



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:24 AM UTC

PDB ID : 4O9C / pdb_00004o9c
Title : Crystal structure of Beta-ketothiolase (PhaA) from Ralstonia eutropha H16
Authors : Kim, E.J.; Kim, J.; Kim, S.; Kim, K.J.
Deposited on : 2014-01-02
Resolution : 2.00 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

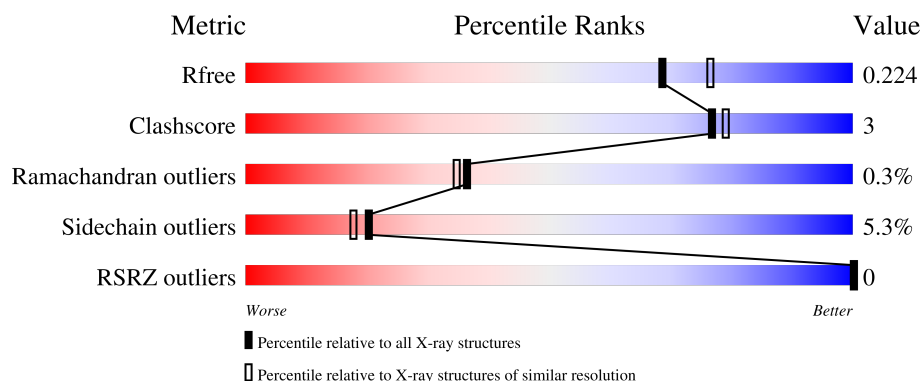
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

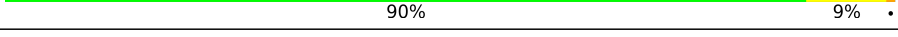
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	393	
1	B	393	
1	C	393	
1	D	393	
1	E	393	

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Mol	Chain	Length	Quality of chain
1	F	393	 88% 10% •
1	G	393	 91% 8% •
1	H	393	 88% 10% ••

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23650 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 Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	0
			2835	1774	502	539	20			
1	B	393	Total	C	N	O	S	0	0	0
			2835	1774	502	539	20			
1	C	393	Total	C	N	O	S	0	0	0
			2835	1774	502	539	20			
1	D	393	Total	C	N	O	S	0	0	0
			2835	1774	502	539	20			
1	E	393	Total	C	N	O	S	0	0	0
			2835	1774	502	539	20			
1	F	393	Total	C	N	O	S	0	0	0
			2835	1774	502	539	20			
1	G	393	Total	C	N	O	S	0	0	0
			2835	1774	502	539	20			
1	H	393	Total	C	N	O	S	0	0	0
			2835	1774	502	539	20			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	SER	CYS	engineered mutation	UNP P14611
B	88	SER	CYS	engineered mutation	UNP P14611
C	88	SER	CYS	engineered mutation	UNP P14611
D	88	SER	CYS	engineered mutation	UNP P14611
E	88	SER	CYS	engineered mutation	UNP P14611
F	88	SER	CYS	engineered mutation	UNP P14611
G	88	SER	CYS	engineered mutation	UNP P14611
H	88	SER	CYS	engineered mutation	UNP P14611

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



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

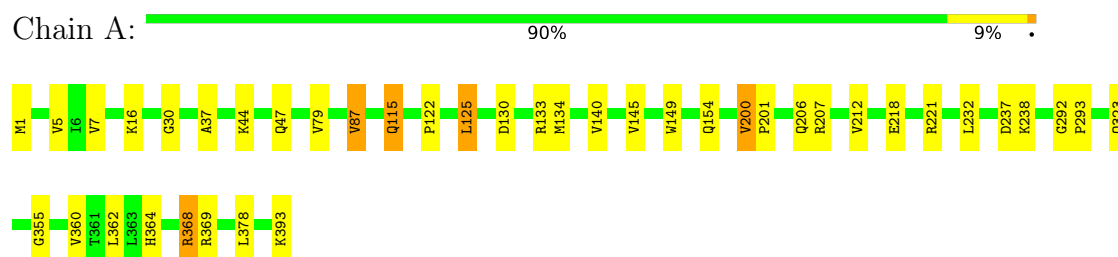
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total	O	0	0
			131	131		
3	B	119	Total	O	0	0
			119	119		
3	C	134	Total	O	0	0
			134	134		
3	D	122	Total	O	0	0
			122	122		
3	E	114	Total	O	0	0
			114	114		
3	F	98	Total	O	0	0
			98	98		
3	G	95	Total	O	0	0
			95	95		
3	H	109	Total	O	0	0
			109	109		

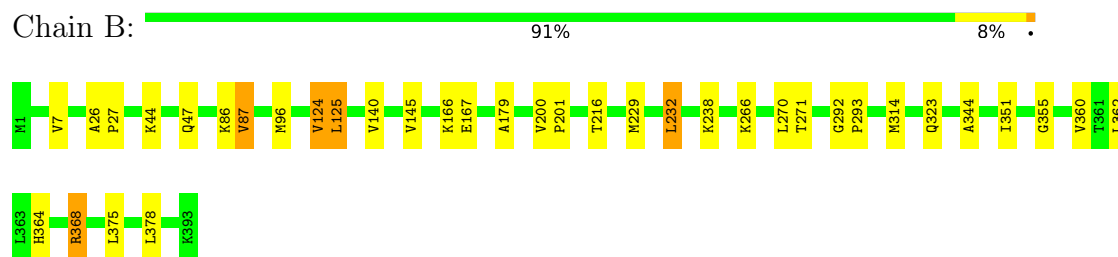
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

