



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:59 AM GMT

PDB ID : 2VJL
Title : FORMYL-COA TRANSFERASE WITH ASPARTYL-COA THIOESTER INTERMEDIATE DERIVED FROM FORMYL-COA
Authors : Berthold, C.L.; Toyota, C.G.; Richards, N.G.J.; Lindqvist, Y.
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
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

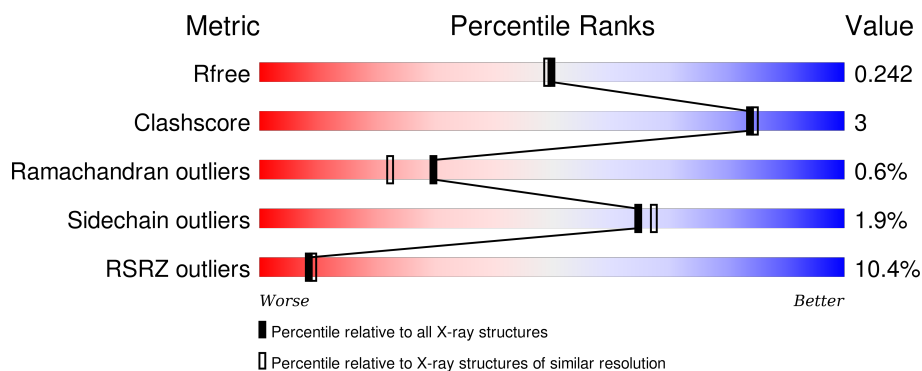
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 ≥ 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.

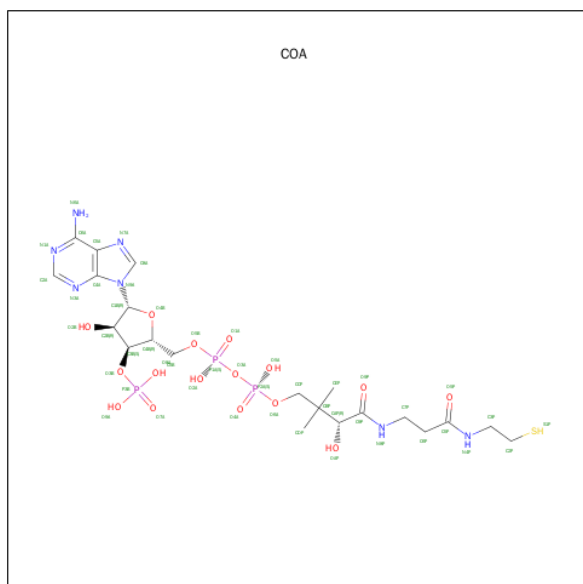
- Molecule 1 is a protein called FORMYL-COENZYME A TRANSFERASE.

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: C₂₁H₃₆N₇O₁₆P₃S).



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		

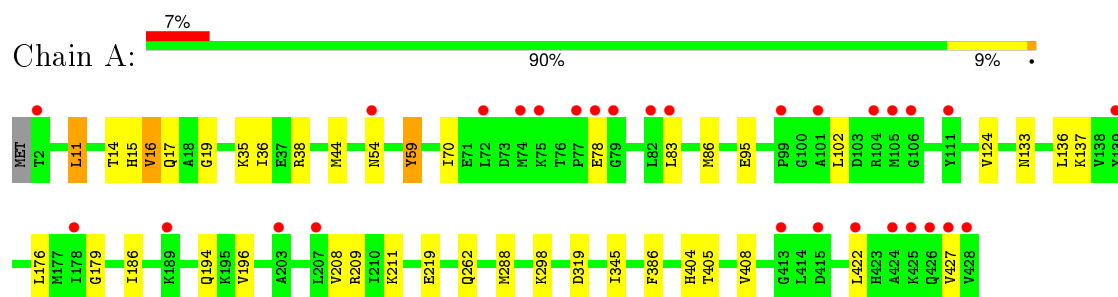
- Molecule 5 is water.

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

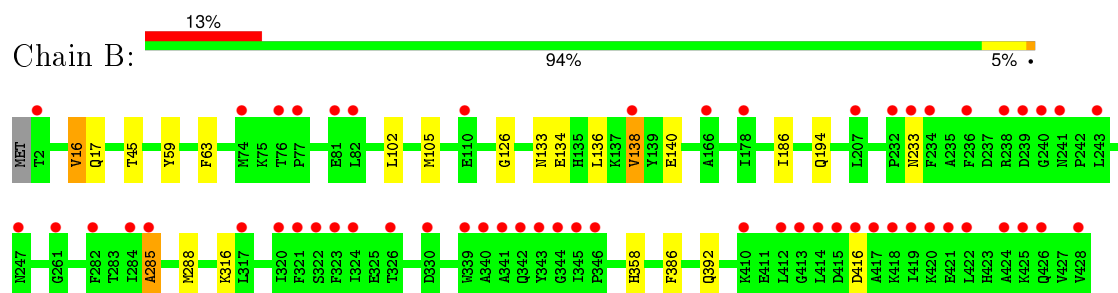
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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



