Full wwPDB X-ray Structure Validation Report ⓘ

Feb 5, 2024 – 03:22 pm GMT

PDB ID	:	8BIT
Title	:	Crystal structure of acyl-CoA synthetase from Metallosphaera sedula in complex with Coenzyme A and acetyl-AMP
Authors	:	Capra, N.; Thunnissen, A.M.W.H.; Janssen, D.B.
Deposited on	:	2022-11-02
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

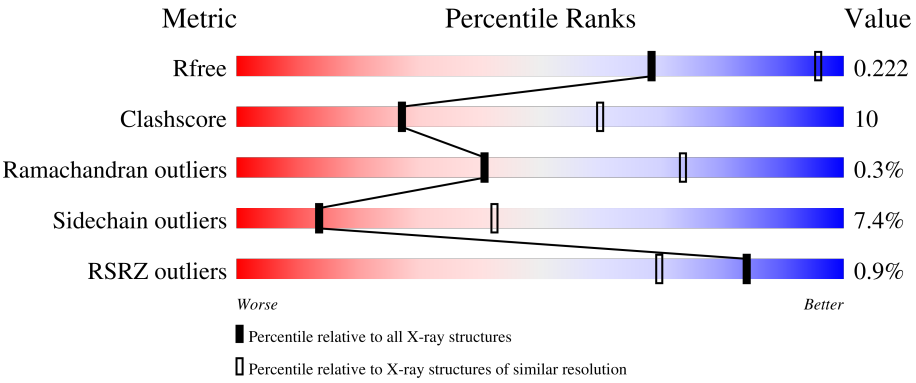
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

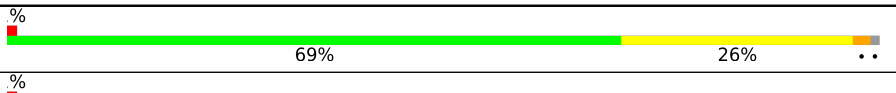
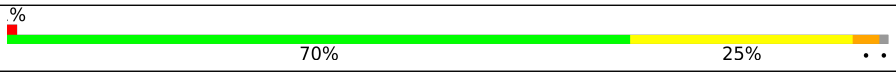
The reported resolution of this entry is 3.10 Å.

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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 <=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	570	
1	B	570	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9185 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.

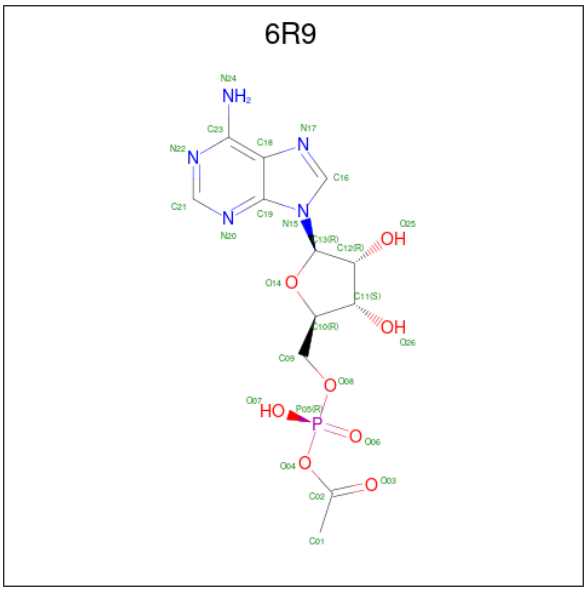
- Molecule 1 is a protein called 4-hydroxybutyrate--CoA ligase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	562	Total	C	N	O	S	0	0	0
			4519	2903	765	838	13			
1	A	562	Total	C	N	O	S	0	0	0
			4518	2902	765	838	13			

There are 14 discrepancies between the modelled and reference sequences:

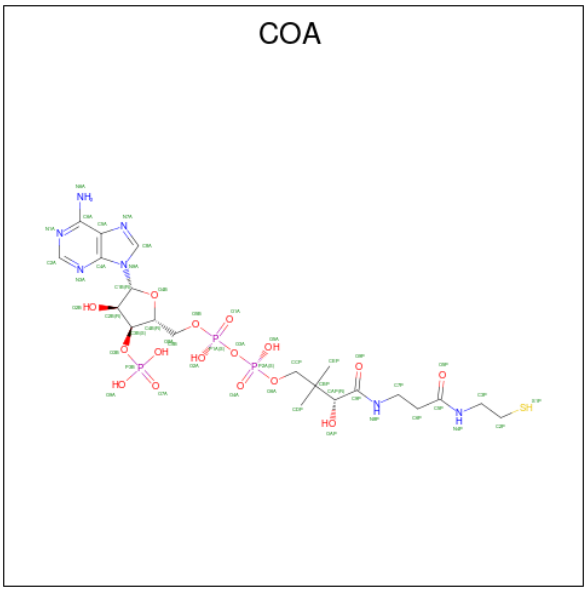
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP A4YDT1
B	2	HIS	-	expression tag	UNP A4YDT1
B	3	HIS	-	expression tag	UNP A4YDT1
B	4	HIS	-	expression tag	UNP A4YDT1
B	5	HIS	-	expression tag	UNP A4YDT1
B	6	HIS	-	expression tag	UNP A4YDT1
B	7	HIS	-	expression tag	UNP A4YDT1
A	1	MET	-	initiating methionine	UNP A4YDT1
A	2	HIS	-	expression tag	UNP A4YDT1
A	3	HIS	-	expression tag	UNP A4YDT1
A	4	HIS	-	expression tag	UNP A4YDT1
A	5	HIS	-	expression tag	UNP A4YDT1
A	6	HIS	-	expression tag	UNP A4YDT1
A	7	HIS	-	expression tag	UNP A4YDT1

- Molecule 2 is [[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] ethanoate (three-letter code: 6R9) (formula: $C_{12}H_{16}N_5O_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			26	12	5	8	1		
2	A	1	Total	C	N	O	P	0	0
			26	12	5	8	1		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



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

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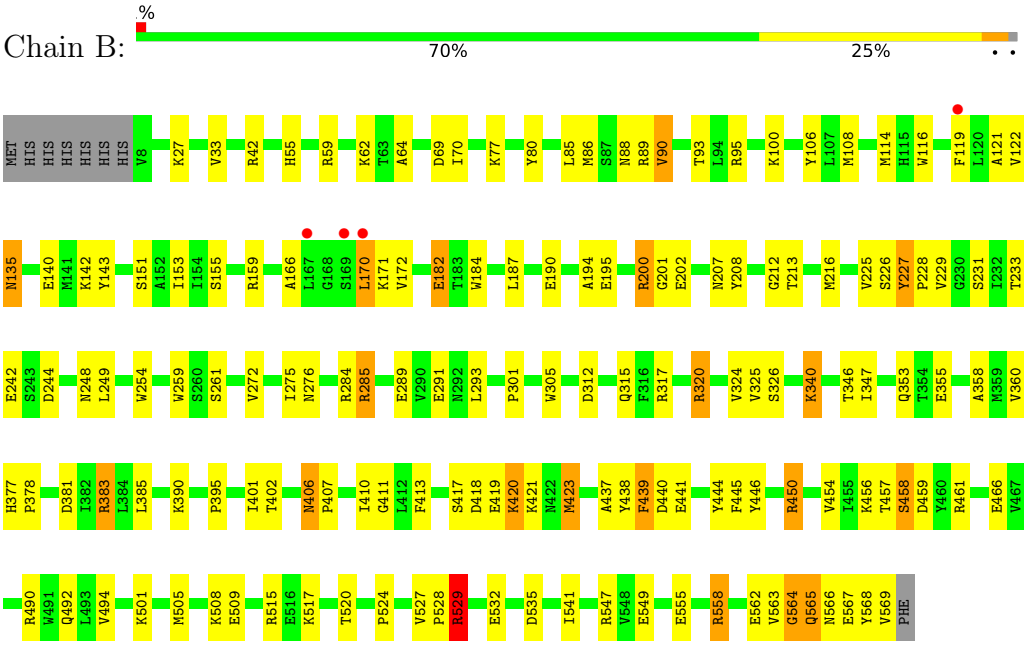
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

3 Residue-property plots (i)

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.