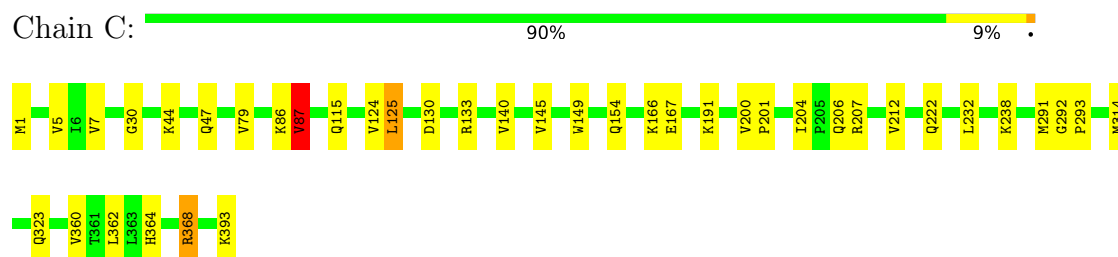
• Molecule 1: Acetyl-CoA acetyltransferase



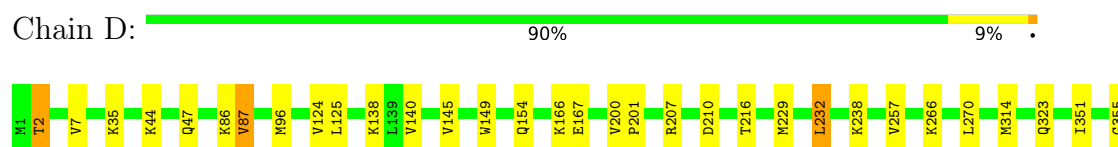
• Molecule 1: Acetyl-CoA acetyltransferase



• Molecule 1: Acetyl-CoA acetyltransferase



• Molecule 1: Acetyl-CoA acetyltransferase





- Molecule 1: Acetyl-CoA acetyltransferase

Chain E: 89% 10% .



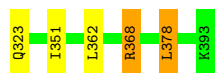
- Molecule 1: Acetyl-CoA acetyltransferase

Chain F: 88% 10% .



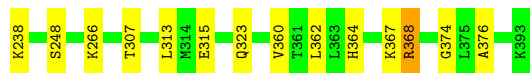
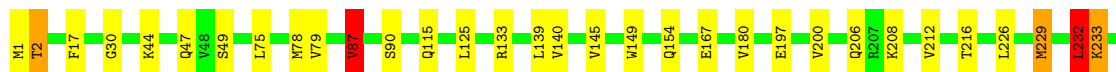
- Molecule 1: Acetyl-CoA acetyltransferase

Chain G: 91% 8% .



- Molecule 1: Acetyl-CoA acetyltransferase

Chain H: 88% 10% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.09Å 157.44Å 114.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.09 – 2.00 102.09 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.4 (102.09-2.00) 98.4 (102.09-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	16.72 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.173 , 0.213 0.186 , 0.224	Depositor DCC
R_{free} test set	11968 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 22.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23650	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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	1.23	3/2875 (0.1%)	1.12	2/3886 (0.1%)
1	B	1.22	3/2875 (0.1%)	1.12	2/3886 (0.1%)
1	C	1.25	3/2875 (0.1%)	1.14	4/3886 (0.1%)
1	D	1.22	2/2875 (0.1%)	1.14	3/3886 (0.1%)
1	E	1.26	3/2875 (0.1%)	1.17	3/3886 (0.1%)
1	F	1.29	7/2875 (0.2%)	1.18	11/3886 (0.3%)
1	G	1.30	6/2875 (0.2%)	1.20	10/3886 (0.3%)
1	H	1.27	5/2875 (0.2%)	1.17	8/3886 (0.2%)
All	All	1.26	32/23000 (0.1%)	1.16	43/31088 (0.1%)

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	E	0	1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	40	ARG	CA-C	-7.43	1.43	1.52
1	H	79	VAL	CA-C	6.28	1.58	1.53
1	H	87	VAL	N-CA	6.24	1.54	1.46
1	E	87	VAL	N-CA	6.12	1.53	1.46
1	F	40	ARG	CA-C	-6.09	1.44	1.52
1	C	124	VAL	N-CA	-5.98	1.39	1.46
1	A	5	VAL	N-CA	-5.85	1.39	1.46
1	B	124	VAL	N-CA	-5.76	1.39	1.46
1	B	271	THR	C-O	-5.69	1.17	1.24
1	F	87	VAL	N-CA	5.68	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	257	VAL	CA-C	5.65	1.59	1.52
1	F	289	MET	C-O	-5.62	1.17	1.24
1	F	265	ALA	CA-C	5.60	1.60	1.52
1	C	5	VAL	N-CA	-5.57	1.39	1.46
1	A	37	ALA	CA-C	5.51	1.59	1.52
1	H	78	MET	C-O	-5.51	1.16	1.24
1	H	233	LYS	CA-C	5.37	1.59	1.53
1	D	35	LYS	C-O	-5.34	1.17	1.24
1	F	2	THR	CA-CB	5.31	1.60	1.53
1	F	108	GLU	CA-C	-5.27	1.47	1.52
1	A	115	GLN	CD-OE1	5.24	1.33	1.23
1	E	274	ALA	CA-C	-5.23	1.46	1.52
1	G	170	ILE	CA-C	-5.17	1.46	1.52
1	E	79	VAL	CA-C	5.14	1.57	1.53
1	G	87	VAL	N-CA	5.13	1.52	1.46
1	G	109	ILE	C-O	-5.11	1.18	1.24
1	F	197	GLU	N-CA	-5.09	1.40	1.46
1	G	265	ALA	CA-C	5.08	1.59	1.52
1	B	179	ALA	N-CA	-5.08	1.40	1.46
1	H	229	MET	N-CA	5.05	1.52	1.46
1	G	108	GLU	CA-C	-5.02	1.47	1.52
1	C	87	VAL	C-O	5.00	1.30	1.24

