



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:59 AM GMT

PDB ID : 2VJK
Title : FORMYL-COA TRANSFERASE WITH ASPARTYL-COA THIOESTER INTERMEDIATE DERIVED FROM OXALYL-COA
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Deposited on : 2007-12-11
Resolution : 1.97 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 ⓘ 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

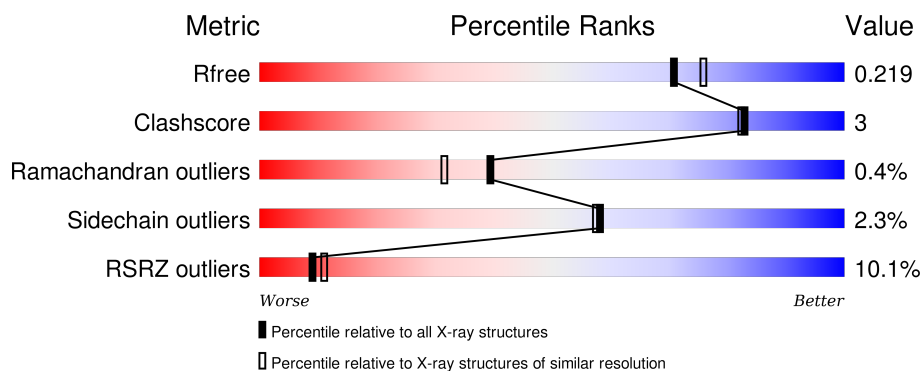
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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 $\leq 5\%$. 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	<div> <div>4%</div> <div>91%</div> <div>8%</div> </div>
1	B	428	<div> <div>16%</div> <div>93%</div> <div>6%</div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7566 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.

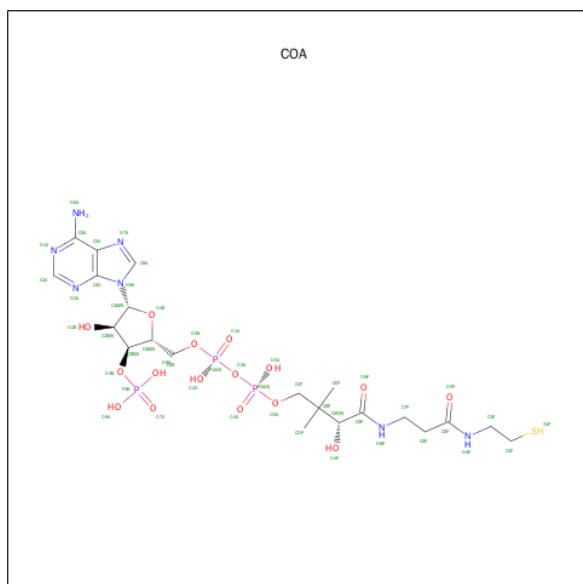
- Molecule 1 is a protein called FORMYL-COENZYME A TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	9	0
			3352	2125	572	631	24			
1	B	427	Total	C	N	O	S	0	3	0
			3327	2106	570	628	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	1	Total	Cl	0	0
			1	1		
3	A	2	Total	Cl	0	0
			2	2		

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

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

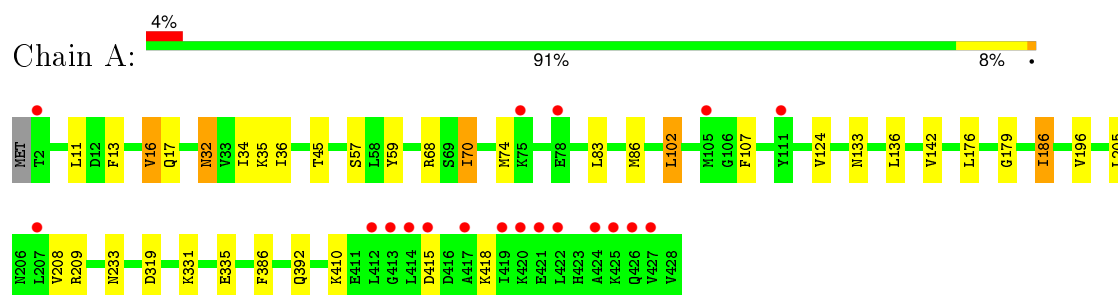
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	440	Total	O	0	0
			440	440		
5	B	347	Total	O	0	0
			347	347		