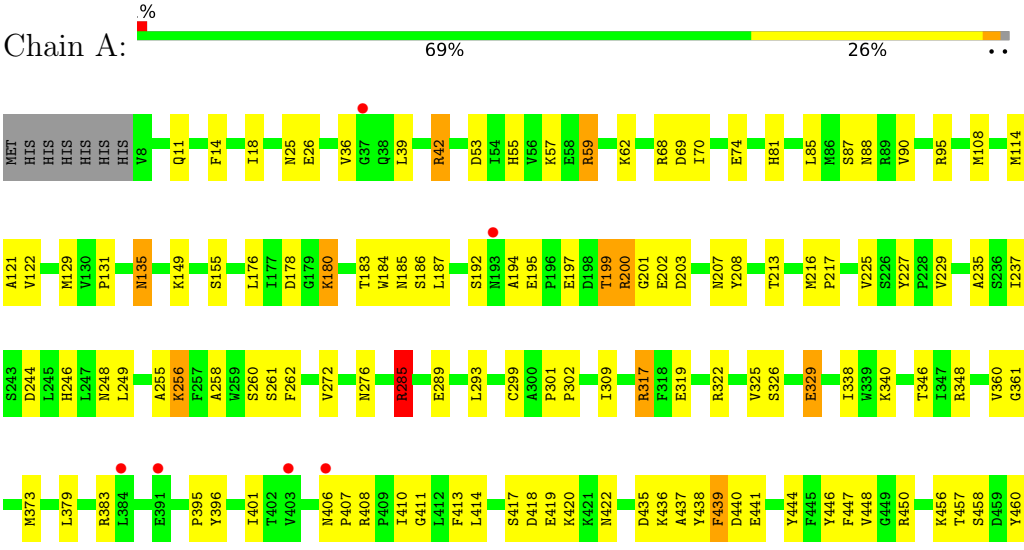
• Molecule 1: 4-hydroxybutyrate--CoA ligase 1

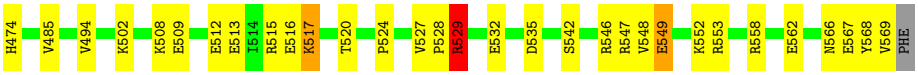
Chain B:



• Molecule 1: 4-hydroxybutyrate--CoA ligase 1

Chain A:




H474
V485
V494
K502
K508
E509
E512
E513
I514
R515
E516
K517
T520
P524
V527
P528
R529
E532
D535
S542
R546
R547
V548
E549
K552
R553
R558
E562
N566
E567
Y568
V569
PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	105.81Å 93.19Å 131.69Å 90.00° 91.12° 90.00°	Depositor
Resolution (Å)	52.95 – 3.10 52.89 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (52.95-3.10) 99.8 (52.89-3.10)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.210 , 0.277 0.218 , 0.222	Depositor DCC
R_{free} test set	1109 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	66.6	Xtriage
Anisotropy	0.686	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9185	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, 6R9

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	0.52	0/4621	1.06	10/6245 (0.2%)
1	B	0.49	0/4623	1.06	19/6248 (0.3%)
All	All	0.50	0/9244	1.06	29/12493 (0.2%)

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	5
1	B	0	4
All	All	0	9

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	529	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	B	565	GLN	N-CA-CB	-7.74	96.67	110.60
1	B	515	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	B	27	LYS	CB-CA-C	-7.41	95.57	110.40
1	B	423	MET	CG-SD-CE	7.13	111.61	100.20
1	B	461	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	A	59	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	135	ASN	CB-CA-C	-6.51	97.37	110.40
1	A	439	PHE	CB-CA-C	-6.44	97.52	110.40
1	B	27	LYS	CA-CB-CG	6.31	127.28	113.40
1	B	439	PHE	CB-CA-C	-6.25	97.91	110.40
1	B	285	ARG	NE-CZ-NH1	6.19	123.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	135	ASN	CB-CA-C	-6.15	98.11	110.40
1	B	461	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	114	MET	CG-SD-CE	5.72	109.36	100.20
1	A	285	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	244	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	B	42	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	B	450	ARG	N-CA-CB	-5.55	100.62	110.60
1	B	42	ARG	CB-CA-C	5.45	121.30	110.40
1	B	450	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	216	MET	CG-SD-CE	5.37	108.79	100.20
1	A	42	ARG	CB-CA-C	5.35	121.09	110.40
1	B	450	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	74	GLU	OE1-CD-OE2	5.29	129.65	123.30
1	A	502	LYS	CB-CA-C	-5.26	99.87	110.40
1	B	42	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	B	320	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	B	27	LYS	N-CA-CB	5.11	119.79	110.60

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	317	ARG	Sidechain
1	A	408	ARG	Sidechain
1	A	450	ARG	Sidechain
1	A	529	ARG	Sidechain
1	A	558	ARG	Sidechain
1	B	200	ARG	Sidechain
1	B	320	ARG	Sidechain
1	B	406	ASN	Peptide
1	B	529	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4518	0	4532	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4519	0	4535	101	0
2	A	26	0	0	0	0
2	B	26	0	0	0	0
3	A	48	0	32	0	0
3	B	48	0	32	2	0
All	All	9185	0	9131	185	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 10.

