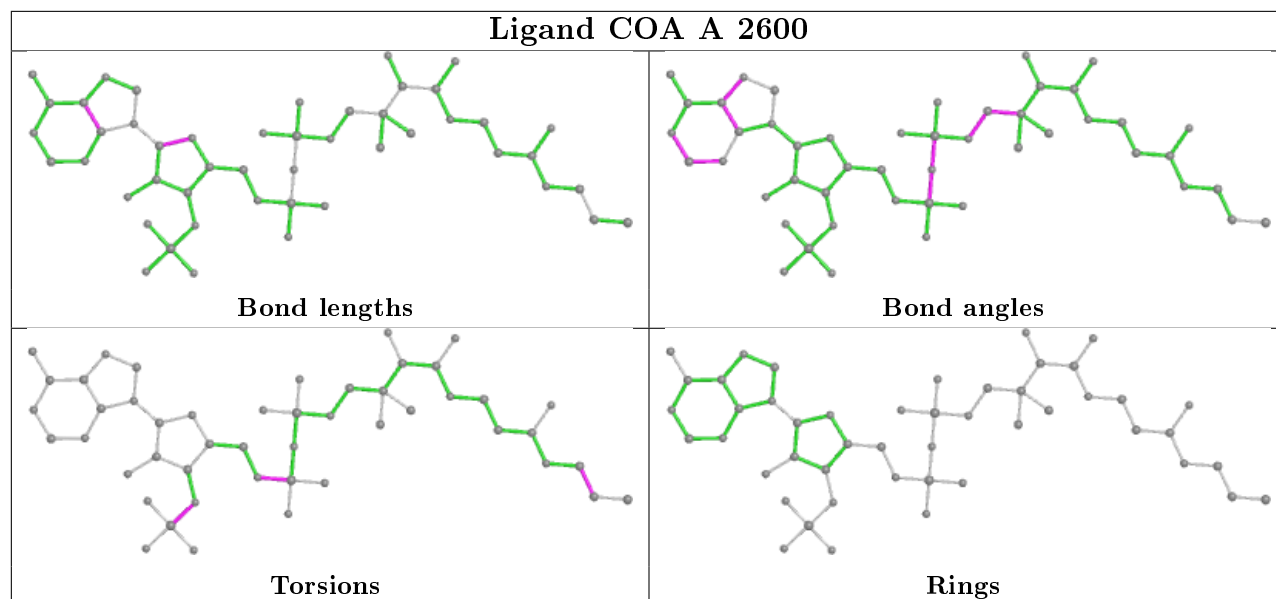
Mol	Chain	Res	Type	Atoms
2	C	2600	COA	OAP-CAP-CBP-CCP
2	C	2600	COA	OAP-CAP-CBP-CDP
2	C	2600	COA	S1P-C2P-C3P-N4P
2	B	2600	COA	OAP-CAP-CBP-CEP
2	C	2600	COA	OAP-CAP-CBP-CEP
2	A	2600	COA	S1P-C2P-C3P-N4P
2	B	2600	COA	C5B-O5B-P1A-O3A
2	A	2600	COA	C5B-O5B-P1A-O2A
2	B	2600	COA	C5B-O5B-P1A-O2A
2	C	2600	COA	C5B-O5B-P1A-O2A
2	B	2600	COA	C9P-CAP-CBP-CEP
2	A	2600	COA	C3B-O3B-P3B-O8A
2	A	2600	COA	C5B-O5B-P1A-O3A
2	B	2600	COA	C3B-O3B-P3B-O8A
2	C	2600	COA	C5B-O5B-P1A-O3A

