



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 05:38 AM GMT

PDB ID : 2REQ  
Title : METHYLMALONYL-COA MUTASE, NON-PRODUCTIVE COA COMPLEX, IN OPEN CONFORMATION REPRESENTING SUBSTRATE-FREE STATE  
Authors : Evans, P.R.; Mancia, F.  
Deposited on : 1997-09-22  
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (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

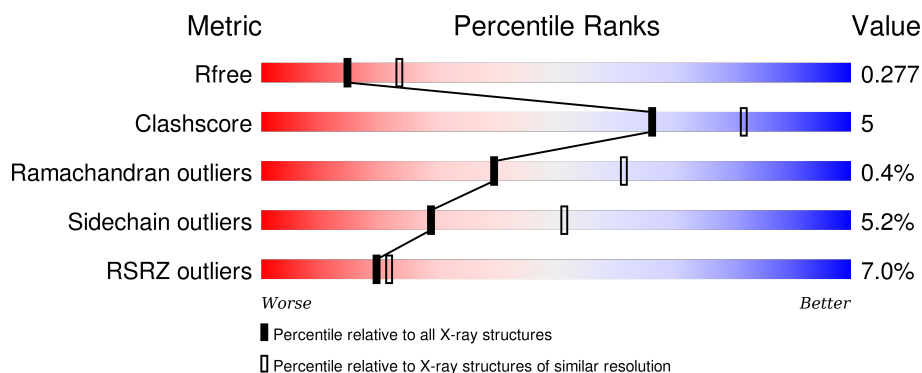
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	727	<div> <div>4%</div> <div>73%</div> <div>24%</div> <div>.</div> </div>
1	C	727	<div> <div>4%</div> <div>73%</div> <div>23%</div> <div>.</div> </div>
2	B	637	<div> <div>12%</div> <div>73%</div> <div>20%</div> <div>.</div> </div>
2	D	637	<div> <div>9%</div> <div>72%</div> <div>22%</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	801	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 21240 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 METHYLMALONYL-COA MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	725	Total	C	N	O	S	0	0	0
			5564	3518	965	1057	24			
1	C	725	Total	C	N	O	S	0	0	0
			5564	3518	965	1057	24			

- Molecule 2 is a protein called METHYLMALONYL-COA MUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	619	Total	C	N	O	S	0	0	0
			4616	2912	795	896	13			
2	D	619	Total	C	N	O	S	0	0	0
			4616	2912	795	896	13			

There are 6 discrepancies between the modelled and reference sequences:

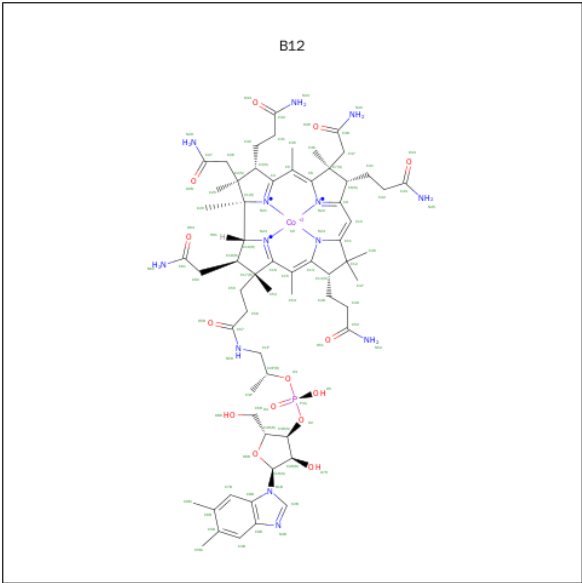
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	SEE REMARK 999	UNP P11652
B	330	GLU	ASP	SEE REMARK 999	UNP P11652
B	331	LEU	VAL	SEE REMARK 999	UNP P11652
D	203	GLY	ALA	SEE REMARK 999	UNP P11652
D	330	GLU	ASP	SEE REMARK 999	UNP P11652
D	331	LEU	VAL	SEE REMARK 999	UNP P11652

- 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	0	0
			31	10	5	13	3		
3	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is COBALAMIN (three-letter code: B12) (formula: C<sub>62</sub>H<sub>89</sub>CoN<sub>13</sub>O<sub>14</sub>P).

