



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:19 PM GMT

PDB ID : 1T4C  
Title : Formyl-CoA Transferase in complex with Oxalyl-CoA  
Authors : Ricagno, S.; Jonsson, S.; Richards, N.G.; Lindqvist, Y.  
Deposited on : 2004-04-29  
Resolution : 2.61 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

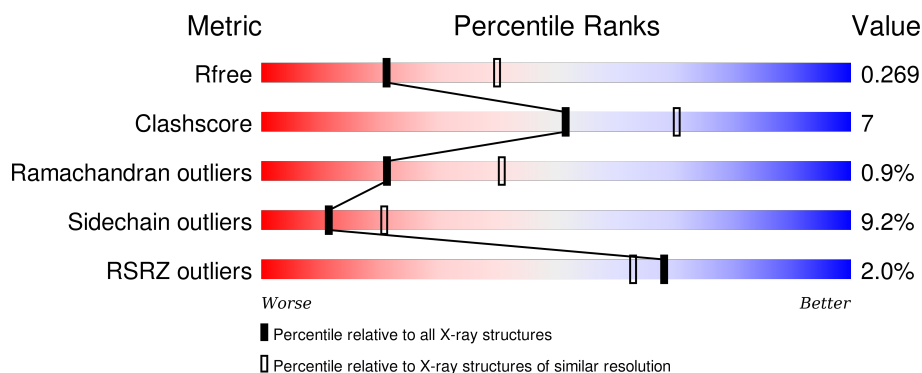
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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))
$R_{free}$	91344	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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	427	<div> <div>2%</div> <div>78%</div> <div>19%</div> <div>•</div> </div>
2	B	427	<div> <div>2%</div> <div>78%</div> <div>21%</div> <div>•</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	COA	A	1	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6857 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 Formyl-coenzyme A transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3313	2096	568	626	23			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	ILE	MET	SEE REMARK 999	UNP O06644

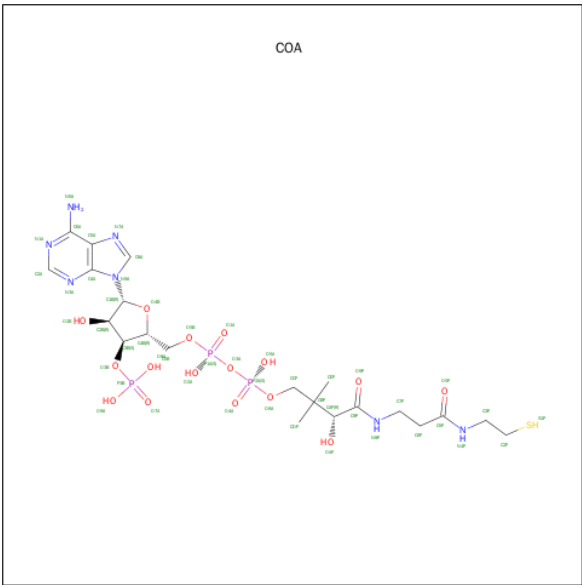
- Molecule 2 is a protein called Formyl-coenzyme A transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	4	0	0
			3318	2098	568	629	23			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	169	OXX	ASP	SEE REMARK 999	UNP O06644
B	186	ILE	MET	SEE REMARK 999	UNP O06644

- Molecule 3 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
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

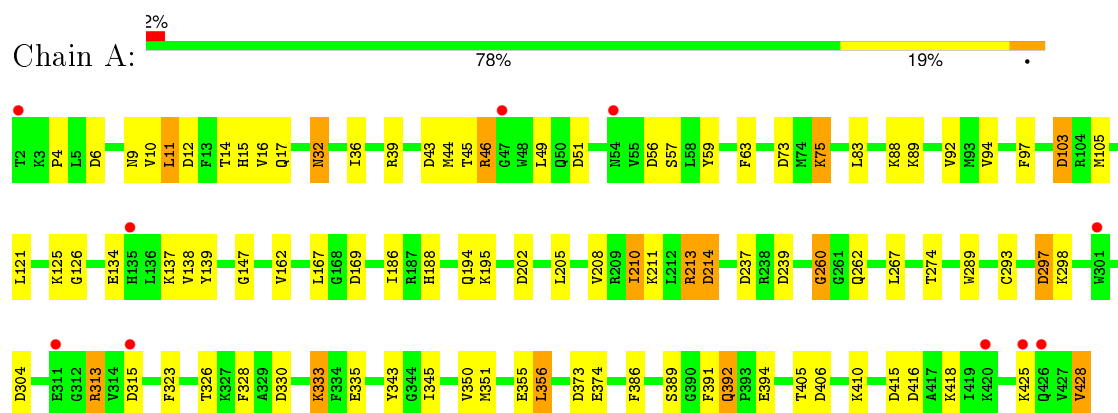
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		
4	B	68	Total	O	0	0
			68	68		