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	294	VAL	CA-C-N	-7.49	111.25	119.19
1	G	294	VAL	C-N-CA	-7.49	111.25	119.19
1	F	86	LYS	N-CA-C	-6.60	102.52	110.44
1	A	79	VAL	CA-C-N	-6.44	114.14	120.52
1	A	79	VAL	C-N-CA	-6.44	114.14	120.52
1	C	79	VAL	CA-C-N	-6.29	114.29	120.52
1	C	79	VAL	C-N-CA	-6.29	114.29	120.52
1	G	200	VAL	CB-CA-C	6.27	117.08	110.37
1	G	86	LYS	CB-CG-CD	6.27	125.71	111.30
1	G	351	ILE	N-CA-C	6.24	116.91	110.36
1	H	75	LEU	CA-C-N	-6.12	114.33	120.21
1	H	75	LEU	C-N-CA	-6.12	114.33	120.21
1	F	86	LYS	CB-CG-CD	5.90	124.88	111.30
1	F	351	ILE	N-CA-C	5.77	116.42	110.36
1	F	294	VAL	CA-C-N	-5.76	113.08	119.19
1	F	294	VAL	C-N-CA	-5.76	113.08	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	210	ASP	CA-C-N	-5.67	113.94	119.78
1	D	210	ASP	C-N-CA	-5.67	113.94	119.78
1	G	79	VAL	N-CA-C	5.67	112.72	107.56
1	B	351	ILE	N-CA-C	5.62	116.26	110.36
1	D	351	ILE	N-CA-C	5.60	116.24	110.36
1	F	200	VAL	CB-CA-C	5.58	116.34	110.37
1	G	86	LYS	N-CA-C	-5.50	103.84	110.44
1	H	232	LEU	CA-C-N	5.47	128.96	120.60
1	H	232	LEU	C-N-CA	5.47	128.96	120.60
1	F	24	ILE	CA-C-N	-5.46	114.16	119.78
1	F	24	ILE	C-N-CA	-5.46	114.16	119.78
1	H	233	LYS	N-CA-CB	-5.42	101.84	110.03
1	E	90	SER	N-CA-C	5.42	117.61	111.11
1	G	24	ILE	CA-C-N	-5.37	114.25	119.78
1	G	24	ILE	C-N-CA	-5.37	114.25	119.78
1	E	197	GLU	N-CA-C	5.35	116.92	111.14
1	F	375	LEU	CA-CB-CG	5.34	134.99	116.30
1	B	344	ALA	N-CA-C	5.27	117.77	111.71
1	H	307	THR	N-CA-C	-5.22	102.56	110.50
1	C	86	LYS	CB-CG-CD	5.20	123.26	111.30
1	H	90	SER	N-CA-C	5.20	117.35	111.11
1	F	232	LEU	CA-C-N	5.18	127.69	120.65
1	F	232	LEU	C-N-CA	5.18	127.69	120.65
1	H	197	GLU	N-CA-C	5.15	116.97	111.36
1	G	314	MET	CG-SD-CE	-5.12	89.64	100.90
1	E	177	GLU	CB-CG-CD	-5.06	103.99	112.60
1	C	204	ILE	CB-CA-C	-5.01	105.02	110.78