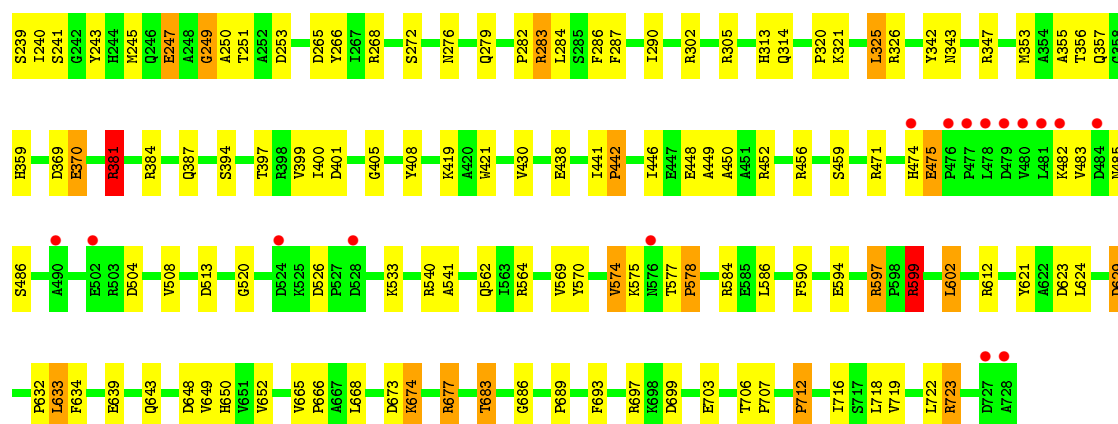


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Co	N	O	P	0
			91	62	1	13	14	1	
4	C	1	Total	C	Co	N	O	P	0
			91	62	1	13	14	1	

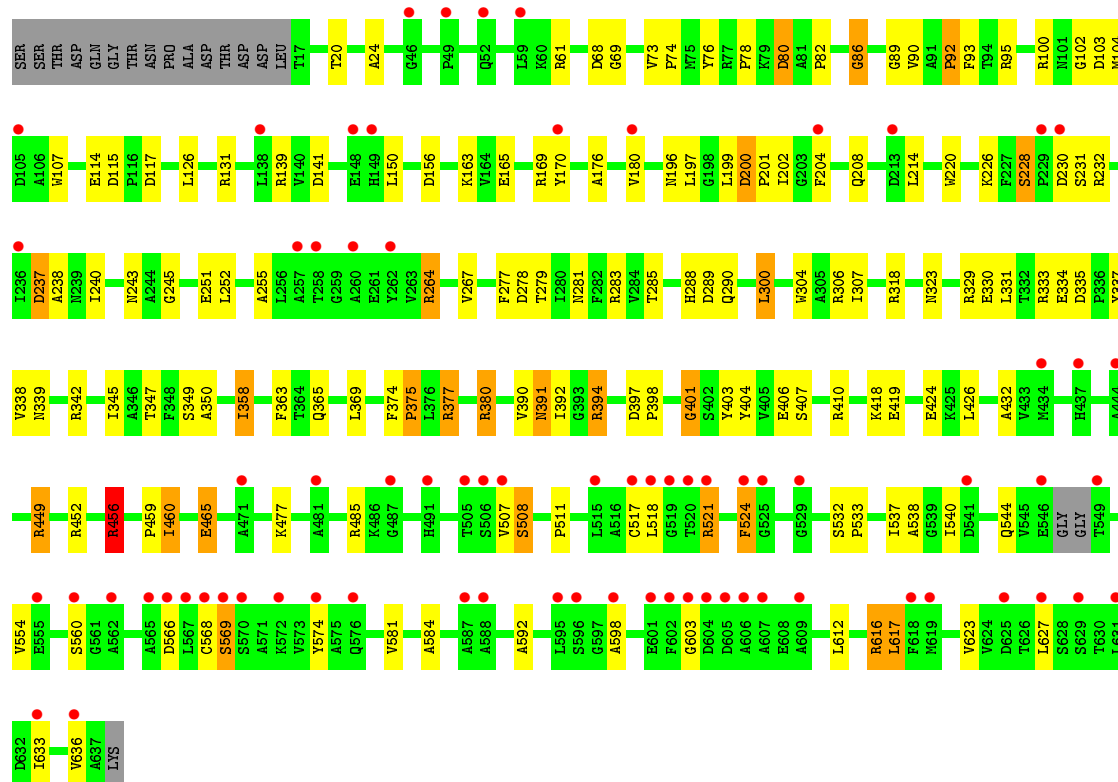
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	206	Total 206	O 206	0	0
5	B	112	Total 112	O 112	0	0
5	C	201	Total 201	O 201	0	0
5	D	117	Total 117	O 117	0	0