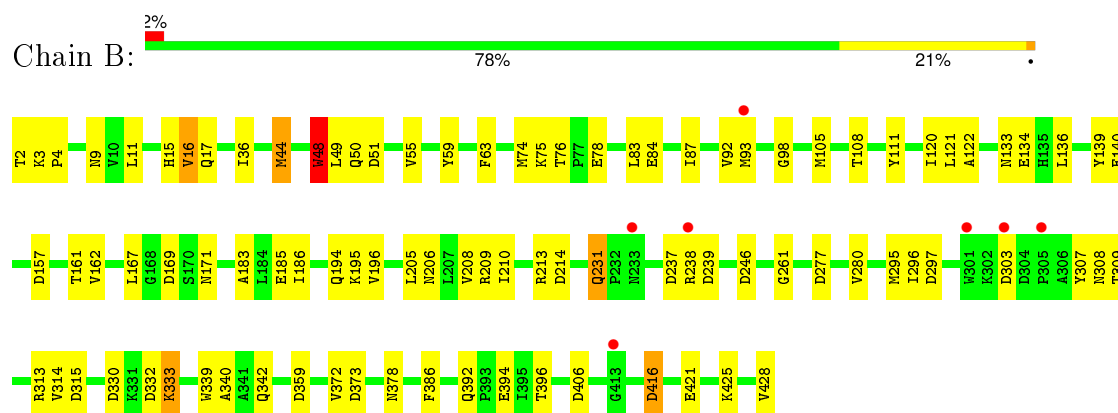
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Formyl-coenzyme A transferase



#### • Molecule 2: Formyl-coenzyme A transferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.16 Å   100.16 Å   196.87 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 2.61 25.47 – 2.61	Depositor EDS
% Data completeness (in resolution range)	96.6 (20.00-2.61) 96.6 (25.47-2.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 2.60 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.200   ,   0.273 0.197   ,   0.269	Depositor DCC
$R_{free}$ test set	1510 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.5	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 31.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 30208 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6857	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, OXX

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	0.91	1/3387 (0.0%)	1.04	21/4580 (0.5%)
2	B	0.90	0/3378	1.02	14/4566 (0.3%)
All	All	0.91	1/6765 (0.0%)	1.03	35/9146 (0.4%)

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
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	GLY	C-O	5.73	1.32	1.23

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	315	ASP	CB-CG-OD2	10.13	127.42	118.30
2	B	214	ASP	CB-CG-OD2	9.91	127.22	118.30
2	B	332	ASP	CB-CG-OD2	9.70	127.03	118.30
1	A	169	ASP	CB-CG-OD2	8.40	125.86	118.30
2	B	406	ASP	CB-CG-OD2	8.14	125.63	118.30
1	A	12	ASP	CB-CG-OD2	7.88	125.39	118.30
1	A	46	ARG	NE-CZ-NH1	7.82	124.21	120.30
2	B	315	ASP	CB-CG-OD2	7.62	125.16	118.30
1	A	121	LEU	CB-CG-CD2	7.62	123.95	111.00
1	A	373	ASP	CB-CG-OD2	7.42	124.98	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	330	ASP	CB-CG-OD2	7.09	124.68	118.30
2	B	157	ASP	CB-CG-OD1	7.09	124.68	118.30
2	B	277	ASP	CB-CG-OD2	6.72	124.35	118.30
1	A	297	ASP	CB-CG-OD2	6.64	124.28	118.30
2	B	297	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	214	ASP	CB-CG-OD2	6.46	124.11	118.30
2	B	48	TRP	CB-CA-C	6.45	123.31	110.40
2	B	359	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	237	ASP	CB-CG-OD2	6.25	123.93	118.30
1	A	73	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	415	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	202	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	406	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	56	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	313	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	B	51	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	46	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	239	ASP	CB-CG-OD1	5.43	123.19	118.30
2	B	332	ASP	OD1-CG-OD2	-5.39	113.06	123.30
2	B	416	ASP	CB-CG-OD2	5.26	123.04	118.30
2	B	48	TRP	CA-CB-CG	5.20	123.57	113.70
1	A	103	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	6	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	51	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	304	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	98	GLY	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	3313	0	3252	49	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3318	0	3251	48	0
3	A	48	0	32	3	0
3	B	48	0	32	1	0
4	A	62	0	0	3	0
4	B	68	0	0	5	0
All	All	6857	0	6567	89	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 7.

