



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 5, 2017 – 12:22 PM EDT

PDB ID : 5WX3  
Title : Alkyldiketide-CoA synthase from Evodia rutaecarpa  
Authors : Matsui, T.; Kodama, T.; Tadakoshi, T.; Morita, H.  
Deposited on : 2017-01-06  
Resolution : 1.80 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029077  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029077

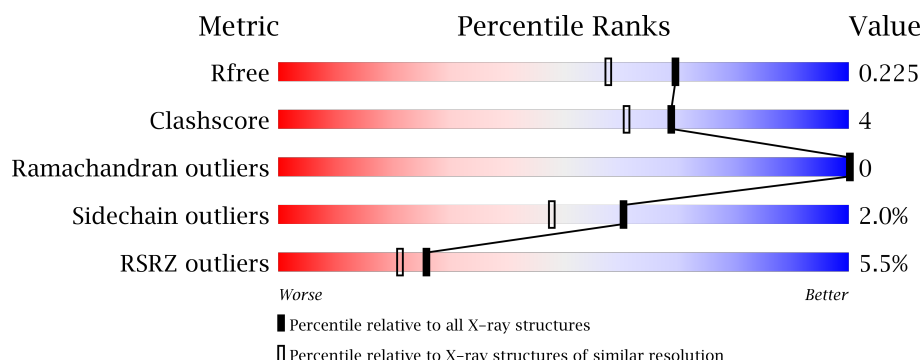
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	4827 (1.80-1.80)
Clashscore	112137	5742 (1.80-1.80)
Ramachandran outliers	110173	5676 (1.80-1.80)
Sidechain outliers	110143	5675 (1.80-1.80)
RSRZ outliers	101464	4906 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	396	<div> <div>4%</div> <div>88%</div> <div>7%</div> <div>5%</div> </div>
1	B	396	<div> <div>4%</div> <div>82%</div> <div>9%</div> <div>8%</div> </div>
1	C	396	<div> <div>6%</div> <div>76%</div> <div>13%</div> <div>11%</div> </div>
1	D	396	<div> <div>7%</div> <div>81%</div> <div>12%</div> <div>7%</div> </div>

## 2 Entry composition [i](#)

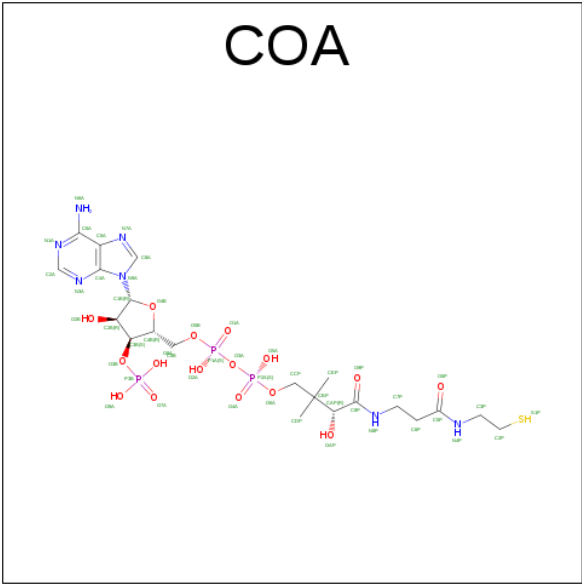
There are 4 unique types of molecules in this entry. The entry contains 12075 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alkyldiketide-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	0	0
			2920	1859	496	539	26			
1	B	363	Total	C	N	O	S	0	1	0
			2845	1815	484	520	26			
1	C	353	Total	C	N	O	S	0	1	0
			2761	1764	466	507	24			
1	D	370	Total	C	N	O	S	0	0	0
			2883	1837	491	529	26			

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: C<sub>21</sub>H<sub>36</sub>N<sub>7</sub>O<sub>16</sub>P<sub>3</sub>S).



