Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:59 AM GMT

PDB ID	:	2VJM
Title	:	FORMYL-COA TRANSFERASE WITH ASPARTYL-FORMYL ANHYDIDE INTERMEDIATE
Authors	:	Berthold, C.L.; Toyota, C.G.; Richards, N.G.J.; Lindqvist, Y.
Deposited on	:	2007-12-11
Resolution	:	1.89 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

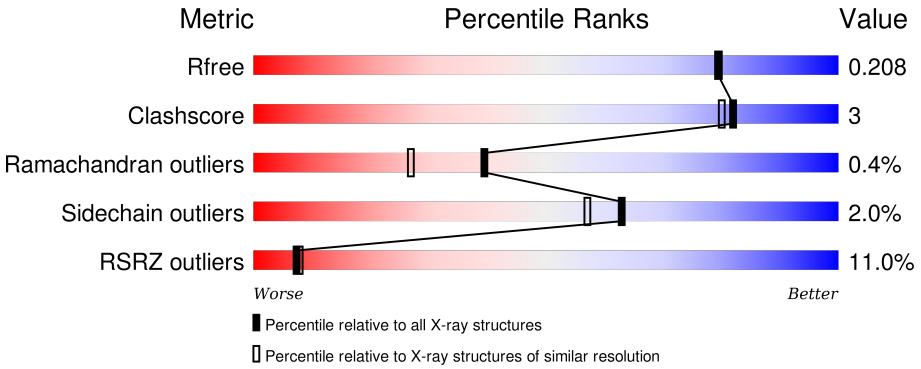
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.89 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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 >=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 <=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	428	4% 93% 6%
2	B	428	18% 92% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7535 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
			Total	C	N	O	S			
1	A	427	3331	2108	569	631	23	7	5	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	186	ILE	MET	CONFLICT SEE REMARK 9	UNP O06644

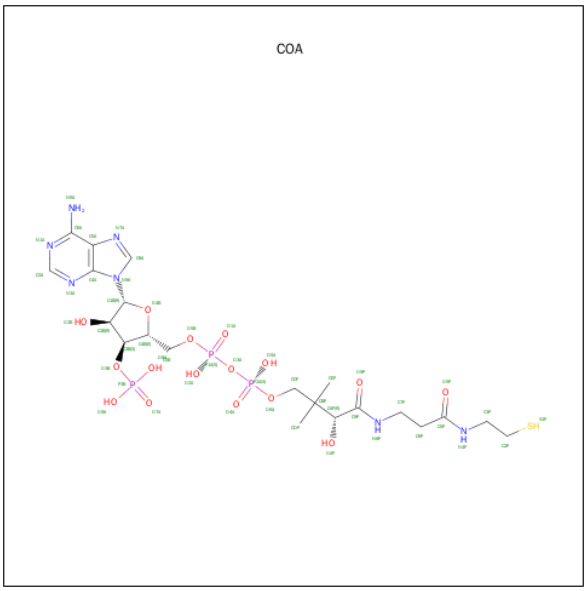
- Molecule 2 is a protein called FORMYL-COENZYME A TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	427	3336	2111	571	630	24	0	4	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	186	ILE	MET	CONFLICT SEE REMARK 9	UNP O06644

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).

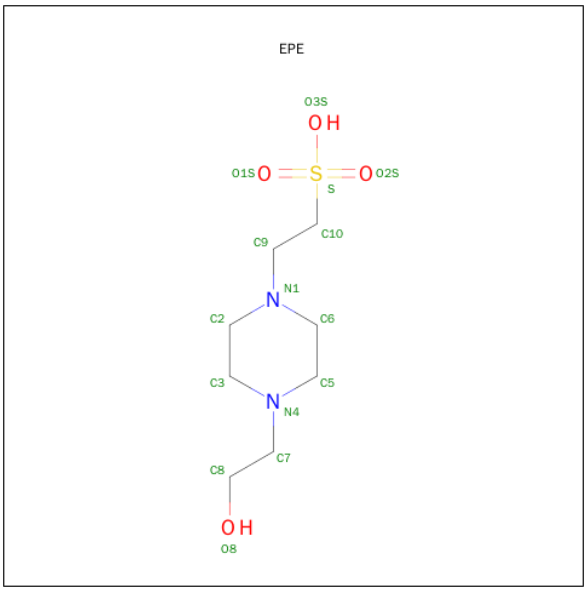


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is water.