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	1	MET	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	2835	0	2907	25	0
1	B	2835	0	2907	18	1
1	C	2835	0	2907	19	0
1	D	2835	0	2907	14	0
1	E	2835	0	2907	19	0
1	F	2835	0	2907	18	1
1	G	2835	0	2907	15	0
1	H	2835	0	2907	20	0
2	C	48	0	32	0	0
3	A	131	0	0	3	0
3	B	119	0	0	2	0
3	C	134	0	0	3	0
3	D	122	0	0	3	0
3	E	114	0	0	3	0
3	F	98	0	0	1	0
3	G	95	0	0	1	0
3	H	109	0	0	3	0
All	All	23650	0	23288	135	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (135) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:VAL:CG2	3:A:605:HOH:O	2.29	0.81
1:C:200:VAL:CG2	3:C:602:HOH:O	2.30	0.80
1:E:2:THR:HG22	3:E:575:HOH:O	1.88	0.74
1:C:368:ARG:CZ	1:C:368:ARG:HB3	2.17	0.74
1:A:368:ARG:HB3	1:A:368:ARG:CZ	2.19	0.71
1:H:2:THR:HG22	3:H:604:HOH:O	1.91	0.69
1:G:44:LYS:H	1:G:47:GLN:HE21	1.44	0.64
1:A:122:PRO:CG	1:B:124:VAL:HG21	2.28	0.63
1:G:46:GLU:HB2	1:G:78:MET:CE	2.31	0.61
1:D:2:THR:HG22	3:D:470:HOH:O	2.01	0.59
1:B:200:VAL:HG23	1:B:201:PRO:HD2	1.84	0.59
1:E:229:MET:HA	1:E:232:LEU:HD22	1.84	0.59
1:F:44:LYS:H	1:F:47:GLN:HE21	1.51	0.57
1:G:96:MET:HE2	3:H:596:HOH:O	2.05	0.57
1:C:140:VAL:CG1	1:C:145:VAL:HG21	2.35	0.57
1:D:229:MET:HA	1:D:232:LEU:HD22	1.86	0.56
1:A:7:VAL:HG12	1:A:7:VAL:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:TRP:HE1	1:A:154:GLN:NE2	2.06	0.54
1:E:368:ARG:CZ	1:E:368:ARG:CB	2.85	0.54
1:E:206:GLN:CG	1:E:212:VAL:HG23	2.37	0.54
1:H:140:VAL:CG1	1:H:145:VAL:HG21	2.37	0.54
1:B:44:LYS:H	1:B:47:GLN:NE2	2.06	0.53
1:A:122:PRO:HG2	1:B:124:VAL:HG21	1.91	0.53
3:A:565:HOH:O	1:B:96:MET:HE2	2.09	0.52
3:C:561:HOH:O	1:D:96:MET:HE2	2.10	0.52
1:E:44:LYS:H	1:E:47:GLN:NE2	2.08	0.52
1:B:360:VAL:O	1:B:364:HIS:HD2	1.93	0.52
1:D:200:VAL:HG23	1:D:201:PRO:HD2	1.92	0.52
1:A:122:PRO:CG	1:B:124:VAL:CG2	2.88	0.51
1:C:368:ARG:HB3	1:C:368:ARG:NH2	2.24	0.51
1:A:44:LYS:H	1:A:47:GLN:NE2	2.08	0.51
1:E:16:LYS:HG3	1:E:218:GLU:HG3	1.93	0.51
1:C:7:VAL:O	1:C:7:VAL:HG12	2.08	0.51
1:D:44:LYS:H	1:D:47:GLN:NE2	2.07	0.51
1:A:368:ARG:HB3	1:A:368:ARG:NH2	2.26	0.51
1:H:368:ARG:CZ	1:H:368:ARG:CB	2.88	0.51
1:B:7:VAL:HG11	1:B:270:LEU:HD13	1.92	0.51
1:C:149:TRP:HE1	1:C:154:GLN:NE2	2.09	0.51
1:C:44:LYS:H	1:C:47:GLN:NE2	2.08	0.51
1:F:216:THR:HG22	3:F:553:HOH:O	2.11	0.51
1:H:229:MET:HA	1:H:232:LEU:HD22	1.93	0.50
1:A:200:VAL:HG22	3:A:605:HOH:O	2.01	0.50
1:H:149:TRP:HE1	1:H:154:GLN:NE2	2.09	0.49
1:H:44:LYS:H	1:H:47:GLN:NE2	2.10	0.49
1:A:16:LYS:HG3	1:A:218:GLU:HG3	1.93	0.49
1:E:2:THR:CG2	3:E:575:HOH:O	2.55	0.49
1:E:315:GLU:O	1:E:376:ALA:HA	2.11	0.49
1:C:200:VAL:HG23	1:C:201:PRO:HD2	1.95	0.48
1:A:30:GLY:HA3	1:A:115:GLN:NE2	2.27	0.48
1:C:360:VAL:O	1:C:364:HIS:HD2	1.96	0.48
1:B:229:MET:HA	1:B:232:LEU:HD22	1.94	0.48
1:D:216:THR:HG22	3:D:437:HOH:O	2.14	0.48
1:H:206:GLN:CG	1:H:212:VAL:HG23	2.44	0.48
1:A:140:VAL:CG1	1:A:145:VAL:HG21	2.44	0.47
1:A:360:VAL:O	1:A:364:HIS:HD2	1.97	0.47
1:F:266:LYS:O	1:F:267:GLU:C	2.58	0.47
1:B:140:VAL:CG1	1:B:145:VAL:HG21	2.45	0.47
1:A:7:VAL:O	1:A:7:VAL:CG1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LEU:HD21	1:H:139:LEU:HD12	1.97	0.46
1:C:30:GLY:HA3	1:C:115:GLN:NE2	2.29	0.46
1:E:17:PHE:CZ	1:F:129:ARG:HD3	2.51	0.46
1:H:360:VAL:O	1:H:364:HIS:HD2	1.99	0.46