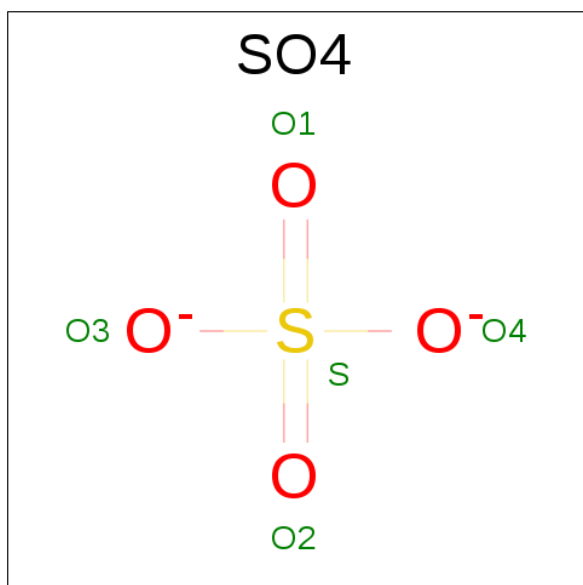
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	140	Total	O	0	0
			140	140		
4	B	122	Total	O	0	0
			122	122		
4	C	130	Total	O	0	0
			130	130		

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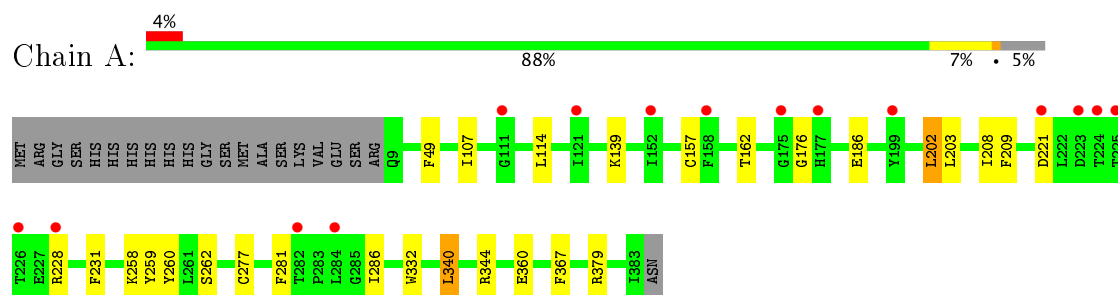
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	62	Total	O	0	0
			62	62		

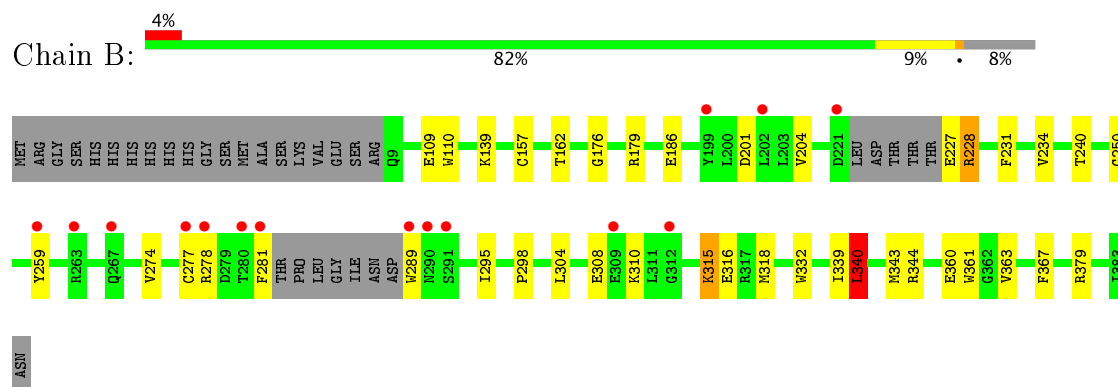
### 3 Residue-property plots [i](#)

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

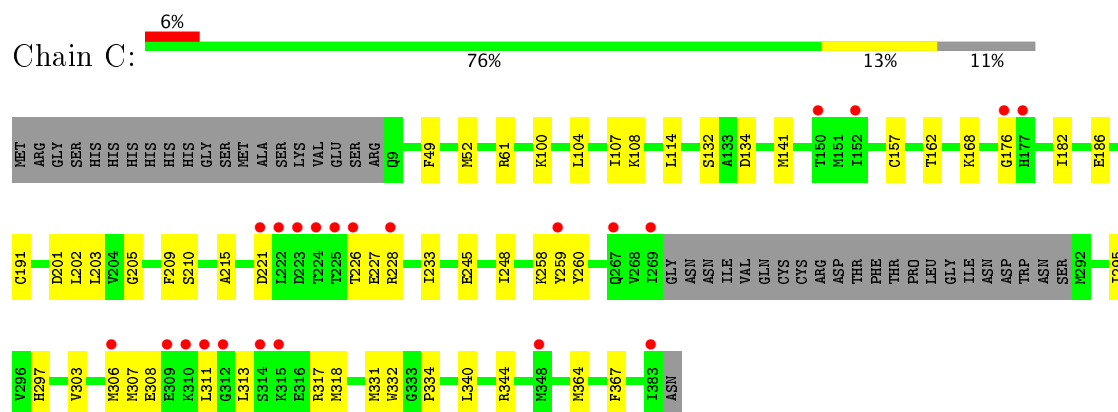
- Molecule 1: Alkyldiketide-CoA synthase



