



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:55 PM UTC

PDB ID : 1EBL / pdb_00001ebl
Title : THE 1.8 Å CRYSTAL STRUCTURE AND ACTIVE SITE ARCHITECTURE OF BETA-KETOACYL-[ACYL CARRIER PROTEIN] SYNTHASE III (FABH) FROM ESCHERICHIA COLI
Authors : Davies, C.; Heath, R.J.; White, S.W.; Rock, C.O.
Deposited on : 2000-01-24
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

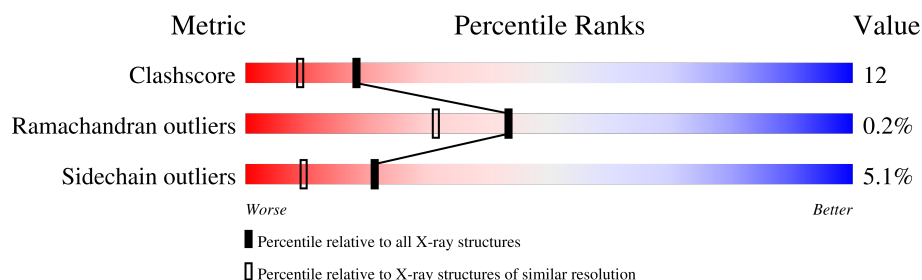
1 Overall quality at a glance

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))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	317	 80% 15% . .
1	B	317	 80% 16% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5502 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.

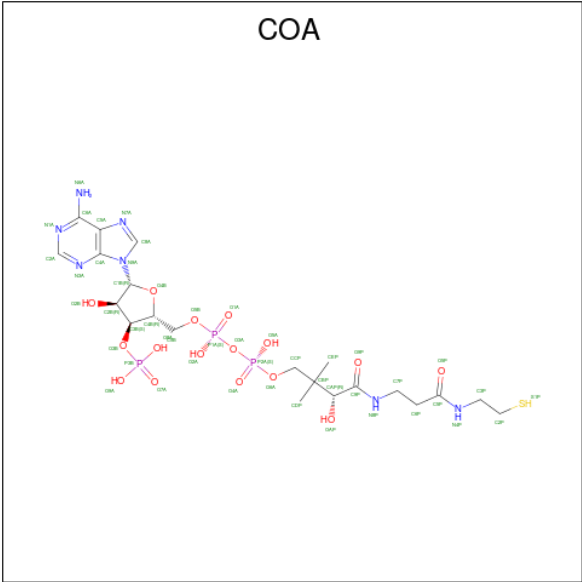
- Molecule 1 is a protein called BETA-KETOACYL-ACP SYNTHASE III.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	Se	0	0	0
			2351	1470	408	460	5	8			
1	B	317	Total	C	N	O	S	Se	0	0	0
			2351	1470	408	460	5	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P0A6R0
A	25	MSE	MET	modified residue	UNP P0A6R0
A	54	MSE	MET	modified residue	UNP P0A6R0
A	65	MSE	MET	modified residue	UNP P0A6R0
A	97	MSE	MET	modified residue	UNP P0A6R0
A	207	MSE	MET	modified residue	UNP P0A6R0
A	260	MSE	MET	modified residue	UNP P0A6R0
A	262	MSE	MET	modified residue	UNP P0A6R0
B	1	MSE	MET	modified residue	UNP P0A6R0
B	25	MSE	MET	modified residue	UNP P0A6R0
B	54	MSE	MET	modified residue	UNP P0A6R0
B	65	MSE	MET	modified residue	UNP P0A6R0
B	97	MSE	MET	modified residue	UNP P0A6R0
B	207	MSE	MET	modified residue	UNP P0A6R0
B	260	MSE	MET	modified residue	UNP P0A6R0
B	262	MSE	MET	modified residue	UNP P0A6R0

- Molecule 2 is COENZYME A (CCD ID: 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	353	Total	O	0	0
			353	353		
3	B	351	Total	O	0	0
			351	351		

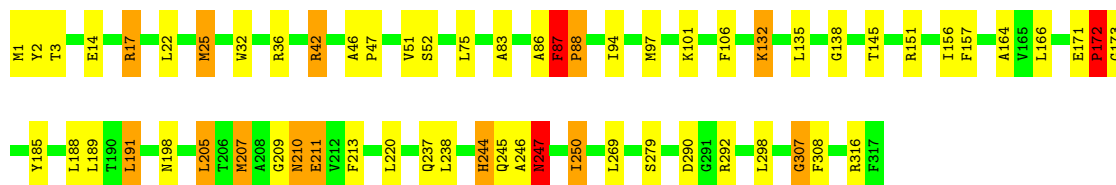
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