All (89) 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:126:GLY:HA3	1:A:138:VAL:HG11	1.52	0.92
2:B:87:ILE:HG12	2:B:93:MET:SD	2.11	0.89
1:A:167:LEU:HD21	2:B:167:LEU:HD21	1.58	0.86
1:A:126:GLY:CA	1:A:138:VAL:HG11	2.13	0.77
1:A:210:ILE:HD13	1:A:213:ARG:HH12	1.56	0.70
2:B:17:GLN:HG3	2:B:63:PHE:CE2	2.26	0.70
1:A:186:ILE:HG21	1:A:194:GLN:HE21	1.59	0.67
1:A:11:LEU:CD2	1:A:36:ILE:HD11	2.27	0.64
1:A:17:GLN:HG3	1:A:63:PHE:CE2	2.35	0.61
1:A:210:ILE:HD13	1:A:213:ARG:NH1	2.16	0.60
1:A:32:ASN:HB2	4:A:436:HOH:O	2.01	0.60
1:A:11:LEU:CD2	1:A:36:ILE:CD1	2.80	0.59
1:A:267:LEU:HD12	1:A:328:PHE:HE2	1.68	0.58
2:B:140:GLU:N	2:B:169:OXX:O1	2.34	0.58
1:A:44:MET:O	1:A:46:ARG:N	2.37	0.58
2:B:295:MET:HE1	2:B:340:ALA:HB2	1.85	0.58
1:A:32:ASN:ND2	4:A:480:HOH:O	2.36	0.57
2:B:48:TRP:HD1	2:B:49:LEU:HG	1.69	0.56
1:A:167:LEU:HD21	2:B:167:LEU:CD2	2.34	0.55
1:A:298:LYS:HE3	1:A:323:PHE:CZ	2.42	0.55
2:B:11:LEU:HB3	2:B:93:MET:HG2	1.89	0.55
1:A:186:ILE:HG21	1:A:194:GLN:NE2	2.22	0.54
1:A:167:LEU:CD2	2:B:167:LEU:HD21	2.33	0.54
1:A:4:PRO:HA	2:B:186:ILE:HG13	1.91	0.53
1:A:267:LEU:HD12	1:A:328:PHE:CE2	2.43	0.53
1:A:9:ASN:ND2	1:A:89:LYS:O	2.32	0.53
2:B:11:LEU:HD11	2:B:36:ILE:HD11	1.92	0.52
1:A:11:LEU:HD21	1:A:36:ILE:HD11	1.90	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:MET:HG3	2:B:48:TRP:CZ3	2.43	0.52
1:A:10:VAL:HG13	1:A:92:VAL:HG22	1.92	0.51
1:A:333:LYS:HE2	1:A:350:VAL:O	2.11	0.51
2:B:93:MET:O	2:B:121:LEU:HD12	2.10	0.51
2:B:307:TYR:O	2:B:313:ARG:HD3	2.10	0.51
2:B:231:GLN:HB2	4:B:1010:HOH:O	2.11	0.51
1:A:186:ILE:HD13	1:A:194:GLN:HE22	1.76	0.51
2:B:120:ILE:HD13	2:B:183:ALA:HB3	1.93	0.51
1:A:205:LEU:HA	1:A:208:VAL:HG22	1.92	0.51
1:A:188:HIS:HE1	2:B:185:GLU:OE1	1.95	0.50
1:A:186:ILE:HD13	1:A:194:GLN:NE2	2.27	0.50
1:A:210:ILE:CD1	1:A:213:ARG:NH1	2.75	0.49
2:B:122:ALA:HA	2:B:196:VAL:O	2.12	0.49
1:A:333:LYS:NZ	1:A:355:GLU:OE2	2.46	0.49
1:A:289:TRP:NE1	1:A:293:CYS:SG	2.85	0.49
1:A:374:GLU:CD	1:A:374:GLU:H	2.15	0.49
1:A:4:PRO:HG3	2:B:186:ILE:HD12	1.95	0.48
2:B:339:TRP:O	2:B:342:GLN:HB2	2.12	0.48