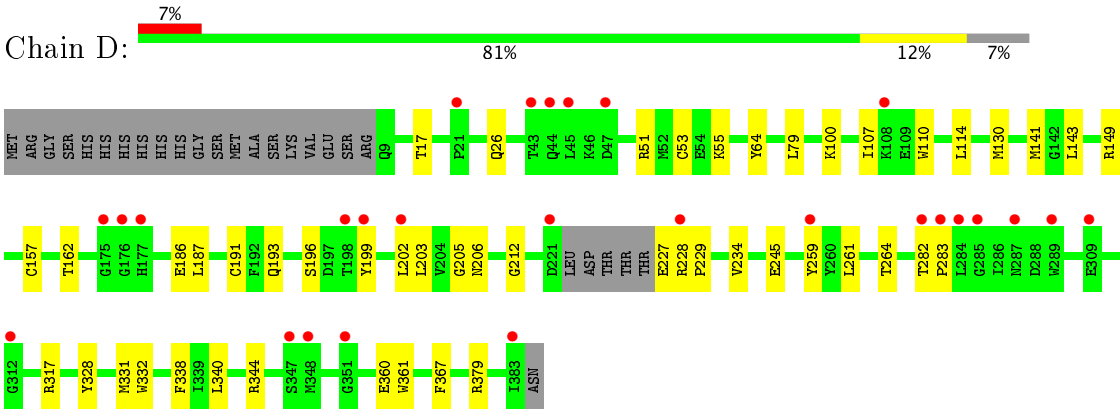
- Molecule 1: Alkyldiketide-CoA synthase



- Molecule 1: Alkyldiketide-CoA synthase



- Molecule 1: Alkyldiketide-CoA synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	164.59 Å   84.12 Å   138.67 Å 90.00°   124.74°   90.00°	Depositor
Resolution (Å)	39.74 – 1.80 39.74 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.74-1.80) 99.5 (39.74-1.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 1.81 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.192 , 0.226 0.188 , 0.225	Depositor DCC
$R_{free}$ test set	7145 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.5	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 44.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.040 for h,-k,-h-l	Depositor
Outliers	1 of 142922 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12075	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: COA, SO4