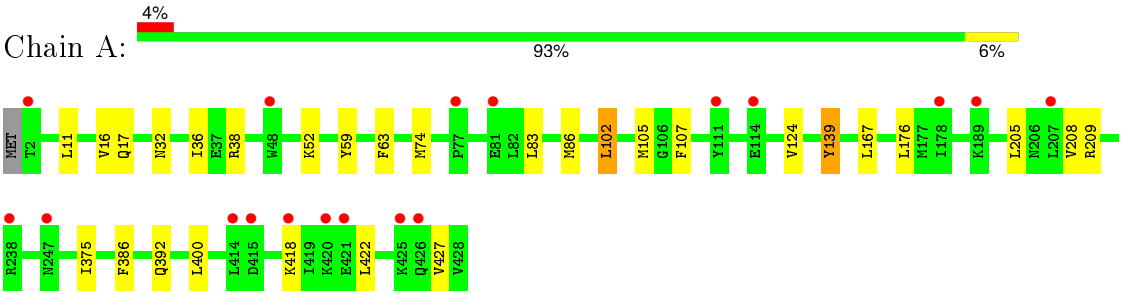
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	432	Total	O	0	0
			432	432		
6	B	324	Total	O	0	0
			324	324		

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.

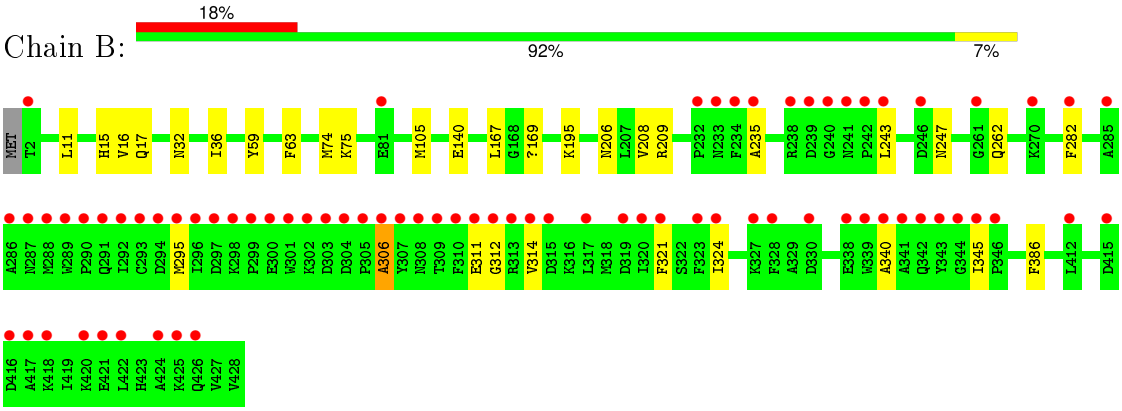
- Molecule 1: FORMYL-COENZYME A TRANSFERASE

Chain A:



- Molecule 2: FORMYL-COENZYME A TRANSFERASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	151.67Å 151.67Å 98.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.89 38.71 – 1.89	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-1.89) 99.3 (38.71-1.89)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.171 , 0.203 0.176 , 0.208	Depositor DCC
R_{free} test set	4455 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	21.8	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.1	EDS
Estimated twinning fraction	0.028 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 89571 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7535	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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, 0.375 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, NA, EPE, A0A

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	0.39	1/3420 (0.0%)	0.56	2/4624 (0.0%)
2	B	0.37	0/3411	0.52	1/4611 (0.0%)
All	All	0.38	1/6831 (0.0%)	0.54	3/9235 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	TYR	CB-CG	-5.98	1.42	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	139	TYR	CB-CG-CD1	-9.16	115.50	121.00
1	A	139	TYR	CB-CG-CD2	8.95	126.37	121.00
2	B	306	ALA	CB-CA-C	5.84	118.86	110.10

There are no chirality outliers.