- 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	151.76Å 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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	28.7	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.9	EDS
Estimated twinning fraction	0.028 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 75233 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7457	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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 [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	431/428 (101%)	420 (97%)	10 (2%)	1 (0%)	52	48
1	B	427/428 (100%)	411 (96%)	12 (3%)	4 (1%)	21	13
All	All	858/856 (100%)	831 (97%)	22 (3%)	5 (1%)	30	22

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%)	55	55
1	B	352/351 (100%)	347 (99%)	5 (1%)	74	77
All	All	708/702 (101%)	694 (98%)	14 (2%)	65	65

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	40,50,50	1.06	1 (2%)	50,75,75	1.76	4 (8%)
2	COA	B	1169	1	40,50,50	1.05	1 (2%)	50,75,75	1.67	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	5.14	1.33	1.23
2	A	1169	COA	O9P-C9P	5.21	1.33	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1169	COA	N3A-C2A-N1A	-10.16	121.12	128.89
2	B	1169	COA	N3A-C2A-N1A	-9.73	121.45	128.89
2	A	1169	COA	P2A-O3A-P1A	-3.30	123.47	132.73
2	B	1169	COA	P2A-O3A-P1A	-2.76	124.97	132.73
2	A	1169	COA	C4A-C5A-N7A	-2.45	107.23	109.48
2	B	1169	COA	C4A-C5A-N7A	-2.35	107.31	109.48
2	A	1169	COA	O4B-C1B-N9A	2.12	112.53	108.10

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.33	29 (6%) 20 22	13, 27, 61, 71	0
1	B	396/428 (92%)	0.72	57 (14%) 3 4	15, 30, 64, 73	0
All	All	823/856 (96%)	0.52	86 (10%) 8 9	13, 28, 62, 73	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	320	ILE	7.8
1	B	323	PHE	7.1
1	B	420	LYS	5.7
1	B	285	ALA	5.6
1	A	427	VAL	5.5
1	B	417	ALA	5.4
1	B	413	GLY	5.3
1	B	424	ALA	5.1
1	B	343	TYR	5.1
1	B	344	GLY	5.0
1	B	421	GLU	4.5
1	B	233	ASN	4.2
1	B	284	ILE	4.2
1	B	238	ARG	4.2
1	B	345	ILE	4.1
1	B	422	LEU	4.1
1	A	106	GLY	4.1
1	B	317	LEU	4.0
1	B	415	ASP	4.0
1	B	240	GLY	3.9
1	B	236	PHE	3.8
1	B	416	ASP	3.7
1	B	342	GLN	3.7
1	A	111	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	419	ILE	3.6
1	A	77	PRO	3.5
1	A	105	MET	3.5
1	A	413	GLY	3.5
1	B	339	TRP	3.4
1	B	428	VAL	3.4
1	A	424	ALA	3.4
1	A	2	THR	3.3
1	B	410	LYS	3.3
1	A	426	GLN	3.3
1	A	74	MET	3.2
1	B	234	PHE	3.1
1	A	75	LYS	3.1
1	A	78	GLU	3.1
1	B	346	PRO	3.1
1	B	77	PRO	3.0
1	A	425	LYS	3.0
1	A	99	PRO	2.9
1	B	418	LYS	2.9
1	A	415	ASP	2.9
1	A	101	ALA	2.9
1	A	72	LEU	2.9
1	A	428	VAL	2.8
1	B	247	ASN	2.8
1	B	414	LEU	2.7
1	B	426	GLN	2.7
1	B	261	GLY	2.7
1	A	422	LEU	2.7
1	B	74	MET	2.7
1	B	324	ILE	2.6
1	A	82	LEU	2.6
1	B	425	LYS	2.6
1	A	178	ILE	2.6
1	B	2	THR	2.6
1	B	239	ASP	2.6
1	A	104	ARG	2.6
1	B	178	ILE	2.5
1	A	207	LEU	2.5
1	B	282	PHE	2.5
1	B	321	PHE	2.4
1	A	54[A]	ASN	2.4
1	B	207	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	326	THR	2.4
1	B	138	VAL	2.3
1	B	241	ASN	2.3
1	B	243	LEU	2.3
1	A	79	GLY	2.3
1	B	340	ALA	2.3
1	B	110	GLU	2.2
1	B	330	ASP	2.2
1	B	412	LEU	2.2
1	B	76	THR	2.2
1	B	232	PRO	2.2
1	A	83	LEU	2.1
1	A	139	TYR	2.1
1	B	81	GLU	2.1
1	B	322	SER	2.1
1	B	82	LEU	2.1
1	A	189	LYS	2.1
1	A	203	ALA	2.1
1	B	341	ALA	2.1
1	B	166	ALA	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	A	1169	48/48	0.91	0.21	0.17	41,58,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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	-3.04	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.