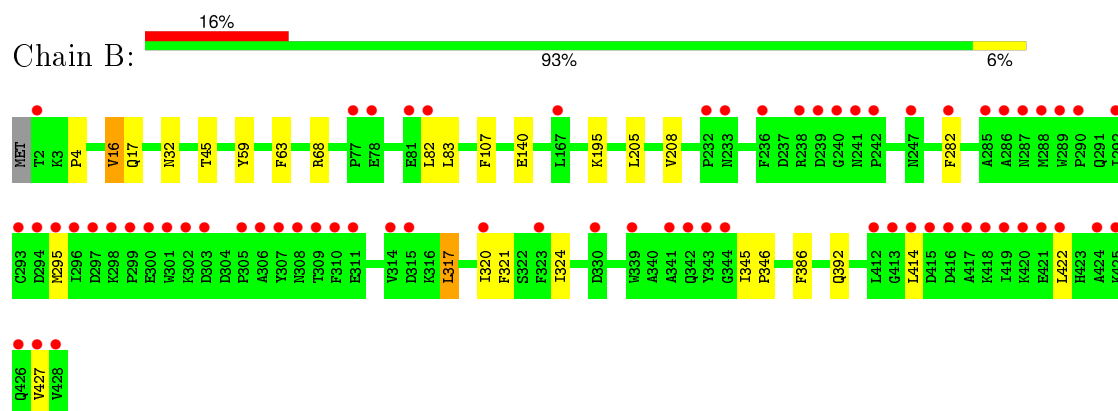
3 Residue-property plots

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 1: FORMYL-COENZYME A TRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	151.91Å 151.91Å 99.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.97 48.04 – 1.97	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.00-1.97) 98.8 (48.04-1.97)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.173 , 0.214 0.175 , 0.219	Depositor DCC
R_{free} test set	3910 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.2	EDS
Estimated twinning fraction	0.034 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 78858 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7566	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, 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	0.40	0/3453	0.55	0/4667
1	B	0.39	0/3411	0.54	0/4612
All	All	0.39	0/6864	0.55	0/9279

There are no bond length outliers.

There are no bond angle outliers.