There are no planarity outliers.

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	3331	0	3277	15	0
2	B	3336	0	3281	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	48	0	31	0	0
3	B	48	0	32	2	0
4	A	1	0	0	0	0
5	B	15	0	17	1	0
6	A	432	0	0	3	0
6	B	324	0	0	2	0
All	All	7535	0	6638	43	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 3.

All (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247[B]:ASN:HD22	2:B:247[B]:ASN:H	1.35	0.72
2:B:306:ALA:O	2:B:312:GLY:O	2.11	0.67
2:B:306:ALA:O	2:B:312:GLY:C	2.33	0.67
2:B:235:ALA:HB1	2:B:243:LEU:HD12	1.77	0.67
1:A:167:LEU:HD21	2:B:167:LEU:HD21	1.81	0.61
2:B:11:LEU:CD1	2:B:36:ILE:HD11	2.30	0.60
1:A:17:GLN:HG3	1:A:63:PHE:CE2	2.37	0.59
2:B:208:VAL:O	2:B:208:VAL:HG12	2.07	0.55
2:B:306:ALA:O	2:B:312:GLY:CA	2.55	0.55
1:A:102:LEU:HD22	1:A:107:PHE:HB2	1.88	0.54
1:A:208:VAL:HG12	1:A:208:VAL:O	2.08	0.54
2:B:32[A]:ASN:ND2	6:B:2022:HOH:O	2.40	0.54
2:B:243:LEU:HD22	6:B:2076:HOH:O	2.07	0.53
2:B:169:A0A:CM1	3:B:1429:COA:S1P	2.98	0.52
2:B:235:ALA:CB	2:B:243:LEU:HD12	2.40	0.51
2:B:295:MET:CE	2:B:345:ILE:HD12	2.40	0.51
1:A:124:VAL:HG23	1:A:176:LEU:HD22	1.93	0.50
1:A:209:ARG:HD2	2:B:63:PHE:CZ	2.47	0.50
2:B:295:MET:HE3	2:B:345:ILE:CD1	2.44	0.48
6:A:2271:HOH:O	5:B:1430:EPE:H82	2.14	0.48
2:B:282:PHE:CZ	2:B:324:ILE:HD11	2.49	0.48
1:A:83:LEU:HD23	1:A:86:MET:HE3	1.96	0.48
1:A:11:LEU:HD11	1:A:36:ILE:HD11	1.96	0.47
1:A:63:PHE:CZ	2:B:209:ARG:HD2	2.51	0.45
2:B:17:GLN:HG3	2:B:63:PHE:CE2	2.52	0.45
2:B:321:PHE:HA	2:B:324:ILE:HG22	1.99	0.44
1:A:32[A]:ASN:ND2	6:A:2020:HOH:O	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:282:PHE:CE2	2:B:324:ILE:HD11	2.53	0.44
1:A:375:ILE:HD13	1:A:400:LEU:HD11	2.00	0.43
1:A:167:LEU:CD2	2:B:167:LEU:HD21	2.49	0.43
2:B:74:MET:SD	2:B:105[A]:MET:HE1	2.58	0.43
2:B:11:LEU:HD12	2:B:36:ILE:HD11	2.00	0.42
2:B:295:MET:HE3	2:B:345:ILE:HD12	2.01	0.42
2:B:311:GLU:O	2:B:314:VAL:HG12	2.20	0.42
1:A:32[B]:ASN:ND2	6:A:2022:HOH:O	2.53	0.42
1:A:74:MET:HB2	1:A:105:MET:HE2	2.01	0.41
2:B:208:VAL:O	2:B:208:VAL:CG1	2.69	0.41
2:B:206:ASN:ND2	2:B:209:ARG:HH21	2.18	0.41
2:B:295:MET:HE2	2:B:340:ALA:HA	2.03	0.41
1:A:422:LEU:HD22	1:A:427:VAL:HG11	2.02	0.40
2:B:306:ALA:O	2:B:312:GLY:HA3	2.20	0.40
2:B:75:LYS:HG3	3:B:1429:COA:H2A	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	430/428 (100%)	422 (98%)	7 (2%)	1 (0%)	52	42
2	B	428/428 (100%)	416 (97%)	10 (2%)	2 (0%)	34	21
All	All	858/856 (100%)	838 (98%)	17 (2%)	3 (0%)	39	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	140	GLU
2	B	16	VAL
1	A	16	VAL