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	0.41	0/2983	0.57	1/4040 (0.0%)
1	B	0.40	0/2906	0.56	1/3929 (0.0%)
1	C	0.42	1/2820 (0.0%)	0.55	0/3815
1	D	0.37	0/2945	0.50	0/3985
All	All	0.40	1/11654 (0.0%)	0.54	2/15769 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	297	HIS	C-N	5.23	1.44	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	LEU	CA-CB-CG	5.13	127.09	115.30
1	B	340	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2920	0	2923	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2845	0	2844	24	0
1	C	2761	0	2774	32	0
1	D	2883	0	2886	31	0
2	A	48	0	32	2	0
2	B	48	0	32	2	0
2	C	48	0	32	2	0
2	D	48	0	32	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	140	0	0	1	0
4	B	122	0	0	0	0
4	C	130	0	0	0	0
4	D	62	0	0	0	0
All	All	12075	0	11555	100	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (100) 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:A:401:COA:O4B	2:A:401:COA:C1B	1.67	1.28
2:B:401:COA:C1B	2:B:401:COA:O4B	1.67	1.27
2:D:401:COA:O4B	2:D:401:COA:C1B	1.66	1.14
2:C:401:COA:O4B	2:C:401:COA:C1B	1.66	1.13
1:D:360:GLU:OE2	1:D:379:ARG:NH1	2.21	0.73
1:B:360:GLU:OE2	1:B:379:ARG:NH1	2.25	0.70
1:D:110:TRP:NE1	1:D:227:GLU:OE1	2.25	0.69
1:A:360:GLU:OE1	1:A:379:ARG:NH1	2.27	0.67
1:D:212:GLY:HA3	1:D:331:MET:HE3	1.77	0.66
1:C:303:VAL:HG11	1:C:367:PHE:HZ	1.60	0.66
1:C:226:THR:HG23	1:C:227:GLU:HG3	1.78	0.65
1:C:52:MET:HE1	1:C:203:LEU:HG	1.81	0.63
1:C:104:LEU:O	1:C:108:LYS:HG2	1.98	0.63
1:D:331:MET:HE1	1:D:338:PHE:CZ	2.34	0.63
1:C:202:LEU:HD23	1:C:259[A]:TYR:O	1.99	0.62
1:D:234:VAL:HG21	1:D:361:TRP:HZ3	1.64	0.61
1:B:295:ILE:HD11	1:B:343:MET:HE2	1.84	0.59
1:D:51:ARG:O	1:D:55:LYS:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:GLU:OE2	1:B:228:ARG:NH2	2.32	0.57
1:C:202:LEU:O	1:C:259[A]:TYR:OH	2.09	0.57
1:B:186:GLU:HG3	1:B:332:TRP:HB2	1.85	0.57
1:A:176:GLY:HA2	1:A:221:ASP:HB2	1.86	0.56
1:C:176:GLY:HA2	1:C:221:ASP:HB2	1.88	0.56
1:D:212:GLY:HA3	1:D:331:MET:CE	2.36	0.56
1:C:157:CYS:HB2	1:C:367:PHE:O	2.05	0.55
1:C:205:GLY:HA3	1:C:259[A]:TYR:CE1	2.42	0.55
1:D:199:TYR:HB3	1:D:202:LEU:HD12	1.88	0.54
1:D:186:GLU:HG3	1:D:332:TRP:HB2	1.89	0.54
1:C:186:GLU:HG3	1:C:332:TRP:HB2	1.92	0.52
1:D:107:ILE:HD13	1:D:114:LEU:HD21	1.91	0.51
1:B:298:PRO:HD3	1:B:339:ILE:HD11	1.93	0.51
1:D:157:CYS:HB2	1:D:367:PHE:O	2.10	0.51
1:C:191:CYS:HB2	1:C:259[A]:TYR:HD2	1.77	0.50
1:D:191:CYS:O	1:D:259:TYR:HE2	1.95	0.50
1:A:157:CYS:HB2	1:A:367:PHE:O	2.12	0.50
1:C:209:PHE:HE2	1:C:259[A]:TYR:CD1	2.30	0.49
1:D:100:LYS:HG3	1:D:141:MET:HG2	1.94	0.49
1:B:281:PHE:CZ	1:B:363:VAL:HB	2.47	0.49
1:B:308:GLU:HG2	1:B:318:MET:HG3	1.95	0.49
1:B:157:CYS:HB2	1:B:367:PHE:O	2.12	0.49
1:C:308:GLU:HG2	1:C:318:MET:HG3	1.94	0.49
1:C:308:GLU:CG	1:C:318:MET:HG3	2.42	0.49
1:D:202:LEU:O	1:D:206:ASN:ND2	2.46	0.48
1:B:278:ARG:HA	1:B:289:TRP:HH2	1.78	0.48
1:C:132:SER:HB2	1:C:134:ASP:OD1	2.13	0.48