All (185) 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:379:LEU:HD23	1:A:379:LEU:O	1.66	0.94
1:A:42:ARG:O	1:A:200:ARG:HG3	1.77	0.83
1:A:90:VAL:HG13	1:A:121:ALA:HB2	1.63	0.80
1:A:116:TRP:CZ2	1:A:116:TRP:CZ3	2.64	0.77
1:B:142:LYS:HD3	1:B:166:ALA:HA	1.66	0.76
1:B:547:ARG:HG3	1:B:547:ARG:HH11	1.52	0.74
1:B:233:THR:HG23	1:B:377:HIS:CG	2.25	0.71
1:B:508:LYS:HA	1:B:567:GLU:HG2	1.71	0.71
1:B:227:TYR:O	1:B:231:SER:HB2	1.94	0.68
1:B:547:ARG:HG3	1:B:547:ARG:NH1	2.09	0.68
1:A:474:HIS:HE2	1:A:513:GLU:HG2	1.60	0.67
1:A:508:LYS:HA	1:A:567:GLU:HG2	1.76	0.67
1:B:373:MET:HE1	1:B:445:PHE:HB3	1.77	0.66
1:B:64:ALA:HB2	1:B:80:TYR:CD1	2.31	0.65
1:A:517:LYS:O	1:A:520:THR:HB	1.98	0.64
1:B:373:MET:CE	1:B:445:PHE:HB3	2.28	0.63
1:B:517:LYS:O	1:B:520:THR:HB	1.99	0.63
1:A:95:ARG:NH2	1:A:195:GLU:O	2.33	0.61
1:B:458:SER:OG	1:B:490:ARG:HG2	2.01	0.60
1:A:62:LYS:NZ	1:A:242:GLU:O	2.34	0.60
1:B:213:THR:HB	1:B:454:VAL:HG23	1.83	0.59
1:A:176:LEU:HD22	1:A:180:LYS:HB2	1.82	0.59
1:A:494:VAL:HB	1:A:528:PRO:HA	1.83	0.59
1:B:93:THR:HG21	1:B:187:LEU:HA	1.84	0.59
1:B:340:LYS:HD2	1:B:346:THR:OG1	2.03	0.59
1:A:248:ASN:HD21	1:A:256:LYS:HG3	1.67	0.59
1:B:86:MET:O	1:B:90:VAL:HG13	2.02	0.58
1:A:366:LEU:HD11	1:A:444:TYR:OH	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:LYS:HE2	1:A:542:SER:HB3	1.86	0.58
1:B:289:GLU:O	1:B:293:LEU:HG	2.04	0.58
1:A:116:TRP:CZ3	1:A:261:SER:O	2.57	0.58
1:B:419:GLU:O	1:B:423:MET:HG2	2.05	0.57
1:B:116:TRP:CZ3	1:B:261:SER:O	2.57	0.57
1:A:419:GLU:H	1:A:419:GLU:CD	2.08	0.56
1:A:88:ASN:HB3	1:A:194:ALA:HB2	1.87	0.56
1:B:249:LEU:O	1:B:301:PRO:HD3	2.06	0.56
1:A:122:VAL:HG11	1:A:129:MET:HB3	1.88	0.56
1:B:70:ILE:HD12	1:B:289:GLU:HG3	1.87	0.56
1:B:233:THR:HG21	1:B:358:ALA:O	2.06	0.56
1:A:401:ILE:HD11	1:A:437:ALA:HB2	1.88	0.56
1:A:81:HIS:CE1	1:A:85:LEU:HD12	2.41	0.55
1:B:90:VAL:HG22	1:B:121:ALA:HB2	1.87	0.55
1:A:395:PRO:HA	1:A:439:PHE:HB2	1.89	0.55
1:B:116:TRP:HZ3	1:B:261:SER:O	1.89	0.54
1:A:200:ARG:N	1:A:203:ASP:OD2	2.40	0.54
1:B:509:GLU:OE1	1:B:509:GLU:N	2.37	0.54
1:A:509:GLU:N	1:A:509:GLU:OE1	2.40	0.54
1:B:366:LEU:HD11	1:B:444:TYR:OH	2.07	0.54
1:B:95:ARG:NH2	1:B:195:GLU:O	2.41	0.54
1:B:395:PRO:HA	1:B:439:PHE:HB2	1.90	0.54
1:A:515:ARG:NH1	1:A:528:PRO:O	2.41	0.53
1:B:248:ASN:HB3	1:B:261:SER:OG	2.08	0.53
1:B:89:ARG:HA	1:B:190:GLU:O	2.09	0.53
1:B:541:ILE:CG2	1:A:414:LEU:HD23	2.38	0.53
1:B:475:PRO:O	1:B:501:LYS:HD2	2.09	0.52
1:A:457:THR:O	1:A:460:TYR:HB2	2.10	0.52
1:A:285:ARG:HH11	1:A:285:ARG:HG3	1.74	0.52
1:A:509:GLU:O	1:A:512:GLU:HB3	2.10	0.52
1:A:309:ILE:HG23	1:A:338:ILE:HG21	1.91	0.52
1:B:116:TRP:CH2	1:B:272:VAL:HG11	2.46	0.51
1:A:11:GLN:HE21	1:A:53:ASP:HB3	1.76	0.51
1:A:362:ASN:HA	1:A:366:LEU:HD23	1.93	0.51
1:B:254:TRP:CG	3:B:602:COA:H32	2.46	0.51
1:B:135:ASN:HB3	1:B:524:PRO:HD2	1.93	0.51
1:B:524:PRO:O	1:B:527:VAL:HG22	2.11	0.51
1:A:419:GLU:HA	1:A:422:ASN:HD22	1.76	0.51
1:B:284:ARG:HD3	1:B:315:GLN:OE1	2.11	0.51
1:A:379:LEU:HD23	1:A:379:LEU:C	2.31	0.51
1:A:131:PRO:HG2	1:A:208:TYR:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASP:OD2	1:A:276:ASN:ND2	2.44	0.50
1:A:238:VAL:O	1:A:348:ARG:NH2	2.39	0.50
1:B:122:VAL:HG11	1:B:129:MET:HB3	1.93	0.50
1:B:450:ARG:HG3	1:B:450:ARG:NH1	2.27	0.49
1:B:131:PRO:HG2	1:B:208:TYR:CE1	2.46	0.49
1:B:457:THR:HG23	1:B:492:GLN:O	2.12	0.49
1:A:68:ARG:NH2	1:A:293:LEU:HD21	2.27	0.49
1:A:532:GLU:HA	1:A:566:ASN:HA	1.93	0.49
1:B:459:ASP:HB3	3:B:602:COA:H62	1.94	0.49
1:A:238:VAL:HG22	1:A:240:VAL:HG22	1.95	0.49
1:A:524:PRO:O	1:A:527:VAL:HG22	2.12	0.49
1:B:88:ASN:HB3	1:B:194:ALA:CB	2.42	0.49
1:A:197:GLU:HG3	1:A:199:THR:HG23	1.93	0.49
1:B:182:GLU:H	1:B:184:TRP:HD1	1.60	0.48
1:B:440:ASP:HB3	1:B:444:TYR:HB2	1.95	0.48
1:B:88:ASN:HB3	1:B:194:ALA:HB2	1.94	0.48
1:B:508:LYS:CA	1:B:567:GLU:HG2	2.43	0.48
1:A:340:LYS:HD2	1:A:346:THR:OG1	2.13	0.48
1:A:90:VAL:CG1	1:A:121:ALA:HB2	2.38	0.48
1:A:237:ILE:HG21	1:A:361:GLY:HA3	1.96	0.48
1:A:246:HIS:HE2	1:A:260:SER:HB3	1.77	0.48
1:A:401:ILE:HD11	1:A:437:ALA:CB	2.42	0.48
1:A:568:TYR:O	1:A:569:VAL:HG23	2.13	0.48
1:A:90:VAL:HG23	1:A:187:LEU:HD22	1.95	0.48
1:A:235:ALA:HA	1:A:238:VAL:HG13	1.94	0.48
1:A:88:ASN:HB3	1:A:194:ALA:CB	2.43	0.47
1:A:418:ASP:OD1	1:A:420:LYS:HE2	2.14	0.47
1:B:85:LEU:HB3	1:B:89:ARG:HH12	1.79	0.47