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	355/351 (101%)	346 (98%)	9 (2%)	55 47
2	B	353/350 (101%)	348 (99%)	5 (1%)	74 71
All	All	708/701 (101%)	694 (98%)	14 (2%)	63 57

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	52	LYS
1	A	59	TYR
1	A	102	LEU
1	A	139	TYR
1	A	205	LEU
1	A	386	PHE
1	A	392	GLN
1	A	418	LYS
2	B	15	HIS
2	B	59	TYR
2	B	195	LYS
2	B	262	GLN
2	B	386	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	GLN
1	A	206	ASN
1	A	247	ASN
1	A	392	GLN
2	B	206	ASN
2	B	262	GLN
2	B	342	GLN

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	A0A	B	169	2	7,9,10	1.14	1 (14%)	5,10,12	1.49	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	A0A	B	169	2	-	0/5/9/11	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	169	A0A	OD2-CM1	2.78	1.46	1.38

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	169	A0A	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	1169	1	40,50,50	1.05	1 (2%)	50,75,75	1.73	5 (10%)
3	COA	B	1429	-	40,50,50	1.73	3 (7%)	50,75,75	1.92	4 (8%)
5	EPE	B	1430	-	14,15,15	0.40	0	18,20,20	1.28	3 (16%)

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	1169	1	-	0/44/64/64	0/3/3/3
3	COA	B	1429	-	-	0/44/64/64	0/3/3/3
5	EPE	B	1430	-	-	0/9/19/19	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1429	COA	C2A-N1A	2.44	1.38	1.33
3	B	1429	COA	C2A-N3A	4.02	1.39	1.32
3	A	1169	COA	O9P-C9P	5.09	1.33	1.23
3	B	1429	COA	O9P-C9P	9.21	1.41	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1429	COA	N3A-C2A-N1A	-11.99	119.71	128.89
3	A	1169	COA	N3A-C2A-N1A	-10.06	121.19	128.89
3	A	1169	COA	C4A-C5A-N7A	-2.95	106.77	109.48
3	B	1429	COA	P2A-O3A-P1A	-2.74	125.03	132.73
3	B	1429	COA	C4A-C5A-N7A	-2.45	107.22	109.48
3	A	1169	COA	P2A-O3A-P1A	-2.31	126.23	132.73
3	B	1429	COA	C7P-C6P-C5P	-2.08	108.88	112.31
5	B	1430	EPE	C6-N1-C2	2.12	113.50	108.90
3	A	1169	COA	O9A-P3B-O7A	2.17	117.56	110.58
3	A	1169	COA	O4B-C1B-N9A	2.24	112.79	108.10
5	B	1430	EPE	O2S-S-C10	2.34	108.90	106.91
5	B	1430	EPE	O1S-S-C10	2.82	109.31	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1429	COA	2	0
5	B	1430	EPE	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^{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	427/428 (99%)	0.18	18 (4%) 40 44	11, 19, 37, 49	1 (0%)
2	B	426/428 (99%)	0.89	76 (17%) 2 2	10, 22, 71, 85	0
