



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 05:47 am GMT

PDB ID : 2VJL  
Title : FORMYL-COA TRANSFERASE WITH ASPARTYL-COA THIOESTER INTERMEDIATE DERIVED FROM FORMYL-COA  
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Deposited on : 2007-12-11  
Resolution : 2.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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	:	trunk28620
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)	:	recalc28949

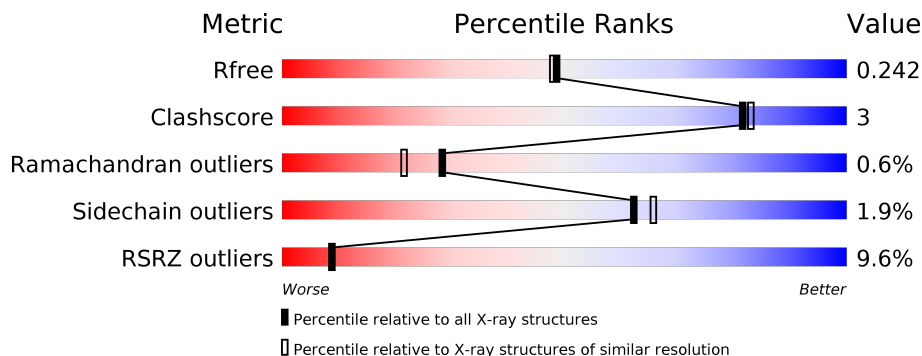
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	428	
1	B	428	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7457 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.

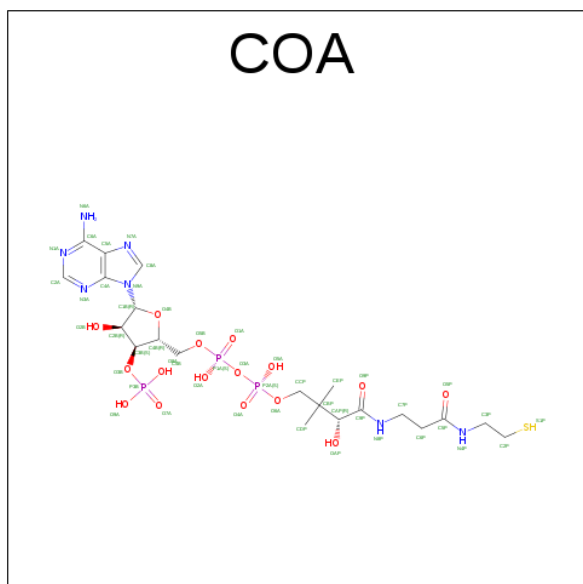
- Molecule 1 is a protein called FORMYL-COENZYME A TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	6	0
			3339	2114	571	631	23			
1	B	427	Total	C	N	O	S	259	2	0
			3323	2103	570	627	23			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cl	0	0
			2	2		
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		

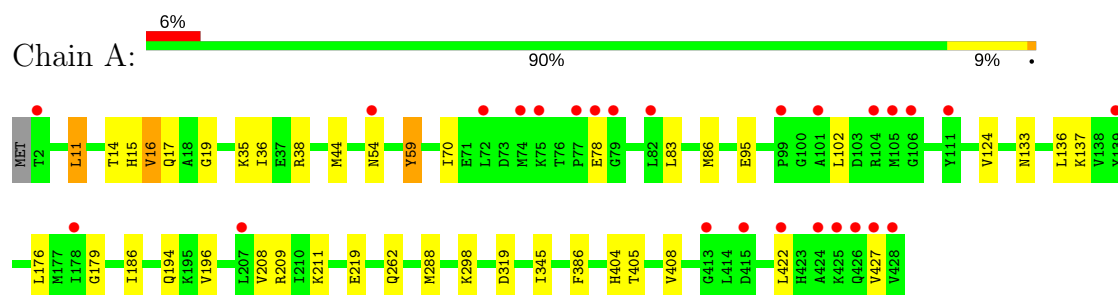
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	369	Total	O	0	0
			369	369		
5	B	325	Total	O	0	0
			325	325		

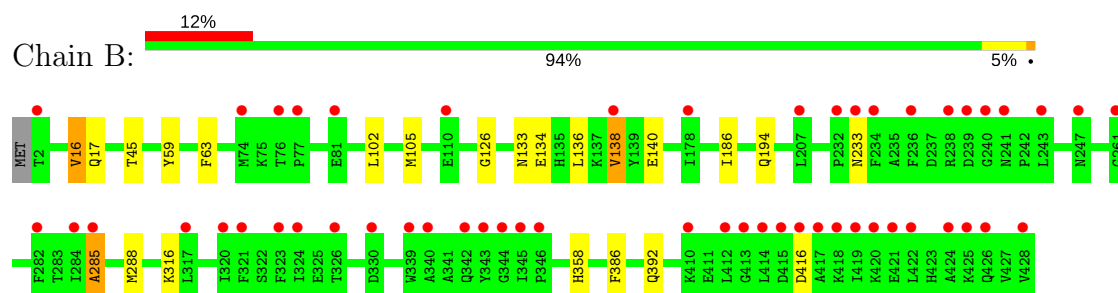
### 3 Residue-property plots [i](#)