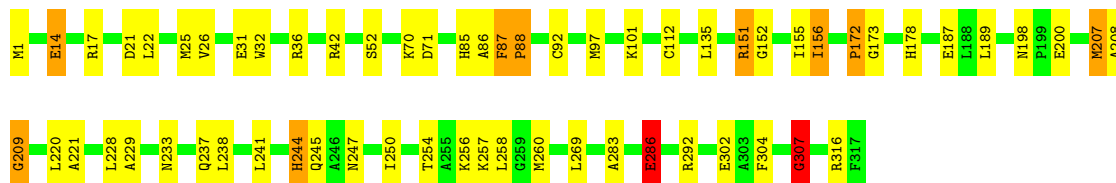
• Molecule 1: BETA-KETOACYL-ACP SYNTHASE III

Chain A: 



• Molecule 1: BETA-KETOACYL-ACP SYNTHASE III

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.13Å 64.30Å 165.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80	Depositor
% Data completeness (in resolution range)	97.2 (20.00-1.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.225	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5502	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

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	0.68	0/2383	1.79	28/3230 (0.9%)
1	B	0.79	3/2383 (0.1%)	1.76	39/3230 (1.2%)
All	All	0.74	3/4766 (0.1%)	1.78	67/6460 (1.0%)

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	4
1	B	0	5
All	All	0	9

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	286	GLU	CA-CB	6.21	1.63	1.53
1	B	286	GLU	CB-CG	5.83	1.70	1.52
1	B	173	GLY	N-CA	-5.40	1.37	1.45

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	ARG	CD-NE-CZ	32.54	169.95	124.40
1	A	17	ARG	CD-NE-CZ	30.09	166.52	124.40
1	B	172	PRO	CA-C-N	26.88	174.09	121.41
1	B	172	PRO	C-N-CA	26.88	174.09	121.41
1	A	307	GLY	CA-C-N	22.69	162.55	121.70
1	A	307	GLY	C-N-CA	22.69	162.55	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	307	GLY	O-C-N	-22.38	96.14	122.33
1	B	17	ARG	CD-NE-CZ	16.56	147.58	124.40
1	A	172	PRO	O-C-N	-16.25	105.81	123.03
1	A	207	MSE	CA-CB-CG	13.73	141.56	114.10
1	B	307	GLY	CA-C-O	-13.43	104.06	118.97
1	B	207	MSE	CA-CB-CG	11.89	137.88	114.10
1	A	172	PRO	CA-C-N	11.67	144.29	121.41
1	A	172	PRO	C-N-CA	11.67	144.29	121.41
1	B	87	PHE	CA-C-O	-10.73	105.46	120.16
1	A	87	PHE	CA-C-O	-10.68	105.53	120.16
1	A	308	PHE	N-CA-CB	10.63	128.57	110.50
1	B	286	GLU	CB-CA-C	-10.48	93.45	110.84
1	B	14	GLU	CB-CG-CD	9.22	128.27	112.60
1	A	307	GLY	O-C-N	-8.80	111.25	122.70
1	B	172	PRO	CA-C-O	8.57	132.13	121.67
1	A	88	PRO	N-CA-CB	8.13	111.54	102.60
1	A	86	ALA	N-CA-C	-7.79	102.87	111.36
1	B	88	PRO	N-CA-CB	7.44	110.79	102.60
1	B	14	GLU	N-CA-C	7.41	119.14	111.14
1	B	88	PRO	CA-N-CD	-7.41	101.13	111.50
1	B	228	LEU	CA-C-O	7.37	128.56	120.82
1	A	210	ASN	CA-CB-CG	-7.25	105.34	112.60
1	A	209	GLY	N-CA-C	6.89	121.24	112.83
1	B	233	ASN	CA-CB-CG	6.56	119.16	112.60
1	A	157	PHE	CA-CB-CG	-6.53	107.27	113.80
1	B	17	ARG	NE-CZ-NH2	-6.45	113.40	119.20
1	B	244	HIS	CA-CB-CG	-6.41	107.39	113.80
1	B	70	LYS	CA-C-N	6.15	129.36	120.38
1	B	70	LYS	C-N-CA	6.15	129.36	120.38
1	A	88	PRO	CA-N-CD	-6.03	103.06	111.50
1	B	228	LEU	O-C-N	-6.00	115.89	122.07
1	B	172	PRO	O-C-N	-5.97	115.72	123.06
1	A	205	LEU	CA-CB-CG	5.87	136.85	116.30
1	B	286	GLU	CG-CD-OE1	5.86	131.89	118.40
1	B	209	GLY	N-CA-C	5.82	119.68	112.64
1	B	31	GLU	CB-CG-CD	5.75	122.37	112.60
1	A	185	TYR	CA-C-N	5.67	126.38	120.03
1	A	185	TYR	C-N-CA	5.67	126.38	120.03
1	B	207	MSE	CB-CA-C	-5.65	100.34	109.89
1	B	307	GLY	N-CA-C	-5.61	106.93	115.00
1	B	316	ARG	CD-NE-CZ	5.54	132.15	124.40
1	B	172	PRO	N-CA-CB	5.49	108.43	103.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	GLY	N-CA-C	-5.46	100.24	113.18
1	B	151	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	B	198	ASN	CA-C-N	5.29	125.01	119.82
1	B	198	ASN	C-N-CA	5.29	125.01	119.82
1	B	208	ALA	CA-C-N	5.26	125.94	119.99
1	B	208	ALA	C-N-CA	5.26	125.94	119.99
1	A	198	ASN	CA-C-N	5.26	124.87	119.56
1	A	198	ASN	C-N-CA	5.26	124.87	119.56
1	A	244	HIS	CA-CB-CG	-5.25	108.56	113.80
1	B	156	ILE	N-CA-C	5.23	116.63	111.67
1	A	247	ASN	O-C-N	-5.22	118.72	123.41
1	B	86	ALA	N-CA-C	-5.19	105.71	111.36
1	A	164	ALA	CA-C-N	-5.17	116.77	123.19
1	A	164	ALA	C-N-CA	-5.17	116.77	123.19
1	B	178	HIS	CA-CB-CG	-5.17	108.63	113.80
1	A	106	PHE	CA-CB-CG	5.16	118.96	113.80
1	B	14	GLU	CB-CA-C	-5.15	102.76	110.90
1	B	228	LEU	CA-C-N	5.09	127.10	120.28
1	B	228	LEU	C-N-CA	5.09	127.10	120.28