1:B:110:TRP:NE1	1:B:227:GLU:OE2	2.40	0.48
1:B:234:VAL:HG21	1:B:361:TRP:HZ3	1.79	0.48
1:C:49:PHE:HA	1:C:52:MET:HE3	1.96	0.47
1:A:209:PHE:CE2	1:A:259:TYR:HD2	2.33	0.47
1:C:49:PHE:HD2	1:C:52:MET:CE	2.29	0.46
1:A:157:CYS:SG	4:A:502:HOH:O	2.34	0.46
1:B:274:VAL:HG21	1:B:310:LYS:HB2	1.97	0.46
1:A:107:ILE:HD13	1:A:114:LEU:HD23	1.96	0.46
1:B:250:GLY:HA3	1:D:130:MET:HE2	1.97	0.46
1:D:328:TYR:HB3	1:D:331:MET:SD	2.56	0.46
1:C:107:ILE:HD13	1:C:114:LEU:CD2	2.46	0.46
1:D:317:ARG:NE	1:D:317:ARG:HA	2.31	0.46
1:D:282:THR:OG1	1:D:283:PRO:HD3	2.16	0.45
1:B:204:VAL:HG13	2:B:401:COA:H133	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:VAL:HG11	1:C:367:PHE:CZ	2.46	0.45
1:C:317:ARG:NE	1:C:317:ARG:HA	2.31	0.45
1:A:186:GLU:HG3	1:A:332:TRP:HB2	1.98	0.45
1:D:228:ARG:NH1	1:D:229:PRO:HD2	2.32	0.45
1:B:201:ASP:N	1:B:201:ASP:OD2	2.48	0.45
1:D:205:GLY:HA3	1:D:259:TYR:CE1	2.52	0.44
1:C:248:ILE:HD11	2:C:401:COA:H22	2.00	0.44
1:A:208:ILE:HD13	2:A:401:COA:H71	2.00	0.44
1:C:258:LYS:HE2	1:C:260:TYR:OH	2.17	0.44
1:A:139:LYS:NZ	1:C:245:GLU:OE2	2.31	0.44
1:C:61:ARG:HD2	1:C:210:SER:HB3	2.00	0.44
1:D:17:THR:HB	1:D:338:PHE:CZ	2.52	0.44
1:A:258:LYS:HE2	1:A:260:TYR:OH	2.18	0.43
1:B:304:LEU:O	1:B:308:GLU:HG3	2.18	0.43
1:C:100:LYS:HG3	1:C:141:MET:HG2	2.00	0.43
1:D:193:GLN:HG3	1:D:202:LEU:HD22	2.00	0.43
1:D:26:GLN:HG3	1:D:53:CYS:HB3	2.00	0.43
1:C:201:ASP:N	1:C:201:ASP:OD2	2.50	0.42
1:B:139:LYS:NZ	1:D:245:GLU:OE2	2.45	0.42
1:B:240:THR:OG1	1:D:149:ARG:NH2	2.43	0.42
1:D:202:LEU:HD23	1:D:259:TYR:CE2	2.55	0.42
1:D:79:LEU:HD22	1:D:196:SER:HB2	2.02	0.42
1:B:176:GLY:O	1:B:179:ARG:NH1	2.52	0.42
1:D:261:LEU:O	2:D:401:COA:N6A	2.51	0.42
1:B:295:ILE:HD11	1:B:343:MET:CE	2.48	0.42
1:B:231:PHE:CE2	1:B:340:LEU:HD22	2.55	0.42
1:B:228:ARG:HD3	1:B:228:ARG:O	2.20	0.42
1:A:231:PHE:CE1	1:A:340:LEU:HD22	2.55	0.41
1:C:311:LEU:HB2	1:C:313:LEU:HG	2.03	0.41
1:B:295:ILE:HG23	1:B:339:ILE:HB	2.02	0.41
1:C:49:PHE:HA	1:C:52:MET:CE	2.51	0.41
1:B:315:LYS:HG2	1:B:316:GLU:N	2.35	0.41
1:C:182:ILE:O	1:C:215:ALA:HA	2.20	0.41
1:C:331:MET:O	1:C:334:PRO:HD2	2.21	0.41
1:C:295:ILE:O	1:C:364:MET:HA	2.21	0.41
1:A:49:PHE:HD1	1:A:203:LEU:HG	1.85	0.40
1:D:228:ARG:CZ	1:D:229:PRO:HD2	2.51	0.40
1:C:168:LYS:HD2	1:C:233:ILE:HG22	2.03	0.40
1:D:64:TYR:HB2	1:D:187:LEU:HD22	2.02	0.40
1:A:281:PHE:HD1	1:A:286:ILE:HD13	1.87	0.40
1:D:114:LEU:HD13	1:D:143:LEU:HD23	2.03	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	373/396 (94%)	363 (97%)	10 (3%)	0	100	100
1	B	358/396 (90%)	351 (98%)	7 (2%)	0	100	100
1	C	350/396 (88%)	341 (97%)	9 (3%)	0	100	100
1	D	366/396 (92%)	357 (98%)	9 (2%)	0	100	100
All	All	1447/1584 (91%)	1412 (98%)	35 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	317/335 (95%)	310 (98%)	7 (2%)	57	44
1	B	307/335 (92%)	299 (97%)	8 (3%)	51	36
1	C	298/335 (89%)	292 (98%)	6 (2%)	60	48
1	D	312/335 (93%)	307 (98%)	5 (2%)	68	58
All	All	1234/1340 (92%)	1208 (98%)	26 (2%)	60	46