1:F:206:GLN:O	1:F:207:ARG:HB2	2.16	0.46
1:E:360:VAL:O	1:E:364:HIS:HD2	1.99	0.46
1:G:44:LYS:H	1:G:47:GLN:NE2	2.13	0.46
1:G:216:THR:HG22	3:G:530:HOH:O	2.16	0.46
1:C:206:GLN:HG3	1:C:212:VAL:HG23	1.96	0.46
1:C:292:GLY:N	1:C:293:PRO:CD	2.78	0.45
1:E:124:VAL:CG2	1:F:122:PRO:CG	2.95	0.45
1:E:216:THR:HG22	3:E:602:HOH:O	2.16	0.45
1:A:122:PRO:HG2	1:B:124:VAL:CG2	2.46	0.45
1:G:140:VAL:CG1	1:G:145:VAL:HG21	2.47	0.45
1:H:313:LEU:O	1:H:374:GLY:HA2	2.17	0.45
1:A:125:LEU:HD21	1:E:139:LEU:CD1	2.46	0.44
1:C:125:LEU:HD21	1:H:139:LEU:CD1	2.47	0.44
1:C:200:VAL:HG22	3:C:602:HOH:O	2.06	0.44
1:D:138:LYS:HE2	1:G:136:ASP:OD2	2.18	0.44
1:B:216:THR:HG22	3:B:532:HOH:O	2.17	0.44
1:G:46:GLU:HB2	1:G:78:MET:HE1	1.98	0.44
1:D:44:LYS:H	1:D:47:GLN:HE21	1.64	0.44
1:G:317:ASN:HB3	1:G:378:LEU:HB3	1.99	0.44
1:C:140:VAL:HG11	1:C:145:VAL:HG21	1.99	0.44
1:H:30:GLY:HA3	1:H:115:GLN:NE2	2.33	0.44
1:E:368:ARG:CZ	1:E:368:ARG:HB3	2.47	0.43
1:G:125:LEU:HD22	1:G:132:PHE:CZ	2.52	0.43
1:B:124:VAL:HG22	1:B:125:LEU:N	2.32	0.43
1:F:365:GLU:OE2	1:F:368:ARG:NH1	2.51	0.43
1:E:149:TRP:HE1	1:E:154:GLN:NE2	2.15	0.43
1:H:368:ARG:HB3	1:H:368:ARG:NH2	2.34	0.43
1:F:140:VAL:CG1	1:F:145:VAL:HG21	2.49	0.43
1:H:315:GLU:O	1:H:376:ALA:HA	2.17	0.43
1:G:129:ARG:HD3	1:H:17:PHE:CZ	2.54	0.43
1:B:26:ALA:HB3	1:B:27:PRO:HD3	2.00	0.43
1:A:134:MET:HE3	1:A:134:MET:HB2	1.82	0.43
1:D:355:GLY:HA2	1:D:378:LEU:HD11	2.01	0.43
1:E:30:GLY:HA3	1:E:115:GLN:NE2	2.34	0.43
1:H:368:ARG:CZ	1:H:368:ARG:HB3	2.49	0.43
1:A:355:GLY:HA2	1:A:378:LEU:HD11	2.00	0.42
1:B:292:GLY:N	1:B:293:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1:MET:O	1:H:2:THR:C	2.63	0.42
1:A:292:GLY:N	1:A:293:PRO:CD	2.82	0.42
1:H:216:THR:HG22	3:H:572:HOH:O	2.19	0.42
1:C:7:VAL:O	1:C:7:VAL:CG1	2.67	0.42
1:E:180:VAL:HG21	1:E:226:LEU:HA	2.01	0.42
1:E:206:GLN:CD	1:E:212:VAL:HG23	2.45	0.42
1:B:368:ARG:HD3	3:B:520:HOH:O	2.20	0.42
1:F:125:LEU:HD22	1:F:132:PHE:HZ	1.85	0.42
1:A:200:VAL:HG23	1:A:201:PRO:HD2	2.02	0.42
1:D:2:THR:CG2	3:D:470:HOH:O	2.66	0.42
1:D:140:VAL:CG1	1:D:145:VAL:HG21	2.50	0.42
1:G:125:LEU:HD22	1:G:132:PHE:HZ	1.84	0.41
1:A:237:ASP:OD1	1:A:237:ASP:C	2.63	0.41
1:D:7:VAL:HG11	1:D:270:LEU:HD13	2.02	0.41
1:G:140:VAL:HG13	1:G:145:VAL:HG21	2.02	0.41
1:D:360:VAL:O	1:D:364:HIS:HD2	2.04	0.41
1:F:9:ALA:HB1	1:F:360:VAL:HG22	2.03	0.41
1:G:368:ARG:CZ	1:G:368:ARG:HB3	2.49	0.41
1:F:325:LEU:HD23	1:F:325:LEU:HA	1.90	0.41
1:G:134:MET:HE3	1:G:134:MET:HB2	1.87	0.41
1:A:122:PRO:HG3	1:B:124:VAL:HG21	1.99	0.41
1:F:306:TRP:CE2	1:F:373:LYS:HD3	2.56	0.41
1:H:180:VAL:HG21	1:H:226:LEU:HA	2.02	0.41
1:A:140:VAL:HG11	1:A:145:VAL:HG21	2.03	0.41
1:H:233:LYS:HB3	1:H:233:LYS:HE3	1.76	0.41
1:D:149:TRP:HE1	1:D:154:GLN:NE2	2.19	0.40
1:B:355:GLY:HA2	1:B:378:LEU:HD11	2.03	0.40
1:F:157:MET:HA	1:F:157:MET:HE2	2.01	0.40
1:C:291:MET:C	1:C:293:PRO:HD2	2.47	0.40
1:E:124:VAL:HG21	1:F:122:PRO:CG	2.51	0.40
1:F:44:LYS:H	1:F:47:GLN:NE2	2.17	0.40
1:A:206:GLN:HG3	1:A:212:VAL:HG23	2.03	0.40
1:C:191:LYS:HE3	1:C:222:GLN:OE1	2.22	0.40
1:F:125:LEU:HD22	1:F:132:PHE:CZ	2.56	0.40
1:F:180:VAL:HG21	1:F:226:LEU:HA	2.02	0.40
1:F:194:LYS:HE2	1:F:368:ARG:CZ	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ARG:NH2	1:F:269:GLY:O[2_556]	2.16	0.04