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	PRO	Mainchain,Peptide
1	A	87	PHE	Mainchain,Peptide
1	B	172	PRO	Peptide
1	B	307	GLY	Mainchain,Peptide
1	B	87	PHE	Mainchain,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	2351	0	2337	49	0
1	B	2351	0	2337	50	3
2	A	48	0	30	17	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	48	0	30	16	0
3	A	353	0	0	4	1
3	B	351	0	0	14	5
All	All	5502	0	4734	115	5

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 12.

All (115) 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)
2:B:2350:COA:C7P	2:B:2350:COA:N8P	1.70	1.51
2:A:1350:COA:N8P	2:A:1350:COA:C7P	1.75	1.47
1:B:286:GLU:CB	3:B:2473:HOH:O	1.68	1.36
1:B:286:GLU:CG	3:B:2473:HOH:O	1.68	1.33
2:B:2350:COA:N8P	2:B:2350:COA:C6P	2.04	1.21
2:A:1350:COA:N8P	2:A:1350:COA:C6P	2.09	1.15
2:B:2350:COA:O3A	2:B:2350:COA:O8A	1.65	1.14
1:B:238:LEU:HD12	1:B:260:MSE:HE1	1.31	1.08
1:B:286:GLU:HG2	1:B:292:ARG:HH22	1.21	1.03
1:B:52:SER:HB3	1:B:97:MSE:HE1	1.40	1.03
1:B:286:GLU:HG2	1:B:292:ARG:NH2	1.72	1.03
2:A:1350:COA:HN8	2:A:1350:COA:C5P	1.80	0.94
2:B:2350:COA:N8P	2:B:2350:COA:H62	1.80	0.93
1:A:132:LYS:HD3	1:A:132:LYS:H	1.37	0.90
2:A:1350:COA:N8P	2:A:1350:COA:C5P	2.35	0.89
2:B:2350:COA:O9P	2:B:2350:COA:H143	1.71	0.88
1:A:52:SER:HB3	1:A:97:MSE:HE1	1.55	0.88
1:A:246:ALA:HB3	1:A:250:ILE:HG21	1.57	0.85
1:A:189:LEU:HD13	1:A:207:MSE:HG2	1.59	0.84
1:B:286:GLU:CD	3:B:2473:HOH:O	2.07	0.83
1:B:189:LEU:HD13	1:B:207:MSE:HG2	1.60	0.81
2:B:2350:COA:O9P	2:B:2350:COA:CEP	2.28	0.80
2:A:1350:COA:N8P	2:A:1350:COA:O5P	2.13	0.77
1:B:286:GLU:CA	3:B:2473:HOH:O	2.09	0.75
2:B:2350:COA:O8A	2:B:2350:COA:P1A	2.47	0.73
2:A:1350:COA:O1A	2:A:1350:COA:H3B	1.87	0.73
1:B:258:LEU:HB3	1:B:260:MSE:HE3	1.70	0.73
1:A:94:ILE:HA	1:A:97:MSE:HE3	1.70	0.73
1:A:88:PRO:HB3	1:B:307:GLY:HA2	1.72	0.72
1:A:52:SER:HB3	1:A:97:MSE:CE	2.19	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:SER:HB3	1:B:97:MSE:CE	2.19	0.71
1:A:307:GLY:HA2	1:B:88:PRO:HB3	1.73	0.71
1:A:210:ASN:OD1	3:A:1609:HOH:O	2.10	0.70
1:A:132:LYS:HD3	1:A:132:LYS:N	2.06	0.70
2:A:1350:COA:H3B	2:A:1350:COA:P1A	2.32	0.69
1:B:151:ARG:HD3	2:B:2350:COA:O2B	1.94	0.68
1:A:247:ASN:ND2	1:A:250:ILE:HG22	2.09	0.68
1:B:112:CYS:HG	2:B:2350:COA:HS1	1.39	0.68
1:B:245:GLN:HB3	1:B:269:LEU:HB3	1.77	0.66
1:A:132:LYS:HG2	3:A:1679:HOH:O	1.95	0.65
1:A:51:VAL:HG21	1:A:83:ALA:HA	1.78	0.65
1:A:17:ARG:HD3	3:A:1468:HOH:O	1.98	0.64
1:A:247:ASN:ND2	1:A:250:ILE:H	1.95	0.64
1:A:247:ASN:OD1	2:A:1350:COA:H143	1.97	0.64
1:B:155:ILE:HD11	2:B:2350:COA:O5A	1.98	0.64
1:B:238:LEU:CD1	1:B:260:MSE:HE1	2.20	0.63
1:B:220:LEU:HD12	1:B:250:ILE:HD11	1.82	0.61
1:A:220:LEU:CD1	1:A:250:ILE:HD11	2.31	0.60
1:B:14:GLU:HG3	3:B:2551:HOH:O	2.01	0.60
1:A:51:VAL:CG2	1:A:83:ALA:HA	2.32	0.60
1:B:286:GLU:CG	1:B:292:ARG:NH2	2.57	0.60