2:B:139:TYR:HE2	3:B:1001:COA:H143	1.79	0.47
1:A:392:GLN:HE21	1:A:392:GLN:HA	1.80	0.47
1:A:389:SER:HB3	2:B:195:LYS:HB3	1.95	0.47
1:A:410:LYS:NZ	1:A:416:ASP:OD1	2.48	0.47
2:B:167:LEU:O	2:B:171:ASN:HB3	2.16	0.46
2:B:139:TYR:HB3	2:B:169:OXX:O1	2.16	0.46
2:B:84:GLU:OE2	2:B:111:TYR:OH	2.29	0.46
2:B:120:ILE:HD13	2:B:183:ALA:CB	2.46	0.46
1:A:147:GLY:O	1:A:205:LEU:HD12	2.16	0.45
2:B:378:ASN:ND2	4:B:1062:HOH:O	2.50	0.45
1:A:405:THR:HG21	1:A:428:VAL:HG13	1.98	0.45
2:B:9:ASN:HB2	4:B:1065:HOH:O	2.17	0.45
2:B:373:ASP:H	2:B:378:ASN:ND2	2.15	0.45
2:B:44:MET:HG3	2:B:48:TRP:HZ3	1.81	0.45
1:A:139:TYR:CZ	3:A:1:COA:H143	2.52	0.44
2:B:208:VAL:O	2:B:208:VAL:HG12	2.16	0.44
2:B:186:ILE:HG21	2:B:194:GLN:HE21	1.82	0.44
2:B:210:ILE:O	2:B:213:ARG:HB3	2.17	0.44
2:B:206:ASN:ND2	2:B:209:ARG:HH21	2.15	0.44
2:B:378:ASN:N	2:B:378:ASN:HD22	2.17	0.43
1:A:49:LEU:HD21	2:B:261:GLY:HA2	2.00	0.43
3:A:1:COA:H131	3:A:1:COA:N4P	2.34	0.43
1:A:210:ILE:HD12	1:A:260:GLY:CA	2.48	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:ASN:OD1	2:B:9:ASN:C	2.57	0.42
2:B:161:THR:HG22	2:B:162:VAL:O	2.19	0.42
1:A:63:PHE:CZ	2:B:209:ARG:HD2	2.54	0.42
2:B:50:GLN:HG2	2:B:55:VAL:O	2.19	0.42
2:B:108:THR:HB	4:B:1057:HOH:O	2.19	0.42
1:A:75:LYS:HG3	3:A:1:COA:H2A	2.02	0.42
2:B:372:VAL:HG12	2:B:372:VAL:O	2.19	0.42
2:B:231:GLN:CB	4:B:1010:HOH:O	2.68	0.42
1:A:211:LYS:NZ	4:A:472:HOH:O	2.45	0.42
2:B:11:LEU:HD12	2:B:11:LEU:HA	1.95	0.41
1:A:11:LEU:HD23	1:A:36:ILE:CD1	2.50	0.41
1:A:343:TYR:HB2	1:A:345:ILE:HD12	2.02	0.41
1:A:213:ARG:CZ	1:A:214:ASP:OD1	2.69	0.41
1:A:351:MET:HB3	1:A:356:LEU:HD13	2.03	0.41
2:B:3:LYS:HA	2:B:4:PRO:HD3	1.94	0.41
1:A:43:ASP:O	1:A:46:ARG:HG3	2.21	0.41
2:B:133:ASN:HB3	2:B:136:LEU:HD12	2.03	0.40
2:B:44:MET:HE2	2:B:44:MET:HB3	2.01	0.40
1:A:14:THR:CG2	1:A:94:VAL:HG12	2.51	0.40
2:B:76:THR:HG22	2:B:78:GLU:H	1.86	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	425/427 (100%)	403 (95%)	18 (4%)	4 (1%)	21	41
2	B	424/427 (99%)	400 (94%)	20 (5%)	4 (1%)	21	41
All	All	849/854 (99%)	803 (95%)	38 (4%)	8 (1%)	21	41