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	3352	0	3318	24	0
1	B	3327	0	3268	19	0
2	A	48	0	31	0	0
2	B	48	0	31	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
5	A	440	0	0	2	0
5	B	347	0	0	1	0
All	All	7566	0	6648	41	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 (41) 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:186:ILE:HG23	1:B:4:PRO:HA	1.41	1.01
1:B:422:LEU:HD22	1:B:427:VAL:HG21	1.57	0.85
1:A:319:ASP:OD1	5:A:2325:HOH:O	2.00	0.79
1:B:295:MET:HE2	1:B:345:ILE:HD12	1.67	0.73
1:B:295:MET:CE	1:B:345:ILE:HD12	2.28	0.63
1:A:233:ASN:ND2	5:A:2227:HOH:O	2.32	0.62
1:B:422:LEU:CD2	1:B:427:VAL:HG21	2.28	0.61
1:A:83:LEU:HD23	1:A:86:MET:CE	2.31	0.61
1:A:16:VAL:HG22	1:A:17:GLN:HE21	1.71	0.56
1:B:282:PHE:CE2	1:B:324:ILE:HD11	2.41	0.55
1:A:32[A]:ASN:HD21	1:A:68:ARG:HH21	1.54	0.55
1:A:124:VAL:HG23	1:A:176:LEU:HD22	1.89	0.54
1:B:83:LEU:HD23	1:B:107:PHE:CE1	2.45	0.52
1:A:102:LEU:HD22	1:A:107:PHE:HB2	1.91	0.51
1:A:13:PHE:HE2	1:A:74:MET:HE3	1.74	0.51
1:A:208:VAL:HG12	1:A:208:VAL:O	2.11	0.50
1:B:321:PHE:HA	1:B:324:ILE:HG22	1.93	0.50
1:A:83:LEU:HD23	1:A:86:MET:HE3	1.91	0.50
1:A:36:ILE:HG12	1:A:70[A]:ILE:HD11	1.94	0.50
1:A:133:ASN:HB3	1:A:136:LEU:HD12	1.95	0.49
1:A:45:THR:O	1:A:57[A]:SER:OG	2.31	0.48
1:B:16:VAL:HA	1:B:45:THR:HG23	1.96	0.47
1:B:295:MET:CE	1:B:345:ILE:CD1	2.92	0.47
1:A:34:ILE:CG2	1:A:70[A]:ILE:HD12	2.45	0.47
1:A:331:LYS:HB3	1:A:335:GLU:HG3	1.98	0.46
1:B:82:LEU:HD21	1:B:414:LEU:HD11	1.99	0.45
1:A:74:MET:CE	1:A:83:LEU:HD11	2.47	0.45
1:B:317:LEU:O	1:B:320:ILE:HG22	2.17	0.45
1:B:422:LEU:HD22	1:B:427:VAL:CG2	2.39	0.44
1:A:179:GLY:HA3	1:A:196:VAL:HG21	2.00	0.44
1:B:205:LEU:HA	1:B:208:VAL:HG22	2.00	0.44
1:B:345:ILE:HG23	1:B:346:PRO:HD2	2.01	0.43
1:A:35:LYS:O	1:A:70[A]:ILE:HD13	2.17	0.43
1:B:17:GLN:HG3	1:B:63:PHE:CE2	2.54	0.43
1:A:13:PHE:CE2	1:A:74:MET:HE3	2.54	0.43
1:A:209:ARG:HD2	1:B:63:PHE:CZ	2.54	0.43
1:B:317:LEU:O	1:B:320:ILE:CG2	2.67	0.42
1:A:34:ILE:HG22	1:A:70[A]:ILE:HD12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ASN:HD21	1:B:68:ARG:HH21	1.66	0.42
1:A:11:LEU:HD11	1:A:36:ILE:HD11	2.01	0.42
1:A:142:VAL:HG23	5:B:2274:HOH:O	2.19	0.42

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	434/428 (101%)	426 (98%)	7 (2%)	1 (0%)	52	47
1	B	428/428 (100%)	418 (98%)	8 (2%)	2 (0%)	34	25
All	All	862/856 (101%)	844 (98%)	15 (2%)	3 (0%)	39	39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	140	GLU
1	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	359/351 (102%)	346 (96%)	13 (4%)	42	36
1	B	353/351 (101%)	348 (99%)	5 (1%)	74	75
All	All	712/702 (101%)	694 (98%)	18 (2%)	58	53

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32[A]	ASN
1	A	32[B]	ASN
1	A	59	TYR
1	A	70[A]	ILE
1	A	70[B]	ILE
1	A	102	LEU
1	A	186	ILE
1	A	205	LEU
1	A	386	PHE
1	A	392	GLN
1	A	410	LYS
1	A	415	ASP
1	A	418	LYS
1	B	59	TYR
1	B	195	LYS
1	B	317	LEU
1	B	386	PHE
1	B	392	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	206	ASN
1	A	233	ASN
1	A	392	GLN
1	B	32	ASN
1	B	113	GLN
1	B	206	ASN
1	B	342	GLN
1	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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 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	40,50,50	1.10	1 (2%)	50,75,75	1.69	3 (6%)
2	COA	B	1169	1	40,50,50	1.06	1 (2%)	50,75,75	1.70	3 (6%)