1:A:245:GLN:HB3	1:A:269:LEU:HB3	1.83	0.60
1:A:188:LEU:HD22	1:A:211:GLU:HG3	1.84	0.59
1:A:36:ARG:HB3	2:A:1350:COA:O5A	2.03	0.58
1:A:132:LYS:H	1:A:132:LYS:CD	2.12	0.58
1:A:290:ASP:OD2	1:A:292:ARG:HD3	2.04	0.57
1:B:189:LEU:CD1	1:B:207:MSE:HG2	2.34	0.57
1:B:152:GLY:O	1:B:156:ILE:HD12	2.04	0.56
1:B:14:GLU:CG	3:B:2551:HOH:O	2.53	0.56
1:B:254:THR:HB	3:B:2633:HOH:O	2.06	0.56
1:B:52:SER:CB	1:B:97:MSE:HE1	2.27	0.56
1:A:207:MSE:HE1	2:A:1350:COA:OAP	2.05	0.56
1:A:210:ASN:CG	3:A:1609:HOH:O	2.49	0.56
1:A:220:LEU:HD11	1:A:250:ILE:HD11	1.89	0.55
1:B:286:GLU:HA	3:B:2473:HOH:O	1.92	0.54
1:A:307:GLY:HA2	1:B:88:PRO:CB	2.37	0.53
1:B:247:ASN:HB3	1:B:250:ILE:HG22	1.91	0.53
2:B:2350:COA:C6P	2:B:2350:COA:HN8	2.12	0.52
1:A:36:ARG:HE	2:A:1350:COA:P1A	2.33	0.52
1:B:238:LEU:HB2	1:B:260:MSE:HE2	1.91	0.52
2:A:1350:COA:N8P	2:A:1350:COA:H61	2.17	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ILE:CA	1:A:97:MSE:HE3	2.37	0.51
1:A:298:LEU:HB2	1:A:316:ARG:NH2	2.26	0.51
1:A:32:TRP:HZ2	2:A:1350:COA:H2B	1.76	0.51
1:A:244:HIS:CD2	1:A:279:SER:HB3	2.45	0.50
1:A:52:SER:CB	1:A:97:MSE:HE1	2.36	0.50
1:B:85:HIS:HE1	3:B:2372:HOH:O	1.93	0.50
2:B:2350:COA:O8A	2:B:2350:COA:O5B	2.31	0.49
1:B:286:GLU:CG	1:B:292:ARG:HH22	2.10	0.49
1:B:247:ASN:O	1:B:250:ILE:HG22	2.12	0.49
1:A:244:HIS:HD2	1:A:279:SER:HB3	1.77	0.48
1:A:22:LEU:HA	1:A:25:MSE:HG3	1.95	0.48
1:B:21:ASP:O	1:B:25:MSE:HG2	2.14	0.47
1:A:3:THR:HG21	1:A:166:LEU:HD13	1.96	0.47
2:B:2350:COA:H72	3:B:2472:HOH:O	2.14	0.46
2:A:1350:COA:C7P	2:A:1350:COA:C9P	2.78	0.46
1:B:207:MSE:SE	2:B:2350:COA:O5P	2.84	0.46
1:B:151:ARG:H	1:B:151:ARG:HG3	1.40	0.45
1:B:1:MSE:HB2	3:B:2460:HOH:O	2.15	0.45
1:A:145:THR:HB	1:A:191:LEU:HD21	1.99	0.45
1:B:256:LYS:HE2	1:B:256:LYS:HB2	1.80	0.45
1:B:258:LEU:HB3	1:B:260:MSE:CE	2.45	0.44
1:A:2:TYR:CD1	1:A:172:PRO:HB3	2.52	0.44
1:A:151:ARG:NH2	2:A:1350:COA:O2B	2.48	0.44
1:A:22:LEU:HA	1:A:25:MSE:CG	2.47	0.44
1:A:247:ASN:CG	1:A:250:ILE:HG22	2.43	0.44
1:B:112:CYS:SG	2:B:2350:COA:S1P	3.00	0.44
1:A:156:ILE:HD11	2:A:1350:COA:O4A	2.18	0.43
1:B:32:TRP:CH2	1:B:36:ARG:HG3	2.54	0.43
1:B:151:ARG:HD3	1:B:151:ARG:HH11	1.62	0.43
1:B:22:LEU:HA	1:B:25:MSE:CG	2.49	0.42
1:A:247:ASN:O	1:A:250:ILE:HG23	2.20	0.42
1:A:46:ALA:HB1	1:A:47:PRO:HD2	2.02	0.42
1:A:188:LEU:HD13	1:A:211:GLU:HG3	2.02	0.42
1:B:92:CYS:HA	3:B:2685:HOH:O	2.20	0.42
1:B:221:ALA:HB1	1:B:257:LYS:HE3	2.02	0.42
1:B:304:PHE:HB3	3:B:2419:HOH:O	2.19	0.42
1:A:189:LEU:CD1	1:A:207:MSE:HG2	2.38	0.41
1:A:87:PHE:HA	1:A:88:PRO:C	2.46	0.41
1:B:250:ILE:HB	3:B:2472:HOH:O	2.20	0.41
1:A:101:LYS:HB3	1:A:101:LYS:HE2	1.85	0.41
1:A:213:PHE:HD1	2:A:1350:COA:O9P	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:GLY:HA3	2:B:2350:COA:H131	2.02	0.40
1:B:112:CYS:HB3	1:B:244:HIS:CE1	2.57	0.40
1:B:283:ALA:O	1:B:286:GLU:HB3	2.21	0.40