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	391/393 (100%)	378 (97%)	11 (3%)	2 (0%)	24	21
1	B	391/393 (100%)	381 (97%)	9 (2%)	1 (0%)	36	35
1	C	391/393 (100%)	380 (97%)	9 (2%)	2 (0%)	24	21
1	D	391/393 (100%)	381 (97%)	9 (2%)	1 (0%)	36	35
1	E	391/393 (100%)	380 (97%)	10 (3%)	1 (0%)	36	35
1	F	391/393 (100%)	380 (97%)	10 (3%)	1 (0%)	36	35
1	G	391/393 (100%)	379 (97%)	11 (3%)	1 (0%)	36	35
1	H	391/393 (100%)	382 (98%)	8 (2%)	1 (0%)	36	35
All	All	3128/3144 (100%)	3041 (97%)	77 (2%)	10 (0%)	36	35

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	207	ARG
1	A	87	VAL
1	B	87	VAL
1	C	87	VAL
1	D	87	VAL
1	E	87	VAL
1	F	87	VAL
1	G	87	VAL
1	H	87	VAL
1	A	207	ARG

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	285/285 (100%)	271 (95%)	14 (5%)	22	20
1	B	285/285 (100%)	272 (95%)	13 (5%)	24	22
1	C	285/285 (100%)	271 (95%)	14 (5%)	22	20
1	D	285/285 (100%)	269 (94%)	16 (6%)	19	16
1	E	285/285 (100%)	266 (93%)	19 (7%)	15	11
1	F	285/285 (100%)	271 (95%)	14 (5%)	22	20
1	G	285/285 (100%)	271 (95%)	14 (5%)	22	20
1	H	285/285 (100%)	269 (94%)	16 (6%)	19	16
All	All	2280/2280 (100%)	2160 (95%)	120 (5%)	20	18

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	87	VAL
1	A	125	LEU
1	A	130	ASP
1	A	133	ARG
1	A	200	VAL
1	A	221	ARG
1	A	232	LEU
1	A	238	LYS
1	A	323	GLN
1	A	362	LEU
1	A	368	ARG
1	A	369	ARG
1	A	393	LYS
1	B	86	LYS
1	B	87	VAL
1	B	125	LEU
1	B	166	LYS
1	B	167	GLU

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Mol	Chain	Res	Type
1	B	232	LEU
1	B	238	LYS
1	B	266	LYS
1	B	314	MET
1	B	323	GLN
1	B	362	LEU
1	B	368	ARG
1	B	375	LEU
1	C	1	MET
1	C	87	VAL
1	C	125	LEU
1	C	130	ASP
1	C	133	ARG
1	C	166	LYS
1	C	167	GLU
1	C	232	LEU
1	C	238	LYS
1	C	314	MET
1	C	323	GLN
1	C	362	LEU
1	C	368	ARG
1	C	393	LYS
1	D	2	THR
1	D	86	LYS
1	D	87	VAL
1	D	124	VAL
1	D	125	LEU
1	D	166	LYS
1	D	167	GLU
1	D	207	ARG
1	D	232	LEU
1	D	238	LYS
1	D	266	LYS
1	D	314	MET
1	D	323	GLN
1	D	362	LEU
1	D	368	ARG
1	D	375	LEU
1	E	2	THR
1	E	49	SER
1	E	65	PRO
1	E	87	VAL

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Mol	Chain	Res	Type
1	E	125	LEU
1	E	133	ARG
1	E	167	GLU
1	E	177	GLU
1	E	200	VAL
1	E	207	ARG
1	E	232	LEU
1	E	238	LYS
1	E	248	SER
1	E	266	LYS
1	E	323	GLN
1	E	333	TRP
1	E	362	LEU
1	E	367	LYS
1	E	368	ARG
1	F	1	MET
1	F	23	LYS
1	F	86	LYS
1	F	87	VAL
1	F	125	LEU
1	F	200	VAL
1	F	232	LEU
1	F	238	LYS
1	F	248	SER
1	F	323	GLN
1	F	362	LEU
1	F	368	ARG
1	F	375	LEU
1	F	378	LEU
1	G	86	LYS
1	G	87	VAL
1	G	125	LEU
1	G	130	ASP
1	G	200	VAL
1	G	208	LYS
1	G	232	LEU
1	G	233	LYS
1	G	238	LYS
1	G	248	SER
1	G	323	GLN
1	G	362	LEU
1	G	368	ARG

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Mol	Chain	Res	Type
1	G	378	LEU
1	H	2	THR
1	H	49	SER
1	H	87	VAL
1	H	125	LEU
1	H	133	ARG
1	H	167	GLU
1	H	200	VAL
1	H	208	LYS
1	H	232	LEU
1	H	238	LYS
1	H	248	SER
1	H	266	LYS
1	H	323	GLN
1	H	362	LEU
1	H	367	LYS
1	H	368	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	115	GLN
1	A	154	GLN
1	A	364	HIS
1	B	47	GLN
1	B	115	GLN
1	B	154	GLN
1	B	184	ASN
1	B	364	HIS
1	C	47	GLN
1	C	115	GLN
1	C	154	GLN
1	C	329	GLN
1	C	330	GLN
1	C	364	HIS
1	D	47	GLN
1	D	115	GLN
1	D	154	GLN
1	D	329	GLN
1	D	330	GLN
1	D	364	HIS

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Mol	Chain	Res	Type
1	E	47	GLN
1	E	115	GLN
1	E	154	GLN
1	E	364	HIS
1	F	47	GLN
1	F	154	GLN
1	F	184	ASN
1	F	222	GLN
1	G	47	GLN
1	G	115	GLN
1	G	154	GLN
1	G	222	GLN
1	G	364	HIS
1	H	47	GLN
1	H	115	GLN
1	H	154	GLN
1	H	190	GLN
1	H	364	HIS