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	5.17	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1169	COA	O9P-C9P	5.32	1.33	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1169	COA	N3A-C2A-N1A	-9.98	121.25	128.89
2	B	1169	COA	N3A-C2A-N1A	-9.69	121.47	128.89
2	B	1169	COA	P2A-O3A-P1A	-3.58	122.67	132.73
2	A	1169	COA	C4A-C5A-N7A	-2.43	107.24	109.48
2	B	1169	COA	C4A-C5A-N7A	-2.40	107.27	109.48
2	A	1169	COA	P2A-O3A-P1A	-2.29	126.29	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th 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%)	0.17	19 (4%) 38 42	12, 22, 48, 69	0
1	B	427/428 (99%)	0.75	67 (15%) 3 3	11, 26, 70, 86	0
All	All	854/856 (99%)	0.46	86 (10%) 9 11	11, 24, 64, 86	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	305	PRO	8.0
1	B	301	TRP	7.2
1	B	424	ALA	6.0
1	A	415	ASP	5.5
1	B	290	PRO	5.5
1	B	415	ASP	5.5
1	B	417	ALA	5.3
1	B	307	TYR	5.1
1	B	299	PRO	5.0
1	B	241	ASN	5.0
1	B	320	ILE	4.9
1	B	306	ALA	4.9
1	B	323	PHE	4.9
1	B	343	TYR	4.5
1	B	422	LEU	4.3
1	B	296	ILE	4.2
1	B	414	LEU	4.2
1	B	288	MET	4.1
1	B	420	LYS	4.1
1	B	294	ASP	4.1
1	B	297	ASP	4.1
1	B	302	LYS	4.1
1	B	416	ASP	4.0
1	B	303	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	413	GLY	3.8
1	B	427	VAL	3.8
1	B	309	THR	3.8
1	B	295	MET	3.8
1	B	298	LYS	3.7
1	B	344	GLY	3.6
1	B	287	ASN	3.6
1	A	2	THR	3.6
1	B	232	PRO	3.5
1	B	421	GLU	3.5
1	A	413	GLY	3.4
1	B	428	VAL	3.4
1	B	341	ALA	3.2
1	B	81	GLU	3.2
1	B	419	ILE	3.2
1	B	342	GLN	3.1
1	A	424	ALA	3.1
1	B	289	TRP	3.1
1	B	236	PHE	3.1
1	A	427	VAL	3.0
1	B	426	GLN	3.0
1	B	412	LEU	3.0
1	B	339	TRP	2.9
1	B	285	ALA	2.9
1	B	425	LYS	2.9
1	A	414	LEU	2.9
1	B	314	VAL	2.8
1	A	420	LYS	2.8
1	A	425	LYS	2.6
1	B	418	LYS	2.6
1	B	292	ILE	2.6
1	A	111	TYR	2.6
1	B	308	ASN	2.6
1	B	240	GLY	2.6
1	B	310	PHE	2.5
1	B	239	ASP	2.5
1	A	426	GLN	2.5
1	A	422	LEU	2.5
1	B	77	PRO	2.5
1	B	242	PRO	2.5
1	A	419	ILE	2.5
1	B	286	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	2	THR	2.4
1	B	233	ASN	2.4
1	B	315	ASP	2.4
1	B	78	GLU	2.3
1	A	207	LEU	2.3
1	B	330	ASP	2.3
1	B	311	GLU	2.3
1	B	247	ASN	2.3
1	B	293	CYS	2.3
1	A	105	MET	2.2
1	A	412	LEU	2.2
1	B	238	ARG	2.2
1	B	82	LEU	2.2
1	A	421	GLU	2.1
1	B	167	LEU	2.1
1	B	300	GLU	2.1
1	A	75	LYS	2.1
1	B	282	PHE	2.1
1	A	417	ALA	2.0
1	A	78	GLU	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, 95th 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	COA	B	1169	48/48	0.90	0.15	0.46	23,48,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	COA	A	1169	48/48	0.94	0.13	-0.34	30,43,45,46	0
3	CL	A	1430	1/1	0.99	0.08	-2.36	24,24,24,24	0
3	CL	B	1430	1/1	0.99	0.05	-3.91	22,22,22,22	0
3	CL	A	1432	1/1	0.98	0.05	-	27,27,27,27	0
4	MG	A	1431	1/1	0.96	0.05	-	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.