1:A:180:LYS:HB3	1:A:184:TRP:CD1	2.48	0.47
1:B:410:ILE:HD12	1:B:411:GLY:H	1.79	0.47
1:B:90:VAL:CG2	1:B:121:ALA:HB2	2.44	0.47
1:B:184:TRP:HA	1:B:184:TRP:CE3	2.49	0.47
1:B:390:LYS:HD3	1:A:542:SER:O	2.15	0.47
1:B:563:VAL:CG1	1:B:564:GLY:N	2.77	0.47
1:A:244:ASP:OD2	1:A:322:ARG:NH2	2.39	0.47
1:A:436:LYS:O	1:A:448:VAL:HG22	2.15	0.47
1:B:116:TRP:CZ3	1:B:272:VAL:HG11	2.51	0.46
1:A:546:ARG:NH2	1:A:549:GLU:HG3	2.30	0.46
1:B:418:ASP:OD1	1:B:420:LYS:HE2	2.16	0.46
1:B:381:ASP:OD1	1:B:383:ARG:NE	2.49	0.46
1:B:563:VAL:HG12	1:B:564:GLY:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:LYS:NZ	1:B:242:GLU:O	2.47	0.46
1:A:435:ASP:HB3	1:A:447:PHE:HE1	1.81	0.46
1:A:244:ASP:CG	1:A:322:ARG:HH12	2.19	0.46
1:B:385:LEU:HD12	1:B:402:THR:HG21	1.98	0.45
1:A:438:TYR:CE1	1:A:446:TYR:HB2	2.51	0.45
1:B:438:TYR:CE1	1:B:446:TYR:HB2	2.51	0.45
1:B:234:THR:HA	1:B:358:ALA:HB2	1.99	0.45
1:A:201:GLY:O	1:A:225:VAL:HG12	2.17	0.45
1:B:142:LYS:CD	1:B:166:ALA:HA	2.43	0.45
1:B:440:ASP:O	1:B:441:GLU:C	2.53	0.45
1:B:529:ARG:HG3	1:B:569:VAL:HG22	1.99	0.45
1:B:140:GLU:O	1:B:143:TYR:HB3	2.18	0.44
1:B:170:LEU:HD13	1:B:172:VAL:HG13	1.99	0.44
1:A:406:ASN:HB3	1:A:407:PRO:CD	2.47	0.44
1:A:362:ASN:HB3	1:A:368:VAL:HG22	1.98	0.44
1:B:494:VAL:HB	1:B:528:PRO:HA	1.99	0.44
1:B:55:HIS:O	1:B:59:ARG:N	2.46	0.44
1:B:233:THR:CG2	1:B:358:ALA:O	2.65	0.44
1:B:401:ILE:HD11	1:B:437:ALA:HB2	1.98	0.44
1:B:406:ASN:HB3	1:B:407:PRO:CD	2.47	0.44
1:A:237:ILE:O	1:A:348:ARG:NH1	2.48	0.44
1:B:69:ASP:OD2	1:B:276:ASN:ND2	2.49	0.44
1:B:233:THR:CG2	1:B:377:HIS:CG	2.99	0.44
1:B:70:ILE:HD11	1:B:275:ILE:HG23	2.00	0.44
1:B:324:VAL:CG1	1:B:347:ILE:HG12	2.47	0.44
1:B:440:ASP:HB2	1:B:446:TYR:HE1	1.83	0.44
1:A:468:GLU:CD	1:A:547:ARG:HH21	2.20	0.43
1:B:291:GLU:OE2	1:B:317:ARG:N	2.47	0.43
1:B:312:ASP:O	1:B:315:GLN:HG2	2.18	0.43
1:B:216:MET:SD	1:B:466:GLU:HA	2.58	0.43
1:B:108:MET:O	1:B:155:SER:HA	2.19	0.43
1:A:108:MET:O	1:A:155:SER:HA	2.18	0.43
1:A:256:LYS:NZ	1:A:299:CYS:SG	2.90	0.42
1:B:450:ARG:HG3	1:B:450:ARG:HH11	1.84	0.42
1:B:532:GLU:HA	1:B:566:ASN:HA	2.01	0.42
1:A:116:TRP:CZ3	1:A:272:VAL:HG11	2.54	0.42
1:A:217:PRO:HD3	1:A:466:GLU:HG2	2.02	0.42
1:A:249:LEU:O	1:A:301:PRO:HD3	2.19	0.42
1:B:70:ILE:CD1	1:B:289:GLU:HG3	2.49	0.42
1:B:90:VAL:HB	1:B:187:LEU:HB3	2.00	0.42
1:B:440:ASP:CB	1:B:444:TYR:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:GLU:O	1:A:516:GLU:HG2	2.18	0.42
1:A:302:PRO:HD2	1:A:329:GLU:HG3	2.00	0.42
1:A:36:VAL:HA	1:A:39:LEU:HD12	2.01	0.42
1:B:456:LYS:HE2	1:B:459:ASP:HA	2.02	0.42
1:A:25:ASN:OD1	1:A:26:GLU:N	2.53	0.42
1:B:555:GLU:HA	1:B:558:ARG:HD2	2.02	0.42
1:B:353:GLN:HB3	1:B:355:GLU:OE1	2.20	0.42
1:A:55:HIS:ND1	1:A:59:ARG:NH1	2.68	0.42
1:A:120:LEU:HD23	1:A:262:PHE:HZ	1.84	0.42
1:B:106:TYR:HB2	1:B:153:ILE:HD13	2.01	0.42
1:B:305:TRP:CH2	1:B:324:VAL:HG13	2.54	0.42
1:A:256:LYS:HZ2	1:A:256:LYS:HG2	1.66	0.42
1:B:151:SER:O	1:B:172:VAL:HB	2.20	0.41
1:A:70:ILE:CD1	1:A:289:GLU:HG3	2.49	0.41
1:A:135:ASN:HB3	1:A:524:PRO:HD2	2.01	0.41
1:A:440:ASP:O	1:A:441:GLU:C	2.54	0.41
1:A:440:ASP:HB3	1:A:444:TYR:HB2	2.02	0.41
1:A:255:ALA:O	1:A:258:ALA:N	2.53	0.41
1:A:410:ILE:HD12	1:A:411:GLY:H	1.84	0.41
1:A:396:TYR:OH	1:A:440:ASP:OD1	2.31	0.41
1:B:212:GLY:HA3	1:B:421:LYS:NZ	2.35	0.41
1:B:226:SER:O	1:B:411:GLY:HA2	2.21	0.41
1:B:468:GLU:HG2	1:B:482:VAL:HG23	2.02	0.41
1:A:14:PHE:O	1:A:18:ILE:HG13	2.20	0.41
1:A:552:LYS:HB2	1:A:552:LYS:HE3	1.95	0.41
1:B:70:ILE:HD11	1:B:275:ILE:CG2	2.51	0.41
1:B:234:THR:O	1:B:238:VAL:HG12	2.21	0.41
1:B:373:MET:HE3	1:B:445:PHE:HB3	2.03	0.41
1:B:201:GLY:O	1:B:225:VAL:HG12	2.21	0.40
1:A:435:ASP:HB3	1:A:447:PHE:CE1	2.56	0.40
1:B:227:TYR:N	1:B:228:PRO:CD	2.84	0.40
1:B:33:VAL:HG21	1:B:378:PRO:HB2	2.03	0.40
1:B:390:LYS:CE	1:A:542:SER:HB3	2.52	0.40
1:A:87:SER:HA	1:A:90:VAL:HG12	2.01	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	560/570 (98%)	516 (92%)	44 (8%)	0	100	100
1	B	560/570 (98%)	512 (91%)	45 (8%)	3 (0%)	29	64
All	All	1120/1140 (98%)	1028 (92%)	89 (8%)	3 (0%)	41	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	239	GLY
1	B	259	TRP
1	B	564	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	493/502 (98%)	452 (92%)	41 (8%)	11	38
1	B	493/502 (98%)	461 (94%)	32 (6%)	17	47
All	All	986/1004 (98%)	913 (93%)	73 (7%)	13	42