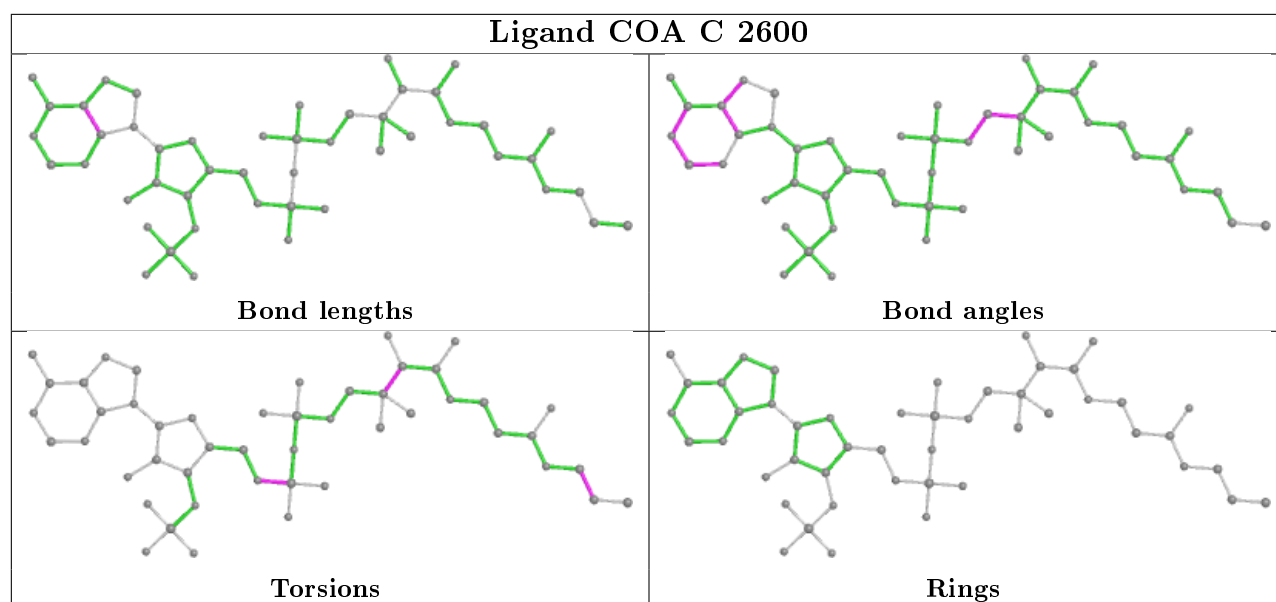
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2600	COA	1	0
2	B	2600	COA	2	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	512/531 (96%)	0.02	14 (2%) 54 63	20, 30, 46, 54	0
1	B	512/531 (96%)	-0.02	13 (2%) 57 65	20, 32, 47, 57	0
1	C	512/531 (96%)	0.14	14 (2%) 54 63	23, 36, 49, 57	0
1	D	487/531 (91%)	0.51	60 (12%) 4 5	21, 40, 59, 64	81 (16%)
All	All	2023/2124 (95%)	0.16	101 (4%) 28 37	20, 34, 52, 64	81 (4%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	489	VAL	7.2
1	D	290	LEU	7.0
1	D	480	LEU	5.1
1	D	516	LEU	4.6
1	D	297	PHE	4.6
1	D	521	ALA	4.2
1	C	429	ASP	4.2
1	D	529	ALA	4.1
1	D	318	VAL	3.9
1	B	428	ALA	3.7
1	D	392	PHE	3.7
1	D	486	ALA	3.6
1	D	467	ILE	3.6
1	D	518	ILE	3.4
1	D	285	LEU	3.4
1	C	4	VAL	3.4
1	D	517	PHE	3.3
1	B	429	ASP	3.3
1	D	511	LEU	3.3
1	D	385	GLY	3.3
1	D	473	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	357	LEU	3.2
1	A	361	SER	3.2
1	D	482	LEU	3.2
1	D	170	ASN	3.1
1	C	61	ARG	3.1
1	D	416	GLY	3.1
1	D	487	PRO	3.1
1	D	443	PHE	3.1
1	A	429	ASP	3.0
1	D	321	GLU	3.0
1	D	512	MET	3.0
1	A	365	PHE	2.9
1	C	360	THR	2.8
1	B	4	VAL	2.8
1	D	447	LEU	2.8
1	A	428	ALA	2.8
1	D	383	GLN	2.7
1	C	357	LEU	2.7
1	D	206	LEU	2.7
1	C	426	GLU	2.7
1	A	56	GLN	2.7
1	B	170	ASN	2.7
1	D	470	ARG	2.6
1	B	309	VAL	2.6
1	C	361	SER	2.6
1	B	357	LEU	2.5
1	D	291	VAL	2.5
1	C	508	GLU	2.5
1	D	156	GLU	2.5
1	D	520	ALA	2.5
1	A	360	THR	2.4
1	D	393	ASN	2.4
1	D	292	ALA	2.4
1	B	210	VAL	2.4
1	C	54	TYR	2.4
1	A	435	VAL	2.4
1	D	210	VAL	2.4
1	A	170	ASN	2.4
1	A	209	LEU	2.4
1	D	61	ARG	2.4
1	D	474	THR	2.4
1	D	169	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	519	ASP	2.3
1	D	357	LEU	2.3
1	D	360	THR	2.3
1	C	209	LEU	2.3
1	A	334	THR	2.3
1	D	293	ARG	2.3
1	B	209	LEU	2.3
1	D	444	ILE	2.3
1	D	469	GLU	2.3
1	B	56	GLN	2.2
1	D	458	LEU	2.2
1	A	210	VAL	2.2
1	D	526	LEU	2.2
1	D	515	ARG	2.2
1	D	471	ALA	2.2
1	C	57	THR	2.2
1	D	507	PRO	2.1
1	D	448	PRO	2.1
1	D	525	VAL	2.1
1	B	360	THR	2.1
1	D	419	THR	2.1
1	B	311	ILE	2.1
1	D	135	ILE	2.1
1	D	317	LEU	2.1
1	D	361	SER	2.1
1	A	363	PHE	2.1
1	D	527	PRO	2.1
1	D	417	THR	2.1
1	C	169	ASP	2.1
1	D	296	LEU	2.0
1	B	439	ARG	2.0
1	D	434	ILE	2.0
1	D	312	ALA	2.0
1	A	304	VAL	2.0
1	D	307	VAL	2.0
1	B	427	ILE	2.0
1	C	206	LEU	2.0
1	C	242	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