All (5) 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)
3:B:2483:HOH:O	3:B:2684:HOH:O[3_755]	1.60	0.60
1:B:229:ALA:N	3:B:2352:HOH:O[3_755]	1.70	0.50
1:B:229:ALA:CA	3:B:2352:HOH:O[3_755]	1.87	0.33
3:A:1644:HOH:O	3:B:2434:HOH:O[4_445]	2.08	0.12
1:B:237:GLN:OE1	3:B:2656:HOH:O[3_755]	2.10	0.10

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	315/317 (99%)	303 (96%)	11 (4%)	1 (0%)	36	25
1	B	315/317 (99%)	307 (98%)	8 (2%)	0	100	100
All	All	630/634 (99%)	610 (97%)	19 (3%)	1 (0%)	43	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	GLY

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	247/239 (103%)	232 (94%)	15 (6%)	17 6
1	B	247/239 (103%)	237 (96%)	10 (4%)	28 15
All	All	494/478 (103%)	469 (95%)	25 (5%)	21 9

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	14	GLU
1	A	25	MSE
1	A	42	ARG
1	A	75	LEU
1	A	132	LYS
1	A	135	LEU
1	A	171	GLU
1	A	191	LEU
1	A	205	LEU
1	A	211	GLU
1	A	237	GLN
1	A	238	LEU
1	A	247	ASN
1	A	250	ILE
1	B	26	VAL
1	B	42	ARG
1	B	71	ASP
1	B	101	LYS
1	B	135	LEU
1	B	187	GLU
1	B	200	GLU
1	B	241	LEU
1	B	286	GLU
1	B	302	GLU