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 ( $\text{RSRZ} > 2$ ). 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



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## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.76Å 151.76Å 100.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 53.66 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.2 (30.00-2.00) 98.2 (53.66-2.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.197 , 0.242 0.199 , 0.242	Depositor DCC
$R_{free}$ test set	3765 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7457	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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

### 5.1 Standard geometry

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

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	0/3431	0.54	0/4638
1	B	0.43	2/3403 (0.1%)	0.54	1/4602 (0.0%)
All	All	0.41	2/6834 (0.0%)	0.54	1/9240 (0.0%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	316	LYS	C-N	-9.36	1.12	1.34
1	B	285	ALA	C-N	7.27	1.50	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	ALA	CA-C-N	-5.73	104.59	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	285	ALA	Mainchain

## 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	3339	0	3291	30	0
1	B	3323	0	3265	11	0
2	A	48	0	31	1	0
2	B	48	0	31	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	A	2	0	0	0	0
5	A	369	0	0	3	0
5	B	325	0	0	2	0
All	All	7457	0	6618	39	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 (39) 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:70:ILE:HG21	1:A:408:VAL:HG21	1.45	0.96
1:B:102:LEU:HD23	1:B:105:MET:HE3	1.69	0.74
1:B:126:GLY:HA3	1:B:138:VAL:HG13	1.70	0.73
1:A:11:LEU:HD21	1:A:36:ILE:HD11	1.72	0.71
1:A:319:ASP:OD1	5:A:2270:HOH:O	2.09	0.69
1:A:422:LEU:HD22	1:A:427:VAL:HG11	1.83	0.61
1:A:219:GLU:OE2	1:B:358:HIS:HE1	1.83	0.61
1:A:208:VAL:HG12	1:A:208:VAL:O	2.02	0.59
1:A:124:VAL:HG23	1:A:176:LEU:HD22	1.87	0.56
1:B:17:GLN:HG3	1:B:63:PHE:CE2	2.42	0.54
1:A:70:ILE:HG21	1:A:408:VAL:CG2	2.30	0.54
1:A:422:LEU:CD2	1:A:427:VAL:HG11	2.39	0.52
1:B:16:VAL:HA	1:B:45:THR:HG23	1.92	0.51
1:B:136:LEU:O	5:B:2138:HOH:O	2.19	0.51
1:A:83:LEU:HD23	1:A:86:MET:HE3	1.93	0.50
1:A:209:ARG:HD2	1:B:63:PHE:CZ	2.47	0.50
1:A:70:ILE:HG22	1:A:405:THR:HA	1.96	0.48
1:A:17:GLN:NE2	1:A:59:TYR:OH	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HD21	1:A:36:ILE:CD1	2.44	0.47
1:A:186:ILE:HD13	1:A:194:GLN:NE2	2.30	0.47
1:A:133:ASN:HB3	1:A:136:LEU:HD12	1.97	0.46
1:A:95:GLU:HG2	1:A:102:LEU:HD22	1.97	0.46
1:B:392:GLN:NE2	5:B:2303:HOH:O	2.48	0.46
1:B:102:LEU:HD23	1:B:105:MET:CE	2.44	0.45
1:A:288:MET:HE1	1:A:345:ILE:HG13	1.99	0.45
1:B:133:ASN:HB3	1:B:136:LEU:HD12	1.98	0.44
1:A:288:MET:HE1	1:A:345:ILE:CG1	2.48	0.43
1:A:298:LYS:NZ	5:A:2247:HOH:O	2.51	0.43
1:A:262:GLN:NE2	5:A:2219:HOH:O	2.51	0.43
1:A:14:THR:HB	1:A:19:GLY:HA3	2.01	0.43
1:A:70:ILE:CG2	1:A:408:VAL:HG21	2.33	0.43
1:B:186:ILE:HG21	1:B:194:GLN:NE2	2.34	0.43
1:A:404:HIS:O	1:A:408:VAL:HG13	2.19	0.42
1:A:36:ILE:HG12	1:A:70:ILE:HD11	2.02	0.42
1:A:208:VAL:HG12	1:A:211:LYS:HB2	2.01	0.42
1:A:137:LYS:HB3	2:A:1169:COA:H142	2.02	0.41
1:A:16:VAL:HG23	1:A:17:GLN:H	1.86	0.41
1:A:179:GLY:HA3	1:A:196:VAL:HG21	2.02	0.41
1:A:15:HIS:O	1:A:16:VAL:HG22	2.21	0.41

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	431/428 (101%)	420 (97%)	10 (2%)	1 (0%)	51	48
1	B	427/428 (100%)	411 (96%)	12 (3%)	4 (1%)	20	12
All	All	858/856 (100%)	831 (97%)	22 (3%)	5 (1%)	28	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	140	GLU
1	B	134	GLU
1	B	233	ASN
1	A	16	VAL
1	B	16	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	356/351 (101%)	347 (98%)	9 (2%)	53	54
1	B	352/351 (100%)	347 (99%)	5 (1%)	71	76
All	All	708/702 (101%)	694 (98%)	14 (2%)	62	64