All	All	853/856 (99%)	0.54	94 (11%) 7 8	10, 20, 50, 85	1 (0%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	301	TRP	11.6
2	B	314	VAL	11.5
2	B	305	PRO	9.9
2	B	307	TYR	9.6
2	B	306	ALA	9.1
2	B	320	ILE	7.8
2	B	303	ASP	7.7
2	B	290	PRO	6.8
2	B	299	PRO	6.6
2	B	298	LYS	6.4
2	B	323	PHE	5.7
2	B	311	GLU	5.6
2	B	341	ALA	5.5
2	B	339	TRP	5.5
2	B	294	ASP	5.3
2	B	289	TRP	5.3
2	B	302	LYS	5.1
2	B	310	PHE	5.0
1	A	2	THR	4.9
2	B	288	MET	4.9
2	B	342	GLN	4.8
2	B	344	GLY	4.7
2	B	297	ASP	4.6
2	B	308	ASN	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	286	ALA	4.5
2	B	300	GLU	4.4
2	B	418	LYS	4.3
2	B	296	ILE	4.3
2	B	295	MET	4.1
2	B	343	TYR	4.0
2	B	417	ALA	4.0
2	B	324	ILE	4.0
2	B	315	ASP	4.0
2	B	240	GLY	3.9
2	B	309	THR	3.9
2	B	238	ARG	3.9
2	B	292	ILE	3.9
2	B	304	ASP	3.9
2	B	415	ASP	3.8
2	B	233	ASN	3.8
2	B	239	ASP	3.7
2	B	420	LYS	3.7
2	B	293	CYS	3.5
2	B	232	PRO	3.5
2	B	313	ARG	3.4
1	A	77	PRO	3.4
2	B	243	LEU	3.4
2	B	340	ALA	3.2
2	B	346	PRO	3.2
2	B	241	ASN	3.2
2	B	317	LEU	3.2
1	A	415	ASP	3.1
2	B	261	GLY	3.1
2	B	285	ALA	3.1
2	B	422	LEU	3.1
2	B	321	PHE	3.0
2	B	291	GLN	3.0
2	B	338	GLU	3.0
2	B	330	ASP	3.0
1	A	207	LEU	3.0
2	B	242	PRO	2.9
2	B	287	ASN	2.9
2	B	234	PHE	2.9
1	A	81	GLU	2.9
2	B	424	ALA	2.8
1	A	114	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	312	GLY	2.7
1	A	111	TYR	2.7
2	B	270	LYS	2.7
1	A	414	LEU	2.6
2	B	412	LEU	2.6
1	A	420	LYS	2.5
1	A	238	ARG	2.5
2	B	416	ASP	2.5
2	B	319	ASP	2.4
1	A	425	LYS	2.4
2	B	235	ALA	2.4
2	B	421	GLU	2.4
2	B	425	LYS	2.4
2	B	327	LYS	2.4
2	B	328	PHE	2.3
1	A	421	GLU	2.3
2	B	426	GLN	2.3
2	B	2	THR	2.2
1	A	418	LYS	2.2
1	A	426	GLN	2.2
1	A	48	TRP	2.2
2	B	282	PHE	2.1
2	B	81	GLU	2.1
2	B	345	ILE	2.1
1	A	189	LYS	2.1
1	A	178	ILE	2.1
2	B	246	ASP	2.1
1	A	247	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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^{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	LLDF	B-factors(Å^2)	Q<0.9
2	A0A	B	169	10/11	0.93	0.18	0.76	13,15,19,19	2

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^{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	LLDF	B-factors(Å^2)	Q<0.9
5	EPE	B	1430	15/15	0.93	0.13	0.11	24,24,26,26	15
3	COA	B	1429	48/48	0.95	0.12	-0.20	19,22,29,30	0
3	COA	A	1169	48/48	0.91	0.13	-0.33	32,37,41,42	0
4	NA	A	1429	1/1	0.96	0.07	-1.56	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.