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	77	LYS
1	B	90	VAL
1	B	100	LYS

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Mol	Chain	Res	Type
1	B	114	MET
1	B	119	PHE
1	B	159	ARG
1	B	170	LEU
1	B	171	LYS
1	B	182	GLU
1	B	200	ARG
1	B	202	GLU
1	B	207	ASN
1	B	227	TYR
1	B	229	VAL
1	B	285	ARG
1	B	325	VAL
1	B	326	SER
1	B	340	LYS
1	B	360	VAL
1	B	383	ARG
1	B	413	PHE
1	B	417	SER
1	B	420	LYS
1	B	458	SER
1	B	505	MET
1	B	529	ARG
1	B	535	ASP
1	B	549	GLU
1	B	558	ARG
1	B	562	GLU
1	B	565	GLN
1	B	568	TYR
1	A	57	LYS
1	A	119	PHE
1	A	149	LYS
1	A	178	ASP
1	A	180	LYS
1	A	183	THR
1	A	185	ASN
1	A	186	SER
1	A	192	SER
1	A	199	THR
1	A	200	ARG
1	A	202	GLU
1	A	207	ASN

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Mol	Chain	Res	Type
1	A	213	THR
1	A	227	TYR
1	A	229	VAL
1	A	238	VAL
1	A	240	VAL
1	A	256	LYS
1	A	285	ARG
1	A	317	ARG
1	A	319	GLU
1	A	325	VAL
1	A	326	SER
1	A	329	GLU
1	A	360	VAL
1	A	367	LYS
1	A	373	MET
1	A	383	ARG
1	A	413	PHE
1	A	417	SER
1	A	456	LYS
1	A	458	SER
1	A	485	VAL
1	A	517	LYS
1	A	529	ARG
1	A	535	ASP
1	A	548	VAL
1	A	549	GLU
1	A	553	ARG
1	A	562	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	11	GLN
1	B	307	GLN
1	A	11	GLN
1	A	248	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	COA	A	602	-	41,50,50	0.72	1 (2%)	52,75,75	0.86	2 (3%)
2	6R9	B	601	-	24,28,28	1.05	1 (4%)	26,42,42	1.29	5 (19%)
2	6R9	A	601	-	24,28,28	0.99	1 (4%)	26,42,42	0.92	2 (7%)
3	COA	B	602	-	41,50,50	0.63	1 (2%)	52,75,75	1.04	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	A	602	-	-	17/44/64/64	0/3/3/3
2	6R9	B	601	-	-	1/9/31/31	0/3/3/3
2	6R9	A	601	-	-	0/9/31/31	0/3/3/3
3	COA	B	602	-	-	8/44/64/64	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	6R9	P05-O04	4.17	1.69	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	6R9	P05-O04	3.48	1.67	1.60
3	A	602	COA	P3B-O3B	2.34	1.63	1.59
3	B	602	COA	P3B-O3B	2.05	1.63	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	COA	C7P-C6P-C5P	-4.32	105.16	112.36
3	A	602	COA	C2B-C3B-C4B	-3.26	97.45	103.22
2	B	601	6R9	O08-P05-O06	-3.10	96.94	109.07
2	B	601	6R9	C18-C23-N24	2.76	124.54	120.35
2	A	601	6R9	C18-C23-N24	2.52	124.18	120.35
2	B	601	6R9	C11-C12-C13	2.28	104.42	100.98
2	A	601	6R9	O07-P05-O04	2.25	111.49	104.14
3	A	602	COA	C5A-C6A-N6A	2.23	123.75	120.35
2	B	601	6R9	O04-P05-O06	2.15	116.09	109.45
2	B	601	6R9	O04-P05-O08	2.08	109.00	102.92

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	COA	C3B-O3B-P3B-O7A
3	A	602	COA	C3B-O3B-P3B-O8A
3	A	602	COA	CCP-O6A-P2A-O3A
3	A	602	COA	CCP-O6A-P2A-O4A
3	A	602	COA	CDP-CBP-CCP-O6A
3	A	602	COA	CAP-CBP-CCP-O6A
3	A	602	COA	CAP-C9P-N8P-C7P
3	A	602	COA	S1P-C2P-C3P-N4P
3	A	602	COA	C4B-C3B-O3B-P3B
3	B	602	COA	C6P-C5P-N4P-C3P
3	B	602	COA	O5P-C5P-N4P-C3P
3	A	602	COA	CEP-CBP-CCP-O6A
3	A	602	COA	O9P-C9P-N8P-C7P
3	A	602	COA	O5P-C5P-N4P-C3P
3	A	602	COA	C4B-C5B-O5B-P1A
3	A	602	COA	O5P-C5P-C6P-C7P
3	B	602	COA	C4B-C5B-O5B-P1A
3	A	602	COA	CCP-O6A-P2A-O5A
3	B	602	COA	CEP-CBP-CCP-O6A
3	A	602	COA	N4P-C5P-C6P-C7P

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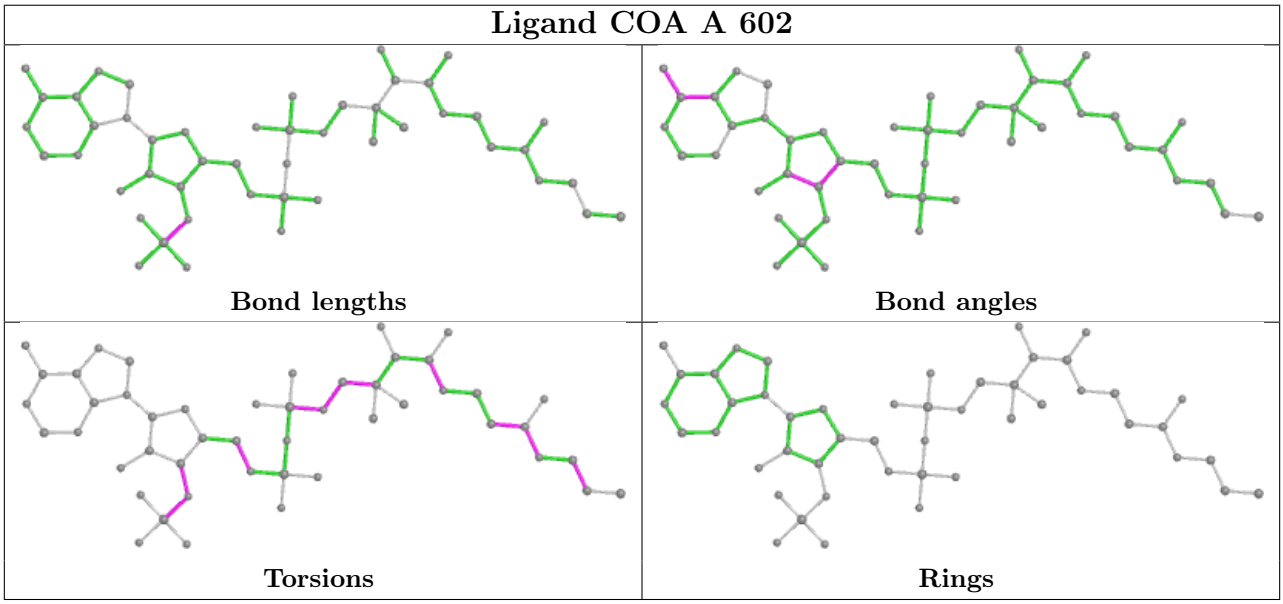
Mol	Chain	Res	Type	Atoms
3	B	602	COA	C5P-C6P-C7P-N8P
3	B	602	COA	C3B-C4B-C5B-O5B
3	B	602	COA	P2A-O3A-P1A-O1A
3	B	602	COA	P2A-O3A-P1A-O2A
3	A	602	COA	CBP-CCP-O6A-P2A
2	B	601	6R9	C09-O08-P05-O06

There are no ring outliers.