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	85	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	93	GLN
1	A	193	ASN
1	A	201	ASN
1	A	204	HIS
1	A	233	ASN
1	A	244	HIS
1	A	247	ASN
1	B	85	HIS
1	B	93	GLN
1	B	231	ASN
1	B	233	ASN
1	B	264	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 oligosaccharides 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	A	1350	-	47,50,50	3.25	7 (14%)	69,75,75	2.57	19 (27%)
2	COA	B	2350	-	47,50,50	3.06	8 (17%)	69,75,75	3.15	23 (33%)

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	1350	-	-	26/48/64/64	0/3/3/3
2	COA	B	2350	-	-	26/48/64/64	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1350	COA	C7P-N8P	13.18	1.75	1.46
2	A	1350	COA	P1A-O3A	12.20	1.72	1.59
2	B	2350	COA	P1A-O3A	11.61	1.72	1.59
2	B	2350	COA	C7P-N8P	10.68	1.70	1.46
2	B	2350	COA	C2P-S1P	-10.26	1.39	1.80
2	A	1350	COA	C2P-S1P	-10.00	1.40	1.80
2	A	1350	COA	P2A-O3A	4.20	1.64	1.59
2	B	2350	COA	C6P-C5P	3.59	1.58	1.51
2	B	2350	COA	P2A-O3A	3.59	1.63	1.59
2	B	2350	COA	CCP-CBP	2.81	1.57	1.52
2	A	1350	COA	C6P-C5P	2.46	1.56	1.51
2	B	2350	COA	O5P-C5P	2.40	1.28	1.23
2	A	1350	COA	C9P-N8P	2.29	1.39	1.33
2	B	2350	COA	C4A-N3A	2.25	1.38	1.34
2	A	1350	COA	CCP-CBP	2.01	1.55	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2350	COA	C6P-C7P-N8P	-16.30	77.31	112.00
2	A	1350	COA	C6P-C7P-N8P	-15.89	78.19	112.00
2	B	2350	COA	C5A-C4A-N3A	-6.96	117.13	126.72
2	B	2350	COA	N3A-C4A-N9A	-6.73	115.72	127.17
2	B	2350	COA	O5P-C5P-C6P	-5.86	111.40	122.02
2	B	2350	COA	O5P-C5P-N4P	-5.69	111.87	123.03
2	A	1350	COA	O9P-C9P-CAP	-5.18	106.43	120.89
2	B	2350	COA	C7P-N8P-C9P	4.96	131.46	122.55
2	B	2350	COA	C2A-N1A-C6A	-4.95	110.59	118.73
2	B	2350	COA	C2A-N3A-C4A	-4.74	100.25	111.83
2	B	2350	COA	N3A-C2A-N1A	-4.59	121.64	128.58
2	B	2350	COA	C3P-N4P-C5P	-4.54	114.38	122.82
2	A	1350	COA	O9P-C9P-N8P	-3.78	114.98	122.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2350	COA	C7P-C6P-C5P	-3.35	106.81	112.39
2	B	2350	COA	P3B-O3B-C3B	-3.29	114.66	123.43
2	B	2350	COA	O8A-P3B-O7A	3.22	123.38	110.83
2	B	2350	COA	C4A-N9A-C1B	-3.15	119.27	126.63
2	B	2350	COA	C6A-C5A-C4A	-3.05	113.02	117.18
2	A	1350	COA	C6A-C5A-C4A	-3.02	113.06	117.18
2	B	2350	COA	C6A-C5A-N7A	-2.97	126.37	132.09
2	A	1350	COA	C2B-C3B-C4B	-2.90	98.16	103.24
2	A	1350	COA	O5P-C5P-N4P	-2.89	117.36	123.03
2	B	2350	COA	O3B-P3B-O7A	-2.78	99.43	109.33
2	B	2350	COA	O2A-P1A-O3A	2.76	114.73	107.27
2	A	1350	COA	O4B-C1B-C2B	-2.64	100.97	106.62
2	A	1350	COA	C5A-C4A-N3A	-2.63	123.09	126.72
2	B	2350	COA	O4B-C4B-C3B	-2.51	99.63	104.92
2	A	1350	COA	C2A-N1A-C6A	-2.45	114.70	118.73
2	A	1350	COA	C3B-C2B-C1B	-2.45	94.50	99.89
2	A	1350	COA	O4B-C1B-N9A	2.29	112.48	108.09
2	A	1350	COA	CEP-CBP-CDP	-2.25	104.72	109.20
2	A	1350	COA	O5P-C5P-C6P	-2.24	117.96	122.02
2	B	2350	COA	C5A-C6A-N1A	-2.24	111.83	117.51
2	A	1350	COA	C4A-N9A-C1B	-2.22	121.43	126.63
2	B	2350	COA	C4A-N9A-C8A	-2.18	103.45	105.74
2	A	1350	COA	C3P-N4P-C5P	-2.14	118.85	122.82
2	A	1350	COA	O3B-P3B-O7A	-2.12	101.78	109.33
2	A	1350	COA	O2A-P1A-O3A	2.09	112.92	107.27
2	B	2350	COA	O9P-C9P-N8P	-2.07	118.60	122.98
2	B	2350	COA	O4B-C4B-C5B	2.05	115.90	109.33
2	A	1350	COA	O3A-P1A-O1A	-2.04	104.58	110.70
2	A	1350	COA	C2P-C3P-N4P	-2.01	107.75	112.31