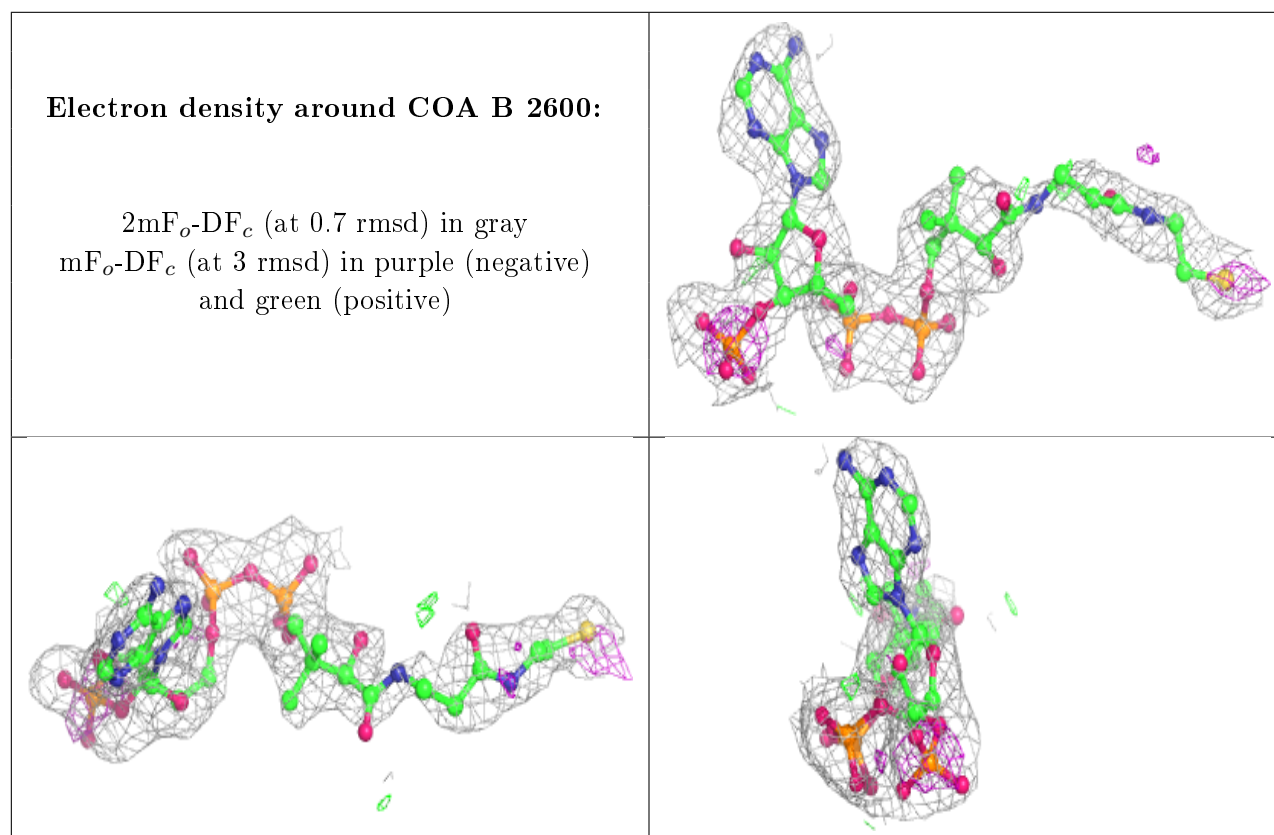
There are no carbohydrates in this entry.