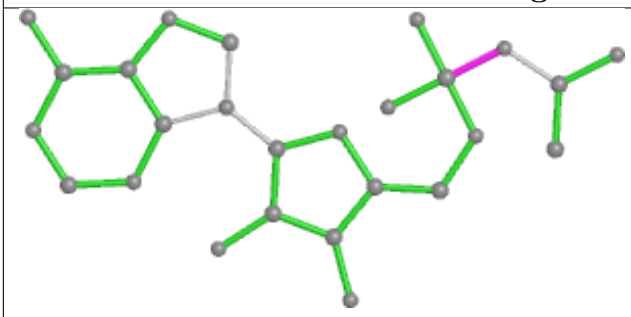
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	COA	2	0

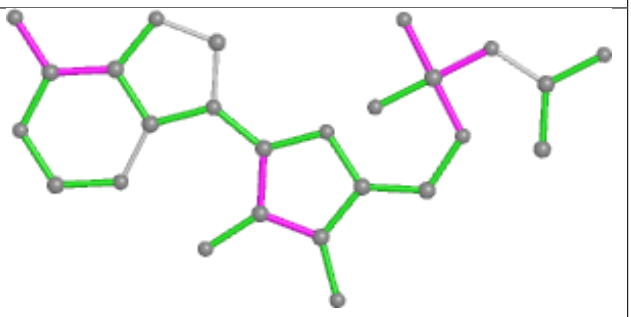
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.