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](#)

1 ligand is 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	C	401	-	47,50,50	2.12	10 (21%)	69,75,75	2.25	19 (27%)

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	C	401	-	-	18/48/64/64	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	COA	P2A-O3A	6.94	1.67	1.59
2	C	401	COA	P1A-O3A	6.78	1.66	1.59
2	C	401	COA	C3P-N4P	5.56	1.58	1.46
2	C	401	COA	C5A-C4A	5.00	1.48	1.39
2	C	401	COA	C2P-S1P	3.51	1.94	1.80
2	C	401	COA	C5A-C6A	2.67	1.48	1.41
2	C	401	COA	P3B-O3B	2.31	1.63	1.59
2	C	401	COA	C8A-N7A	2.28	1.36	1.31
2	C	401	COA	C5A-N7A	-2.24	1.35	1.39
2	C	401	COA	C4A-N3A	2.09	1.38	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	COA	C5A-C4A-N3A	-7.38	116.55	126.72
2	C	401	COA	N3A-C4A-N9A	6.71	138.57	127.17
2	C	401	COA	O5P-C5P-C6P	-5.13	112.72	122.02
2	C	401	COA	C2P-C3P-N4P	4.99	123.62	112.31
2	C	401	COA	C2A-N3A-C4A	4.56	122.97	111.83
2	C	401	COA	CDP-CBP-CCP	-4.24	101.23	108.22
2	C	401	COA	C7P-C6P-C5P	-4.01	105.72	112.39
2	C	401	COA	N3A-C2A-N1A	-3.99	122.53	128.58
2	C	401	COA	CEP-CBP-CDP	3.60	116.38	109.20
2	C	401	COA	C6P-C5P-N4P	3.21	122.19	116.34
2	C	401	COA	O4B-C1B-N9A	2.79	113.46	108.09
2	C	401	COA	CAP-C9P-N8P	2.76	121.72	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	COA	C5A-C6A-N6A	-2.61	116.83	123.29
2	C	401	COA	C4A-N9A-C8A	2.58	108.44	105.74
2	C	401	COA	C5A-N7A-C8A	2.52	107.42	103.45
2	C	401	COA	C4A-C5A-N7A	-2.42	107.82	110.58
2	C	401	COA	N6A-C6A-N1A	2.39	123.69	118.38
2	C	401	COA	C3B-C2B-C1B	2.22	104.78	99.89
2	C	401	COA	O9A-P3B-O8A	2.06	115.51	107.80

There are no chirality outliers.

All (18) torsion outliers are listed below:

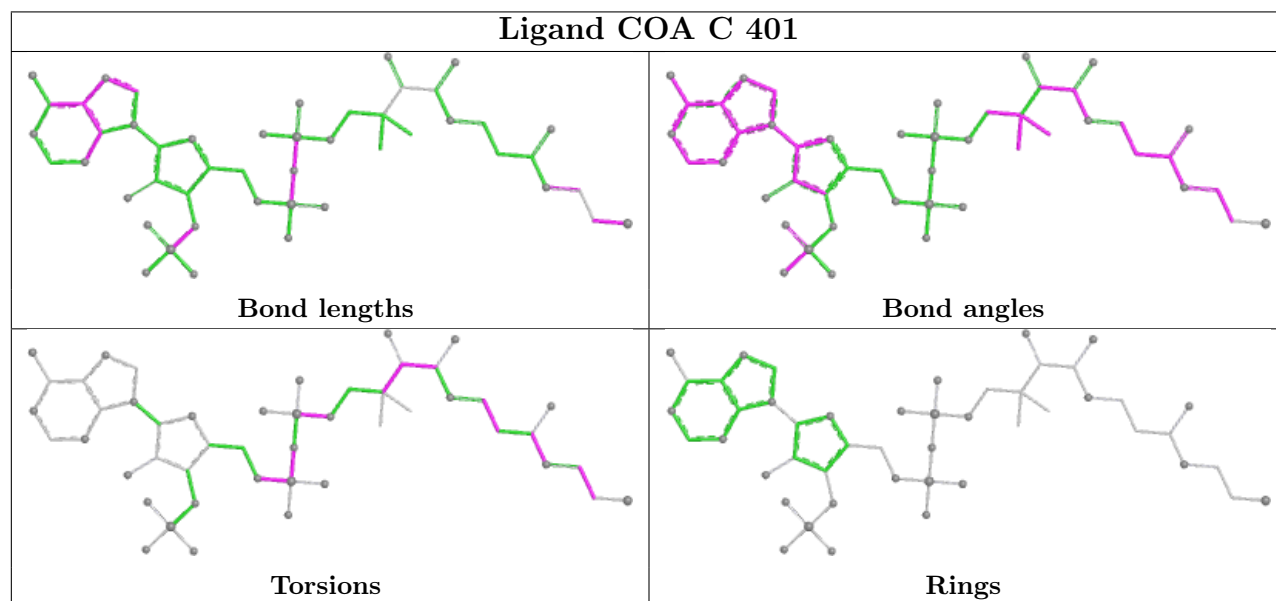
Mol	Chain	Res	Type	Atoms
2	C	401	COA	C5B-O5B-P1A-O2A
2	C	401	COA	C5B-O5B-P1A-O3A
2	C	401	COA	CCP-O6A-P2A-O3A
2	C	401	COA	CCP-O6A-P2A-O4A
2	C	401	COA	OAP-CAP-CBP-CCP
2	C	401	COA	C9P-CAP-CBP-CCP
2	C	401	COA	OAP-CAP-CBP-CDP
2	C	401	COA	OAP-CAP-CBP-CEP
2	C	401	COA	C9P-CAP-CBP-CEP
2	C	401	COA	N8P-C9P-CAP-OAP
2	C	401	COA	C5P-C6P-C7P-N8P
2	C	401	COA	S1P-C2P-C3P-N4P
2	C	401	COA	C5B-O5B-P1A-O1A
2	C	401	COA	C6P-C5P-N4P-C3P
2	C	401	COA	O9P-C9P-CAP-OAP
2	C	401	COA	C9P-CAP-CBP-CDP
2	C	401	COA	P2A-O3A-P1A-O2A
2	C	401	COA	P2A-O3A-P1A-O1A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	393/393 (100%)	-1.43	0 100 100	12, 19, 32, 82	0
1	B	393/393 (100%)	-1.45	0 100 100	12, 19, 32, 70	0
1	C	393/393 (100%)	-1.43	0 100 100	12, 19, 33, 77	0
1	D	393/393 (100%)	-1.44	0 100 100	12, 19, 32, 71	0
1	E	393/393 (100%)	-1.40	0 100 100	12, 20, 36, 77	0
1	F	393/393 (100%)	-1.34	0 100 100	13, 22, 41, 80	0
1	G	393/393 (100%)	-1.35	0 100 100	13, 22, 42, 82	0
1	H	393/393 (100%)	-1.39	0 100 100	12, 20, 37, 81	0
All	All	3144/3144 (100%)	-1.40	0 100 100	12, 20, 36, 82	0