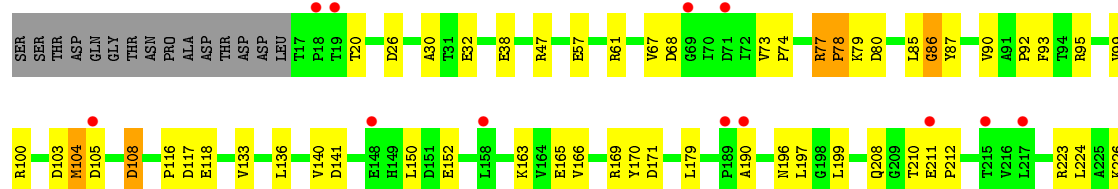




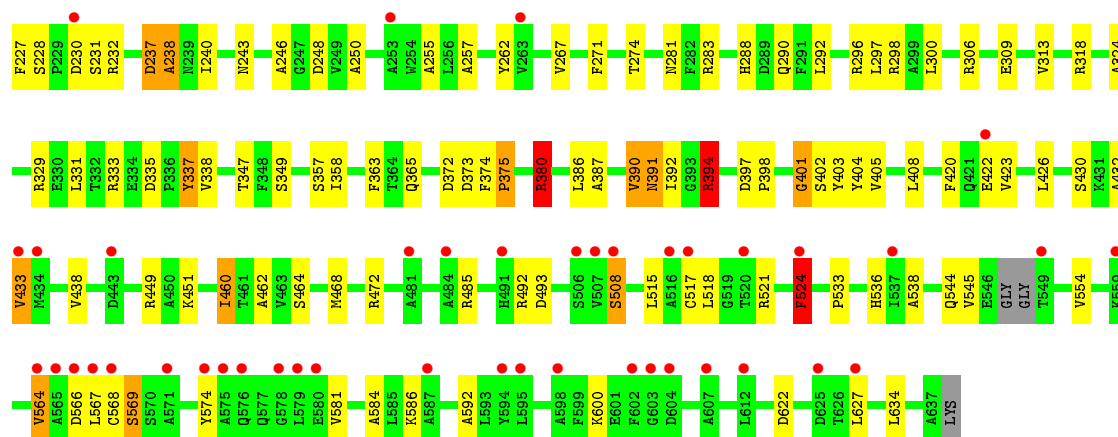
• Molecule 2: METHYLMALONYL-COA MUTASE



• Molecule 2: METHYLMALONYL-COA MUTASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	104.95Å 162.06Å 104.20Å 90.00° 108.75° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.50) 99.8 (19.98-2.50)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.28 (at 2.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.259 , 0.325 0.224 , 0.277	Depositor DCC
$R_{free}$ test set	4538 reflections (4.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.0	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.9	EDS
Estimated twinning fraction	0.009 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 113303 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	21240	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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, B12

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	0.65	0/5680	1.86	123/7715 (1.6%)
1	C	0.68	0/5680	1.95	131/7715 (1.7%)
2	B	0.60	0/4706	1.77	88/6414 (1.4%)
2	D	0.57	0/4706	1.74	90/6414 (1.4%)
All	All	0.63	0/20772	1.84	432/28258 (1.5%)

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	A	0	19
1	C	0	23
2	B	0	18
2	D	0	10
All	All	0	70

There are no bond length outliers.

The worst 5 of 432 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	540	ARG	CD-NE-CZ	21.55	153.77	123.60
1	C	384	ARG	NE-CZ-NH2	-19.09	110.76	120.30
2	B	283	ARG	NE-CZ-NH1	16.99	128.79	120.30
2	B	264	ARG	NE-CZ-NH2	-16.78	111.91	120.30
1	C	540	ARG	NE-CZ-NH2	16.69	128.65	120.30

There are no chirality outliers.

5 of 70 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ALA	Mainchain
1	A	167	MET	Mainchain
1	A	20	ASP	Mainchain
1	A	40	THR	Mainchain
1	A	70	PHE	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	5564	0	5472	42	0
1	C	5564	0	5472	45	0
2	B	4616	0	4428	47	0
2	D	4616	0	4428	49	0
3	A	31	0	11	1	0
3	C	31	0	11	1	0
4	A	91	0	88	19	0
4	C	91	0	88	12	0
5	A	206	0	0	1	0
5	B	112	0	0	0	0
5	C	201	0	0	0	0
5	D	117	0	0	0	0
All	All	21240	0	19998	200	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 5.