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	THR
1	A	202	LEU
1	A	228	ARG
1	A	262	SER
1	A	277	CYS
1	A	340	LEU
1	A	344	ARG
1	B	162	THR
1	B	228	ARG
1	B	259[A]	TYR
1	B	259[B]	TYR
1	B	277	CYS
1	B	315	LYS
1	B	340	LEU
1	B	344	ARG
1	C	162	THR
1	C	228	ARG
1	C	306	MET
1	C	307	MET
1	C	340	LEU
1	C	344	ARG
1	D	162	THR
1	D	203	LEU
1	D	264	THR
1	D	340	LEU
1	D	344	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	GLN
1	D	19	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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	401	-	43,50,50	4.17	14 (32%)	48,75,75	2.21	10 (20%)
3	SO4	A	402	-	4,4,4	0.22	0	6,6,6	0.11	0
2	COA	B	401	-	43,50,50	4.23	15 (34%)	48,75,75	2.09	7 (14%)
3	SO4	B	402	-	4,4,4	0.21	0	6,6,6	0.17	0
2	COA	C	401	-	43,50,50	4.15	15 (34%)	48,75,75	2.24	5 (10%)
3	SO4	C	402	-	4,4,4	0.22	0	6,6,6	0.15	0
2	COA	D	401	-	43,50,50	4.15	15 (34%)	48,75,75	2.28	8 (16%)
3	SO4	D	402	-	4,4,4	0.16	0	6,6,6	0.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COA	A	401	-	-	0/44/64/64	0/3/3/3
3	SO4	A	402	-	-	0/0/0/0	0/0/0/0
2	COA	B	401	-	-	0/44/64/64	0/3/3/3
3	SO4	B	402	-	-	0/0/0/0	0/0/0/0
2	COA	C	401	-	-	0/44/64/64	0/3/3/3
3	SO4	C	402	-	-	0/0/0/0	0/0/0/0
2	COA	D	401	-	-	0/44/64/64	0/3/3/3
3	SO4	D	402	-	-	0/0/0/0	0/0/0/0