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.

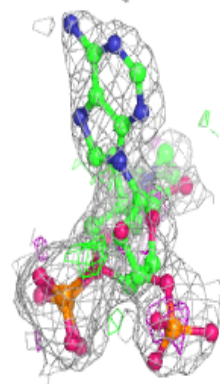
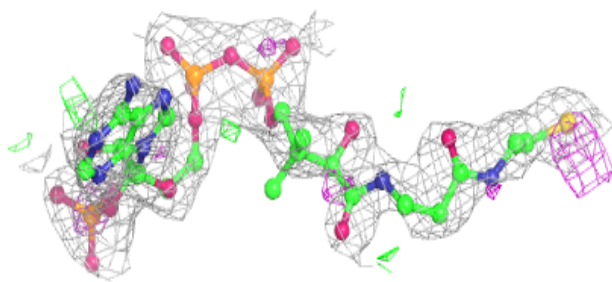
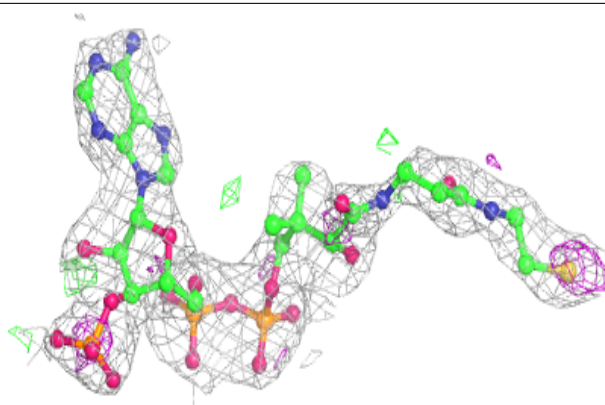
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	COA	B	2600	48/48	0.86	0.18	53,66,76,77	0
2	COA	A	2600	48/48	0.89	0.18	51,62,72,72	0
2	COA	C	2600	48/48	0.93	0.12	43,48,57,58	0

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.

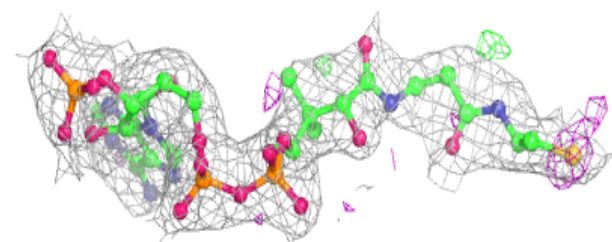
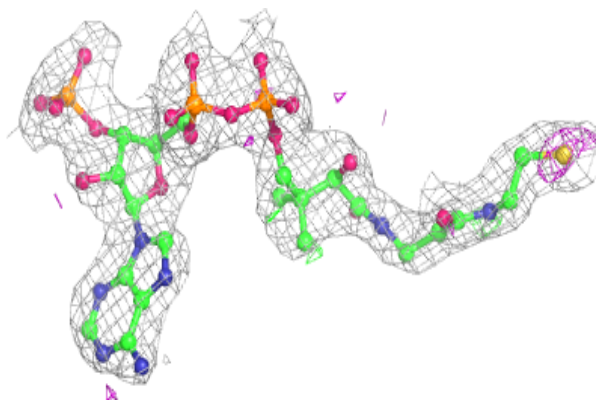


Electron density around COA A 2600:

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

**Electron density around COA C 2600:**

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



6.5 Other polymers

There are no such residues in this entry.