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	333	LYS
1	A	16	VAL
2	B	16	VAL
1	A	45	THR
2	B	134	GLU
1	A	134	GLU
1	A	262	GLN
2	B	314	VAL

### 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	350/350 (100%)	317 (91%)	33 (9%)	11	20
2	B	349/349 (100%)	318 (91%)	31 (9%)	12	22
All	All	699/699 (100%)	635 (91%)	64 (9%)	11	21

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	15	HIS
1	A	32	ASN
1	A	39	ARG
1	A	57	SER
1	A	59	TYR
1	A	75	LYS
1	A	83	LEU
1	A	88	LYS
1	A	97	PHE
1	A	103	ASP
1	A	105	MET
1	A	125	LYS
1	A	137	LYS
1	A	162	VAL
1	A	195	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	210	ILE
1	A	213	ARG
1	A	274	THR
1	A	297	ASP
1	A	313	ARG
1	A	326	THR
1	A	330	ASP
1	A	333	LYS
1	A	335	GLU
1	A	356	LEU
1	A	386	PHE
1	A	391	PHE
1	A	392	GLN
1	A	394	GLU
1	A	418	LYS
1	A	425	LYS
1	A	428	VAL
2	B	2	THR
2	B	15	HIS
2	B	16	VAL
2	B	44	MET
2	B	48	TRP
2	B	59	TYR
2	B	74	MET
2	B	75	LYS
2	B	83	LEU
2	B	92	VAL
2	B	105	MET
2	B	205	LEU
2	B	231	GLN
2	B	237	ASP
2	B	238	ARG
2	B	239	ASP
2	B	246	ASP
2	B	280	VAL
2	B	296	ILE
2	B	303	ASP
2	B	308	ASN
2	B	309	THR
2	B	333	LYS
2	B	386	PHE
2	B	392	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	394	GLU
2	B	396	THR
2	B	416	ASP
2	B	421	GLU
2	B	425	LYS
2	B	428	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	32	ASN
1	A	188	HIS
1	A	194	GLN
1	A	392	GLN
2	B	206	ASN
2	B	231	GLN
2	B	358	HIS
2	B	378	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	OXX	B	169	3,2	8,12,13	1.79	2 (25%)	4,15,17	1.76	1 (25%)

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	OXX	B	169	3,2	-	0/8/14/16	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	169	OXX	OD1-CG	2.50	1.46	1.37
2	B	169	OXX	OD1-C2	3.97	1.45	1.37

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	169	OXX	O-C-CA	-3.17	117.24	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	169	OXX	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	COA	A	1	-	40,50,50	1.90	3 (7%)	50,75,75	2.03	5 (10%)
3	COA	B	1001	2	40,50,50	1.69	3 (7%)	50,75,75	1.82	6 (12%)

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	1	-	-	0/44/64/64	0/3/3/3
3	COA	B	1001	2	-	0/44/64/64	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	COA	C2A-N1A	2.69	1.39	1.33
3	B	1001	COA	C2A-N1A	2.70	1.39	1.33
3	B	1001	COA	C2A-N3A	3.82	1.39	1.32
3	A	1	COA	C2A-N3A	4.04	1.39	1.32
3	B	1001	COA	O9P-C9P	8.86	1.40	1.23
3	A	1	COA	O9P-C9P	10.10	1.43	1.23

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	COA	N3A-C2A-N1A	-11.72	119.92	128.89
3	B	1001	COA	N3A-C2A-N1A	-8.44	122.44	128.89
3	B	1001	COA	C4A-C5A-N7A	-3.58	106.19	109.48
3	A	1	COA	CDP-CBP-CCP	-3.50	103.97	108.50
3	B	1001	COA	P2A-O3A-P1A	-3.45	123.05	132.73
3	B	1001	COA	CDP-CBP-CCP	-3.31	104.22	108.50
3	A	1	COA	P2A-O3A-P1A	-2.58	125.47	132.73
3	A	1	COA	C4A-C5A-N7A	-2.00	107.64	109.48
3	B	1001	COA	O4B-C1B-N9A	2.07	112.43	108.10
3	A	1	COA	P3B-O3B-C3B	2.73	128.12	121.56
3	B	1001	COA	O9A-P3B-O8A	3.03	118.93	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	COA	3	0
3	B	1001	COA	1	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	427/427 (100%)	-0.25	10 (2%) 64 57	16, 28, 56, 64	0
2	B	425/427 (99%)	-0.22	7 (1%) 74 69	12, 28, 56, 64	0
All	All	852/854 (99%)	-0.24	17 (1%) 68 63	12, 28, 56, 64	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	238	ARG	4.1
1	A	135	HIS	3.6
2	B	233	ASN	3.5
2	B	93	MET	3.0
1	A	2	THR	2.8
2	B	413	GLY	2.7
1	A	426	GLN	2.5
1	A	54	ASN	2.5
1	A	47	GLY	2.5
1	A	301	TRP	2.4
1	A	315	ASP	2.4
1	A	425	LYS	2.4
2	B	305	PRO	2.2
2	B	301	TRP	2.2
1	A	420	LYS	2.2
2	B	303	ASP	2.2
1	A	311	GLU	2.2

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

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( $\text{\AA}^2$ )	Q<0.9
2	OXX	B	169	13/14	0.94	0.19	-	22,27,47,50	0

### 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( $\text{\AA}^2$ )	Q<0.9
3	COA	A	1	48/48	0.81	0.35	3.67	98,102,106,107	0
3	COA	B	1001	48/48	0.91	0.19	0.65	62,75,88,89	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.