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	COA	C2B-C1B	-13.05	1.32	1.53
2	B	401	COA	C2B-C1B	-12.82	1.33	1.53
2	A	401	COA	C2B-C1B	-12.44	1.33	1.53
2	C	401	COA	C2B-C1B	-12.34	1.34	1.53
2	C	401	COA	O4B-C4B	-6.21	1.31	1.45
2	B	401	COA	O4B-C4B	-6.18	1.31	1.45
2	A	401	COA	O4B-C4B	-5.99	1.31	1.45
2	D	401	COA	O4B-C4B	-5.91	1.31	1.45
2	D	401	COA	O3B-C3B	-2.58	1.34	1.44
2	C	401	COA	O9P-C9P	-2.57	1.18	1.23
2	B	401	COA	O3B-C3B	-2.53	1.34	1.44
2	A	401	COA	O3B-C3B	-2.27	1.35	1.44
2	C	401	COA	O3B-C3B	-2.26	1.35	1.44
2	B	401	COA	O9P-C9P	-2.16	1.19	1.23
2	D	401	COA	O9P-C9P	-2.09	1.19	1.23
2	C	401	COA	C2P-C3P	2.02	1.59	1.50
2	B	401	COA	C2P-C3P	2.04	1.59	1.50
2	A	401	COA	C2P-C3P	2.08	1.60	1.50
2	D	401	COA	C2A-N1A	2.10	1.37	1.33
2	C	401	COA	C2A-N1A	2.10	1.37	1.33
2	A	401	COA	CCP-CBP	2.18	1.55	1.52
2	D	401	COA	C2P-C3P	2.20	1.60	1.50
2	A	401	COA	C2A-N1A	2.20	1.38	1.33
2	B	401	COA	C2A-N1A	2.32	1.38	1.33
2	C	401	COA	C3B-C4B	2.32	1.59	1.52
2	D	401	COA	C3B-C4B	2.35	1.59	1.52
2	B	401	COA	P2A-O6A	2.36	1.69	1.59
2	C	401	COA	P2A-O6A	2.37	1.69	1.59
2	D	401	COA	P2A-O6A	2.39	1.69	1.59
2	B	401	COA	C3B-C4B	2.43	1.59	1.52
2	A	401	COA	P2A-O6A	2.50	1.69	1.59
2	D	401	COA	CCP-CBP	2.50	1.56	1.52
2	A	401	COA	C3B-C4B	2.55	1.59	1.52
2	C	401	COA	CCP-CBP	2.61	1.56	1.52
2	C	401	COA	C2A-N3A	2.64	1.36	1.32
2	B	401	COA	CCP-CBP	2.74	1.56	1.52
2	D	401	COA	C2A-N3A	2.78	1.36	1.32
2	A	401	COA	C2A-N3A	2.85	1.36	1.32
2	B	401	COA	C2A-N3A	2.88	1.37	1.32
2	A	401	COA	C6A-N6A	4.24	1.51	1.34
2	C	401	COA	C6A-N6A	4.26	1.51	1.34
2	B	401	COA	P3B-O3B	4.31	1.67	1.59
2	D	401	COA	C6A-N6A	4.31	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	COA	P3B-O3B	4.37	1.67	1.59
2	B	401	COA	C6A-N6A	4.46	1.52	1.34
2	C	401	COA	P3B-O3B	5.20	1.68	1.59
2	A	401	COA	P3B-O3B	5.45	1.69	1.59
2	A	401	COA	C5P-N4P	6.09	1.47	1.33
2	D	401	COA	C5P-N4P	6.27	1.48	1.33
2	C	401	COA	C5P-N4P	6.29	1.48	1.33
2	B	401	COA	C5P-N4P	6.49	1.48	1.33
2	C	401	COA	C9P-N8P	7.02	1.47	1.33
2	D	401	COA	C9P-N8P	7.10	1.48	1.33
2	A	401	COA	C9P-N8P	7.19	1.48	1.33
2	B	401	COA	C9P-N8P	7.45	1.48	1.33
2	D	401	COA	O4B-C1B	18.34	1.66	1.41
2	C	401	COA	O4B-C1B	18.58	1.66	1.41
2	A	401	COA	O4B-C1B	18.73	1.67	1.41
2	B	401	COA	O4B-C1B	18.75	1.67	1.41