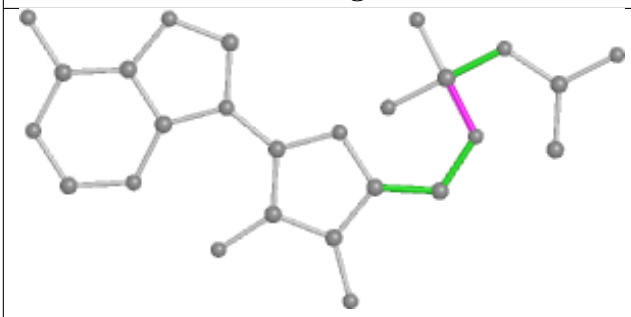
Ligand 6R9 B 601



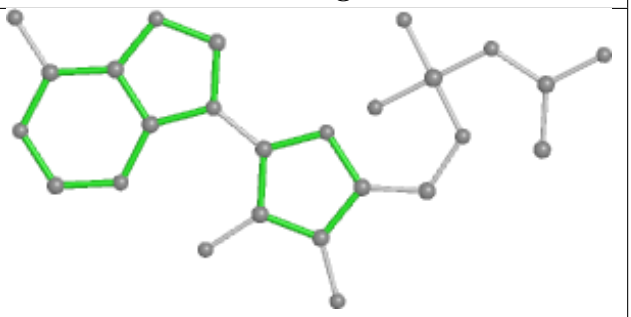
Bond lengths



Bond angles

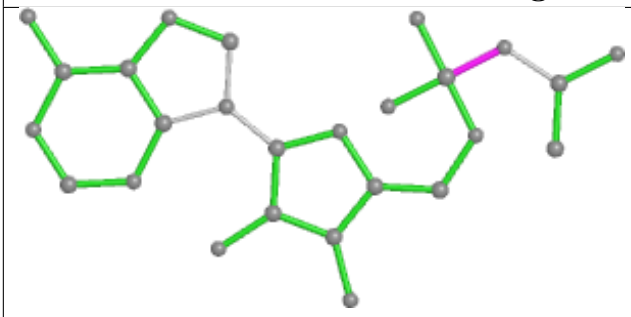


Torsions

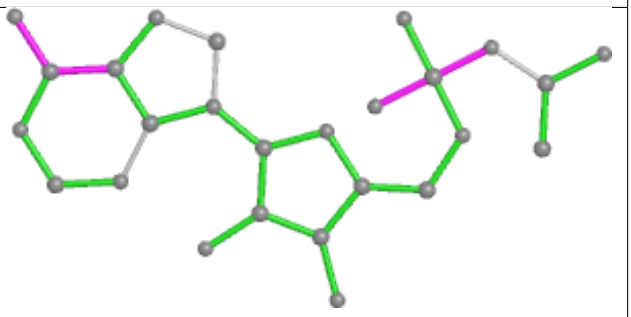


Rings

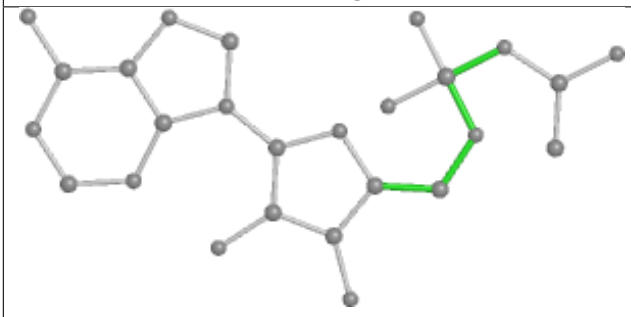
Ligand 6R9 A 601



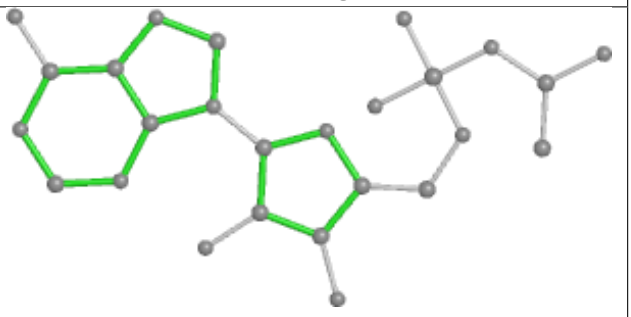
Bond lengths



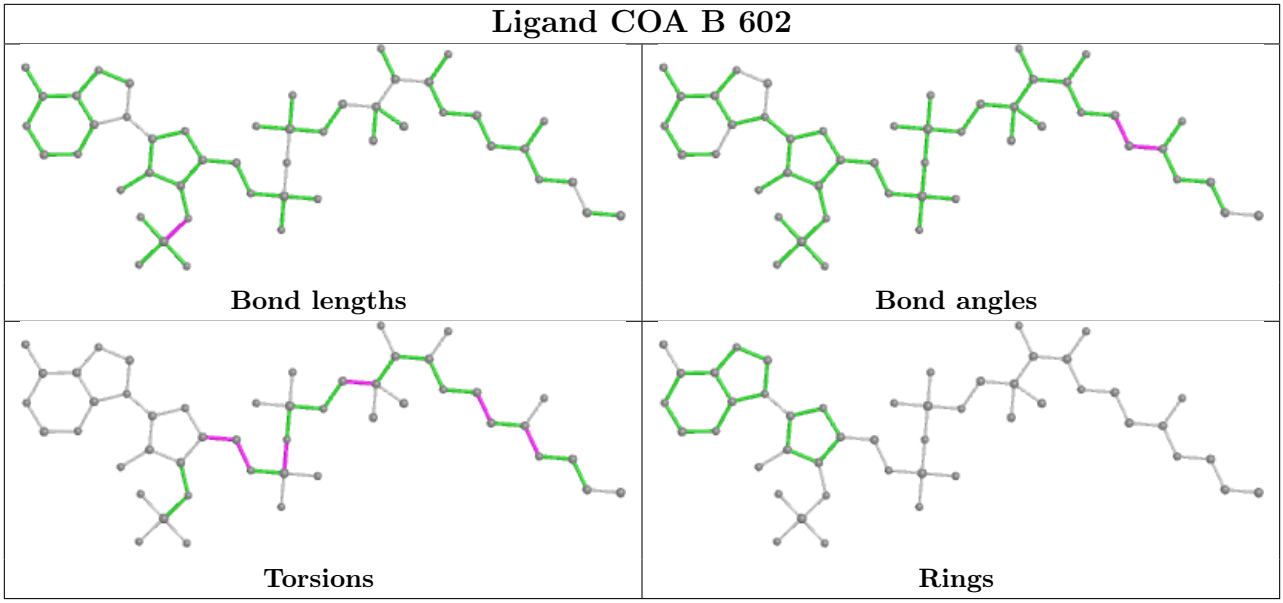
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	562/570 (98%)	-0.01	6 (1%)	80	64	47, 81, 120, 159	0
1	B	562/570 (98%)	-0.01	4 (0%)	87	75	51, 84, 123, 191	0
All	All	1124/1140 (98%)	-0.01	10 (0%)	84	69	47, 82, 121, 191	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	193	ASN	6.5
1	A	37	GLY	3.6
1	B	167	LEU	3.0
1	A	403	VAL	3.0
1	A	406	ASN	3.0
1	B	169	SER	2.6
1	B	119	PHE	2.5
1	B	170	LEU	2.3
1	A	391	GLU	2.2
1	A	384	LEU	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

There are no monosaccharides in this entry.

6.4 Ligands (i)

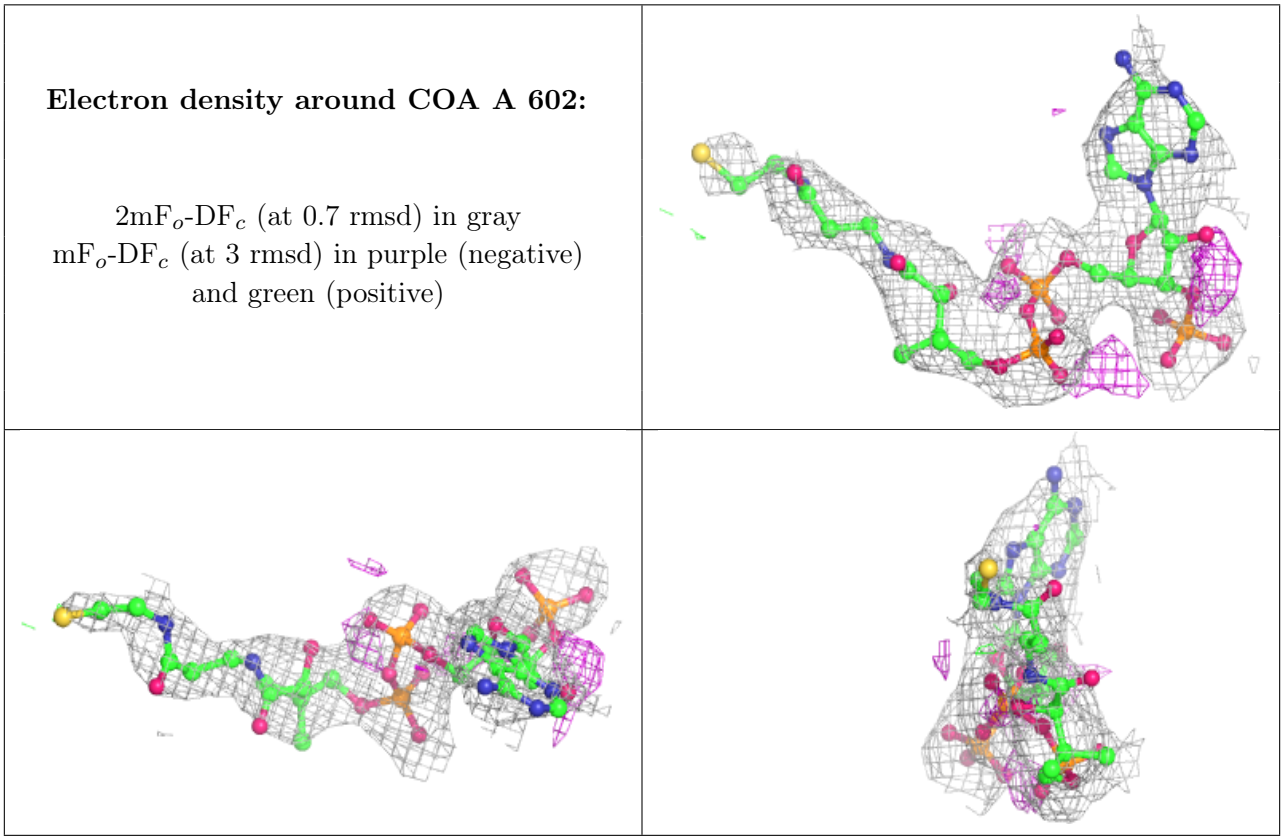
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	COA	A	602	48/48	0.92	0.23	73,96,134,143	0
3	COA	B	602	48/48	0.93	0.21	71,98,158,200	0
2	6R9	A	601	26/26	0.93	0.22	47,67,88,98	0
2	6R9	B	601	26/26	0.97	0.19	53,68,78,86	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.