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1350	COA	C2B-C1B-N9A-C4A
2	A	1350	COA	C5B-O5B-P1A-O2A
2	A	1350	COA	C5B-O5B-P1A-O3A
2	A	1350	COA	CCP-O6A-P2A-O5A
2	A	1350	COA	CDP-CBP-CCP-O6A
2	A	1350	COA	OAP-CAP-CBP-CCP
2	A	1350	COA	C9P-CAP-CBP-CCP
2	A	1350	COA	C9P-CAP-CBP-CDP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1350	COA	OAP-CAP-CBP-CEP
2	A	1350	COA	C9P-CAP-CBP-CEP
2	A	1350	COA	CAP-C9P-N8P-C7P
2	A	1350	COA	S1P-C2P-C3P-N4P
2	B	2350	COA	C2B-C1B-N9A-C4A
2	B	2350	COA	C5B-O5B-P1A-O2A
2	B	2350	COA	C5B-O5B-P1A-O3A
2	B	2350	COA	P1A-O3A-P2A-O6A
2	B	2350	COA	CDP-CBP-CCP-O6A
2	B	2350	COA	CEP-CBP-CCP-O6A
2	B	2350	COA	CAP-CBP-CCP-O6A
2	B	2350	COA	OAP-CAP-CBP-CCP
2	B	2350	COA	C9P-CAP-CBP-CCP
2	B	2350	COA	OAP-CAP-CBP-CDP
2	B	2350	COA	C9P-CAP-CBP-CDP
2	B	2350	COA	OAP-CAP-CBP-CEP
2	B	2350	COA	C9P-CAP-CBP-CEP
2	B	2350	COA	N8P-C9P-CAP-OAP
2	B	2350	COA	CAP-C9P-N8P-C7P
2	B	2350	COA	C6P-C5P-N4P-C3P
2	A	1350	COA	C6P-C5P-N4P-C3P
2	B	2350	COA	O4B-C4B-C5B-O5B
2	A	1350	COA	O9P-C9P-CAP-OAP
2	B	2350	COA	O9P-C9P-CAP-OAP
2	A	1350	COA	OAP-CAP-CBP-CDP
2	A	1350	COA	O9P-C9P-CAP-CBP
2	B	2350	COA	O9P-C9P-CAP-CBP
2	B	2350	COA	N8P-C9P-CAP-CBP
2	B	2350	COA	CBP-CCP-O6A-P2A
2	A	1350	COA	CEP-CBP-CCP-O6A
2	A	1350	COA	CAP-CBP-CCP-O6A
2	B	2350	COA	S1P-C2P-C3P-N4P
2	A	1350	COA	C5B-O5B-P1A-O1A
2	A	1350	COA	CCP-O6A-P2A-O3A
2	A	1350	COA	CCP-O6A-P2A-O4A
2	B	2350	COA	C5B-O5B-P1A-O1A
2	A	1350	COA	C4B-C5B-O5B-P1A
2	B	2350	COA	C3B-O3B-P3B-O8A
2	A	1350	COA	C2B-C1B-N9A-C8A
2	A	1350	COA	C2P-C3P-N4P-C5P
2	B	2350	COA	C5P-C6P-C7P-N8P
2	A	1350	COA	O4B-C1B-N9A-C8A

Continued on next page...

Continued from previous page...