There are no RSRZ outliers to report.

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](#)

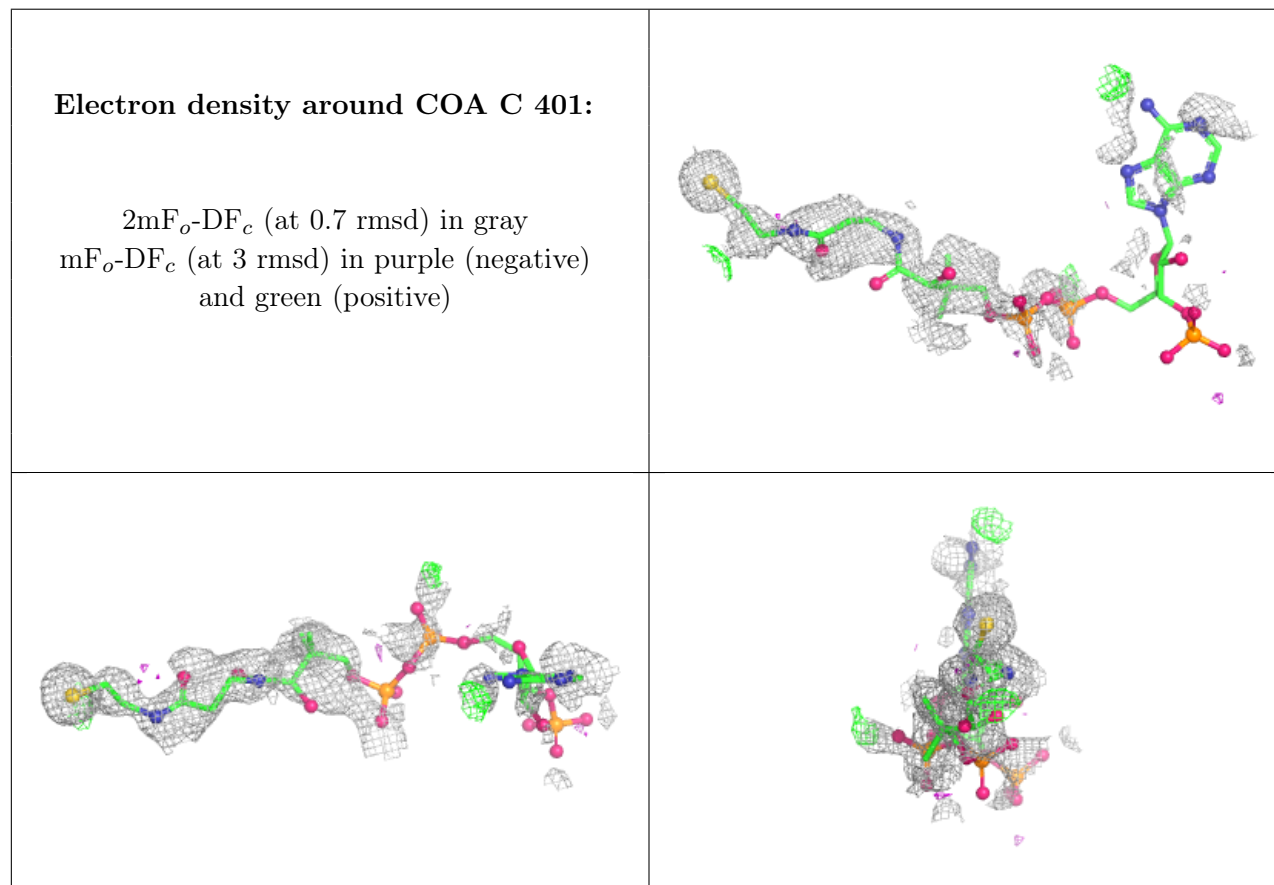
There are no oligosaccharides in this entry.

6.4 Ligands [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($\text{\AA}^2$)	Q<0.9
2	COA	C	401	48/48	0.97	0.10	24,125,158,164	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.