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

Mol	Chain	Res	Type
1	A	11	LEU
1	A	35	LYS
1	A	38	ARG
1	A	44	MET
1	A	54[A]	ASN
1	A	54[B]	ASN
1	A	59	TYR
1	A	78	GLU
1	A	386	PHE
1	B	59	TYR
1	B	138	VAL
1	B	288	MET
1	B	386	PHE
1	B	416	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	262	GLN
1	A	363	GLN
1	B	358	HIS
1	B	392	GLN

### 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](#)

Of 7 ligands modelled in this entry, 5 are monoatomic - leaving 2 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	$\# Z  > 2$
2	COA	A	1169	1	43,50,50	1.05	1 (2%)	48,75,75	1.52	2 (4%)
2	COA	B	1169	1	43,50,50	1.02	1 (2%)	48,75,75	1.46	2 (4%)

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	1169	1	-	0/44/64/64	0/3/3/3
2	COA	B	1169	1	-	0/44/64/64	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1169	COA	O9P-C9P	5.15	1.33	1.23
2	A	1169	COA	O9P-C9P	5.22	1.33	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1169	COA	N3A-C2A-N1A	-8.89	121.12	128.86
2	B	1169	COA	N3A-C2A-N1A	-8.51	121.45	128.86
2	A	1169	COA	C4A-C5A-N7A	-2.26	107.23	109.41
2	B	1169	COA	C4A-C5A-N7A	-2.17	107.31	109.41

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	A	1169	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	427/428 (99%)	0.27	26 (6%) 22 22	13, 27, 61, 71	0
1	B	396/428 (92%)	0.65	53 (13%) 4 4	15, 30, 64, 73	0
All	All	823/856 (96%)	0.45	79 (9%) 9 9	13, 28, 62, 73	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	320	ILE	7.4
1	B	323	PHE	6.7
1	B	420	LYS	5.5
1	B	285	ALA	5.3
1	A	427	VAL	5.1
1	B	417	ALA	5.1
1	B	413	GLY	5.0
1	B	343	TYR	4.9
1	B	424	ALA	4.8
1	B	344	GLY	4.8
1	B	421	GLU	4.3
1	B	233	ASN	4.1
1	B	238	ARG	4.0
1	A	106	GLY	3.9
1	B	422	LEU	3.9
1	B	284	ILE	3.9
1	B	345	ILE	3.9
1	B	415	ASP	3.8
1	B	317	LEU	3.8
1	B	240	GLY	3.7
1	B	342	GLN	3.6
1	B	236	PHE	3.6
1	B	416	ASP	3.6
1	A	111	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	77	PRO	3.4
1	A	105	MET	3.4
1	B	419	ILE	3.3
1	A	413	GLY	3.3
1	B	339	TRP	3.2
1	B	410	LYS	3.2
1	A	424	ALA	3.2
1	A	426	GLN	3.2
1	A	2	THR	3.2
1	B	428	VAL	3.2
1	A	74	MET	3.1
1	A	75	LYS	3.0
1	A	78	GLU	3.0
1	B	234	PHE	2.9
1	B	346	PRO	2.9
1	B	77	PRO	2.9
1	A	425	LYS	2.9
1	B	418	LYS	2.8
1	A	99	PRO	2.8
1	A	415	ASP	2.7
1	A	72	LEU	2.7
1	A	101	ALA	2.7
1	B	247	ASN	2.7
1	B	426	GLN	2.6
1	A	428	VAL	2.6
1	B	74	MET	2.6
1	B	261	GLY	2.6
1	B	414	LEU	2.6
1	A	422	LEU	2.5
1	B	425	LYS	2.5
1	B	2	THR	2.5
1	A	104	ARG	2.5
1	B	239	ASP	2.5
1	A	82	LEU	2.4
1	B	324	ILE	2.4
1	A	178	ILE	2.4
1	A	207	LEU	2.4
1	B	178	ILE	2.4
1	A	54[A]	ASN	2.3
1	B	282	PHE	2.3
1	B	321	PHE	2.3
1	B	207	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	326	THR	2.2
1	B	241	ASN	2.2
1	B	110	GLU	2.2
1	A	79	GLY	2.2
1	B	243	LEU	2.1
1	B	138	VAL	2.1
1	B	330	ASP	2.1
1	B	76	THR	2.1
1	B	340	ALA	2.1
1	B	412	LEU	2.1
1	B	232	PRO	2.1
1	B	81	GLU	2.0
1	A	139	TYR	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	A	1169	48/48	0.91	0.21	0.17	41,58,65,65	0
4	MG	A	4001	1/1	1.00	0.12	0.14	20,20,20,20	0
2	COA	B	1169	48/48	0.92	0.13	-0.32	23,39,45,46	0
4	MG	A	4000	1/1	0.96	0.10	-1.33	40,40,40,40	0
3	CL	B	3000	1/1	0.99	0.07	-3.02	26,26,26,26	0
3	CL	A	3000	1/1	0.99	0.07	-3.17	35,35,35,35	0
3	CL	B	3001	1/1	0.99	0.04	-	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.