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	COA	N3A-C2A-N1A	-10.15	120.02	128.86
2	C	401	COA	N3A-C2A-N1A	-9.83	120.30	128.86
2	A	401	COA	N3A-C2A-N1A	-9.80	120.33	128.86
2	B	401	COA	N3A-C2A-N1A	-8.96	121.05	128.86
2	C	401	COA	N6A-C6A-N1A	-6.24	106.39	118.77
2	B	401	COA	N6A-C6A-N1A	-6.19	106.50	118.77
2	D	401	COA	N6A-C6A-N1A	-6.18	106.52	118.77
2	A	401	COA	N6A-C6A-N1A	-5.61	107.65	118.77
2	C	401	COA	C7P-C6P-C5P	-4.56	104.88	112.22
2	D	401	COA	C4B-O4B-C1B	-4.03	105.48	109.77
2	A	401	COA	C7P-C6P-C5P	-3.61	106.41	112.22
2	D	401	COA	C7P-C6P-C5P	-3.06	107.30	112.22
2	A	401	COA	O6A-CCP-CBP	-2.91	105.86	110.55
2	A	401	COA	C4B-O4B-C1B	-2.91	106.67	109.77
2	D	401	COA	C2P-C3P-N4P	-2.78	106.45	112.50
2	C	401	COA	C7P-N8P-C9P	-2.74	117.48	122.59
2	A	401	COA	C2P-C3P-N4P	-2.46	107.15	112.50
2	B	401	COA	O6A-CCP-CBP	-2.40	106.69	110.55
2	D	401	COA	C7P-N8P-C9P	-2.27	118.36	122.59
2	D	401	COA	C6P-C7P-N8P	-2.04	107.65	111.87
2	A	401	COA	C7P-N8P-C9P	-2.03	118.80	122.59
2	B	401	COA	C6P-C7P-N8P	-2.01	107.72	111.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	COA	O9P-C9P-N8P	-2.01	119.20	123.07
2	B	401	COA	C4A-C5A-N7A	-2.01	107.47	109.41
2	B	401	COA	CDP-CBP-CCP	2.47	111.99	108.37
2	A	401	COA	CDP-CBP-CAP	3.21	114.39	108.82
2	A	401	COA	C5A-C6A-N6A	5.85	132.39	120.47
2	D	401	COA	C5A-C6A-N6A	6.30	133.32	120.47
2	C	401	COA	C5A-C6A-N6A	6.43	133.58	120.47
2	B	401	COA	C5A-C6A-N6A	6.54	133.81	120.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	COA	2	0
2	B	401	COA	2	0
2	C	401	COA	2	0
2	D	401	COA	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	375/396 (94%)	-0.00	15 (4%)	39 33	14, 22, 40, 68	0
1	B	363/396 (91%)	0.02	15 (4%)	38 32	15, 24, 50, 70	0
1	C	353/396 (89%)	0.16	23 (6%)	20 16	13, 23, 52, 82	0
1	D	370/396 (93%)	0.34	27 (7%)	16 13	17, 37, 60, 80	0
All	All	1461/1584 (92%)	0.13	80 (5%)	26 21	13, 25, 52, 82	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	199	TYR	6.5
1	B	259[A]	TYR	6.2
1	C	223	ASP	5.6
1	D	176	GLY	5.4
1	C	224	THR	5.4
1	C	312	GLY	5.3
1	C	259[A]	TYR	5.2
1	A	225	THR	5.1
1	C	225	THR	4.9
1	D	202	LEU	4.3
1	C	311	LEU	4.2
1	B	278	ARG	4.1
1	B	199	TYR	4.0
1	D	175	GLY	4.0
1	D	348	MET	3.9
1	D	259	TYR	3.8
1	C	309	GLU	3.7
1	D	383	ILE	3.6
1	A	224	THR	3.6
1	B	289	TRP	3.5
1	A	177	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	221	ASP	3.3
1	A	226	THR	3.2
1	D	177	HIS	3.2
1	D	44	GLN	3.2
1	C	222	LEU	3.1
1	D	228	ARG	3.0
1	D	287	ASN	3.0
1	D	347	SER	3.0
1	B	267	GLN	2.9
1	C	383	ILE	2.9
1	C	226	THR	2.9
1	B	277	CYS	2.8
1	B	221	ASP	2.8
1	C	177	HIS	2.8
1	D	285	GLY	2.7
1	A	111	GLY	2.6
1	C	267	GLN	2.6
1	C	176	GLY	2.6
1	C	228	ARG	2.6
1	B	291	SER	2.6
1	C	315	LYS	2.6
1	C	152	ILE	2.6
1	D	21	PRO	2.5
1	A	228	ARG	2.5
1	C	348	MET	2.5
1	D	309	GLU	2.5
1	C	314	SER	2.5
1	D	283	PRO	2.4
1	D	351	GLY	2.4
1	C	306	MET	2.4
1	D	43	THR	2.4
1	D	312	GLY	2.4
1	D	108	LYS	2.4
1	A	199	TYR	2.3
1	B	312	GLY	2.3
1	A	221	ASP	2.3
1	D	198	THR	2.2
1	B	280	THR	2.2
1	A	121	ILE	2.2
1	C	310	LYS	2.2
1	B	202	LEU	2.2
1	B	263	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	282	THR	2.1
1	A	175	GLY	2.1
1	B	290	ASN	2.1
1	A	223	ASP	2.1
1	D	47	ASP	2.1
1	A	152	ILE	2.1
1	C	150	THR	2.1
1	C	221	ASP	2.1
1	A	284	LEU	2.1
1	D	284	LEU	2.1
1	B	309	GLU	2.1
1	D	289	TRP	2.1
1	B	281	PHE	2.1
1	A	158	PHE	2.1
1	D	45	LEU	2.0
1	C	269	ILE	2.0
1	D	282	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	COA	D	401	48/48	0.81	0.20	1.80	59,73,75,76	0
2	COA	B	401	48/48	0.78	0.19	1.73	46,64,76,79	0
2	COA	A	401	48/48	0.85	0.16	1.48	21,43,56,61	0
2	COA	C	401	48/48	0.86	0.19	1.31	37,50,57,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	D	402	5/5	0.94	0.14	-0.21	50,57,59,61	0
3	SO4	A	402	5/5	0.96	0.10	-0.30	40,48,50,52	0
3	SO4	B	402	5/5	0.95	0.13	-	56,58,62,64	0
3	SO4	C	402	5/5	0.92	0.13	-	51,55,57,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.