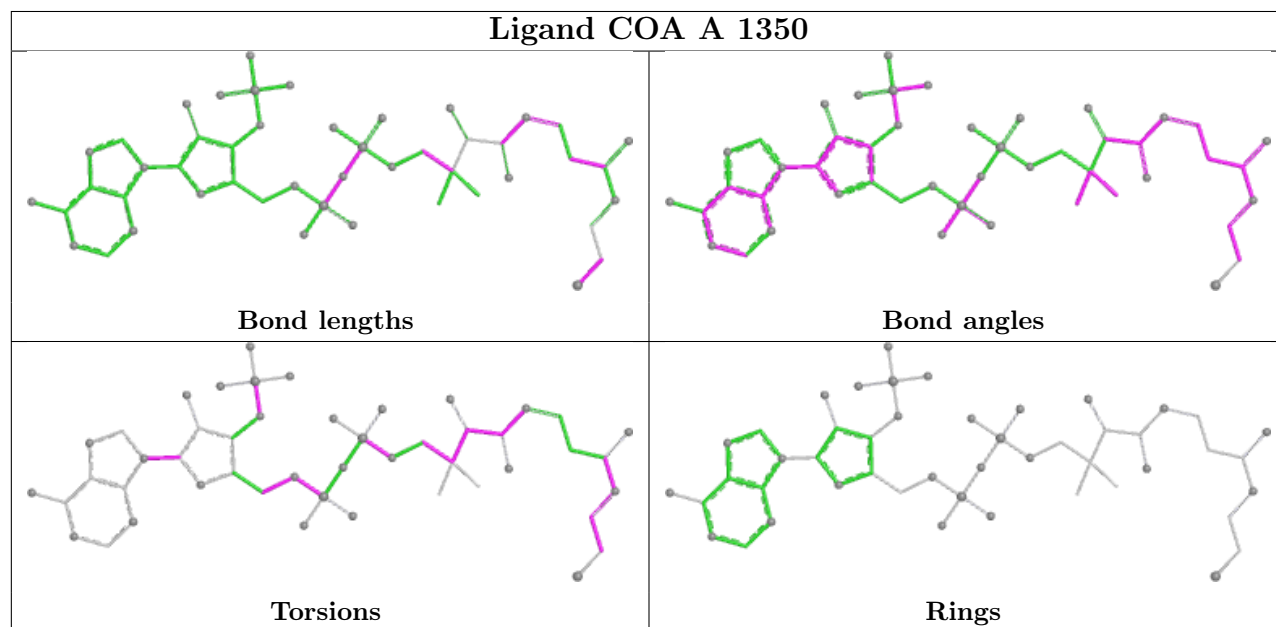
Mol	Chain	Res	Type	Atoms
2	B	2350	COA	O4B-C1B-N9A-C8A
2	A	1350	COA	C3B-O3B-P3B-O9A

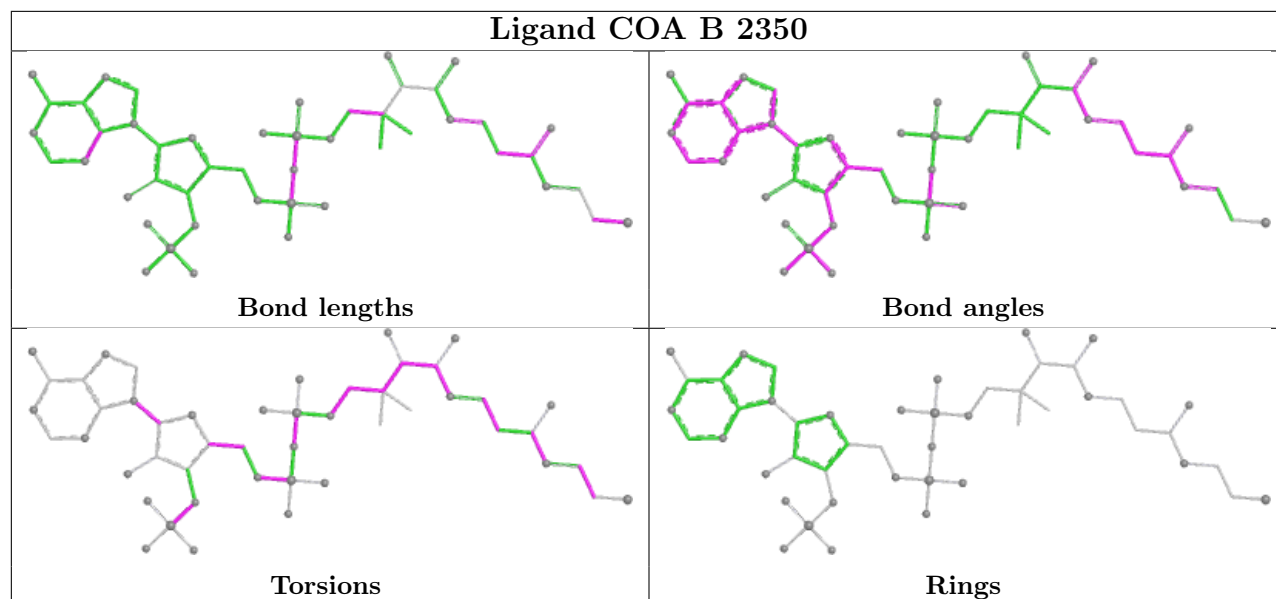
There are no ring outliers.

2 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1350	COA	17	0
2	B	2350	COA	16	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.