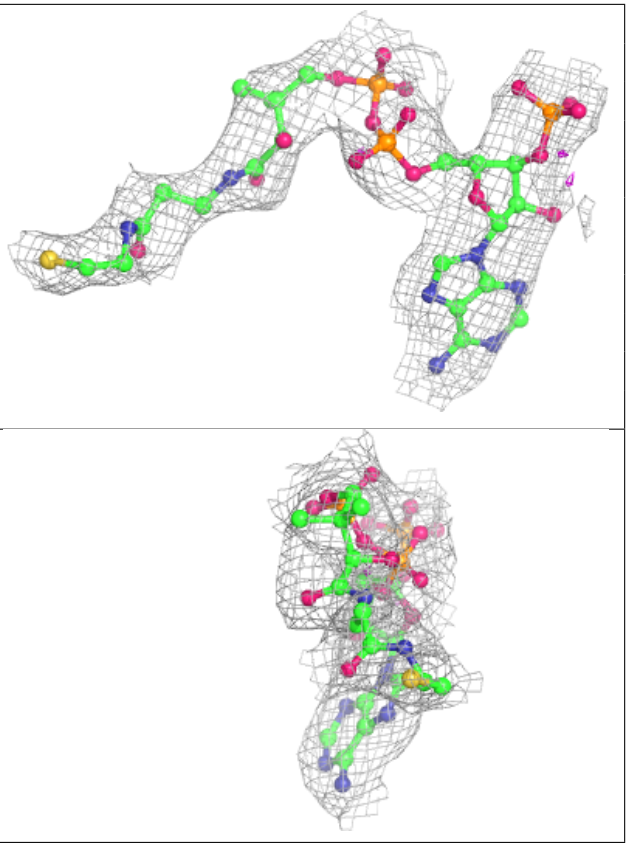
Electron density around COA A 602:

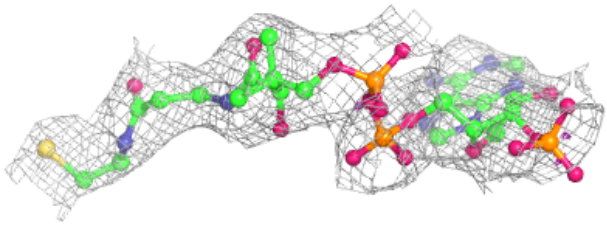
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around COA B 602:

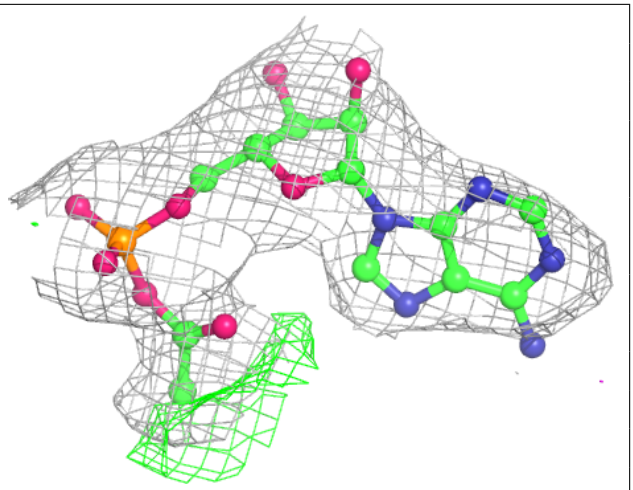
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

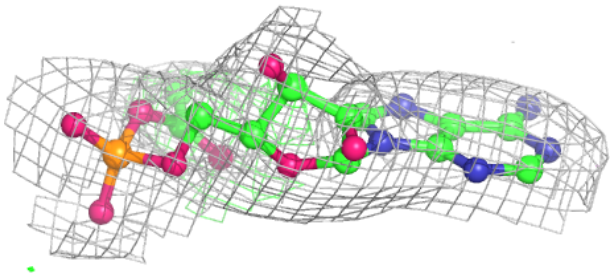


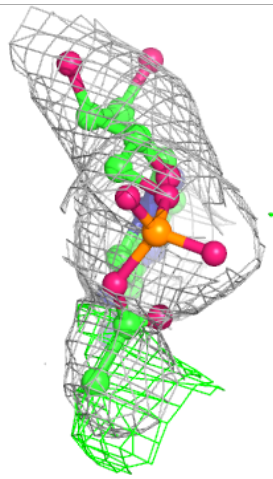


Electron density around 6R9 A 601:

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

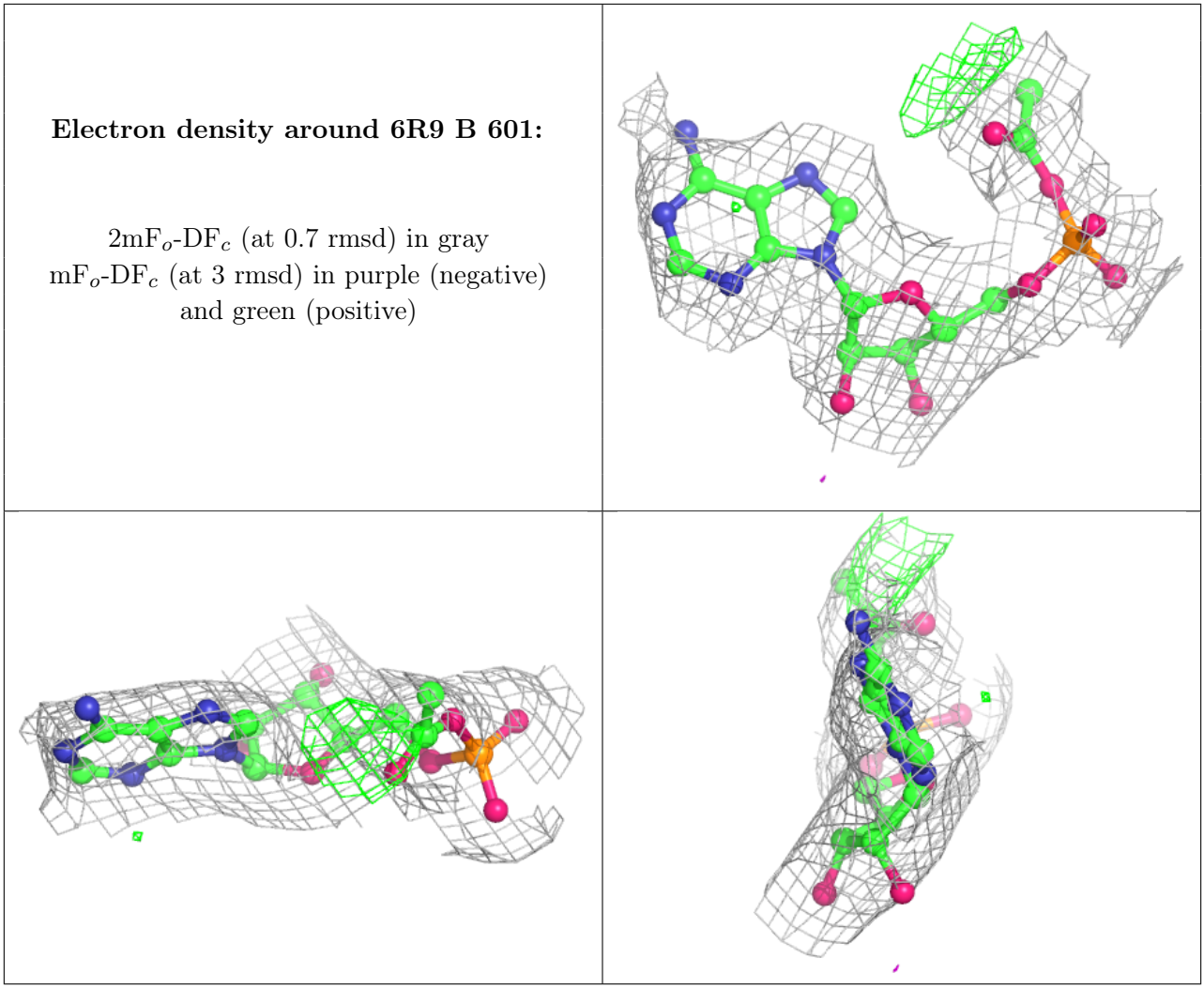






Electron density around 6R9 B 601:

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



6.5 Other polymers (i)

There are no such residues in this entry.