The worst 5 of 200 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)
4:A:800:B12:H362	4:A:800:B12:H351	1.22	1.11
4:C:800:B12:H362	4:C:800:B12:H351	1.17	1.09
4:A:800:B12:H531	4:A:800:B12:H552	1.09	1.09
4:A:800:B12:C53	4:A:800:B12:H552	1.98	0.93
2:B:281:ASN:HD22	2:B:323:ASN:HD21	1.21	0.88

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	723/727 (99%)	682 (94%)	36 (5%)	5 (1%)	26	46
1	C	723/727 (99%)	688 (95%)	33 (5%)	2 (0%)	46	68
2	B	615/637 (96%)	569 (92%)	43 (7%)	3 (0%)	34	55
2	D	615/637 (96%)	576 (94%)	38 (6%)	1 (0%)	52	75
All	All	2676/2728 (98%)	2515 (94%)	150 (6%)	11 (0%)	39	61

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	486	SER
1	A	10	VAL
1	A	486	SER
1	A	542	MET
1	A	575	LYS

### 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	571/590 (97%)	541 (95%)	30 (5%)	28	50
1	C	571/590 (97%)	544 (95%)	27 (5%)	32	56
2	B	457/509 (90%)	438 (96%)	19 (4%)	36	62
2	D	457/509 (90%)	427 (93%)	30 (7%)	21	38
All	All	2056/2198 (94%)	1950 (95%)	106 (5%)	29	51

5 of 106 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	612	LEU
1	C	276	ASN
2	D	464	SER
1	C	9	SER
1	C	171	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	391	ASN
1	C	246	GLN
2	D	323	ASN
1	C	198	ASN
1	C	359	HIS

### 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](#)

4 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
4	B12	A	800	1	74,101,101	1.10	7 (9%)	111,166,166	1.67	23 (20%)
3	COA	A	801	-	26,33,50	0.92	0	33,52,75	0.96	1 (3%)
4	B12	C	800	1	74,101,101	1.06	4 (5%)	111,166,166	1.55	22 (19%)
3	COA	C	801	-	26,33,50	0.81	0	33,52,75	0.96	1 (3%)

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
4	B12	A	800	1	-	0/51/223/223	0/3/11/11
3	COA	A	801	-	-	0/17/37/64	0/3/3/3
4	B12	C	800	1	-	0/51/223/223	0/3/11/11
3	COA	C	801	-	-	0/17/37/64	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	800	B12	O6R-C1R	-3.71	1.36	1.41
4	A	800	B12	C11-C10	-2.75	1.36	1.41
4	C	800	B12	C11-C10	-2.66	1.36	1.41
4	C	800	B12	O2-C3R	-2.22	1.37	1.44
4	A	800	B12	O2-C3R	-2.21	1.37	1.44

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	B12	O58-C57-C56	-4.10	114.92	121.98
4	C	800	B12	C9-C10-C11	-4.09	122.01	132.28
4	C	800	B12	C2-C1-C19	-3.98	111.68	118.56
4	A	800	B12	C3-C4-C5	-3.37	120.50	131.88
4	A	800	B12	C13-C14-C15	-3.35	120.58	131.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	800	B12	19	0
3	A	801	COA	1	0
4	C	800	B12	12	0
3	C	801	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	725/727 (99%)	0.14	31 (4%) 39 44	18, 35, 68, 125	0
1	C	725/727 (99%)	0.17	28 (3%) 43 48	14, 34, 68, 125	0
2	B	619/637 (97%)	0.66	74 (11%) 6 6	19, 51, 99, 129	0
2	D	619/637 (97%)	0.52	55 (8%) 12 13	19, 52, 99, 130	0
All	All	2688/2728 (98%)	0.36	188 (6%) 19 22	14, 42, 87, 130	0

The worst 5 of 188 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	519	GLY	7.6
2	D	568	CYS	6.6
1	C	474	HIS	6.4
2	B	520	THR	6.1
1	A	92	PHE	6.1

### 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( $\text{\AA}^2$ )	Q<0.9
3	COA	A	801	31/48	0.87	0.27	2.11	48,79,100,101	0
3	COA	C	801	31/48	0.83	0.22	1.88	43,77,100,101	0
4	B12	A	800	91/91	0.96	0.12	-0.40	14,27,39,45	0
4	B12	C	800	91/91	0.97	0.13	-0.49	9,22,33,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.