



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2019 – 05:08 PM EDT

PDB ID : 5N2A  
Title : METHYL-COENZYME M REDUCTASE III FROM METHANOTORRIS  
FORMICICUS TRIGONAL FORM  
Authors : Wagner, T.; Wegner, C.E.; Ermler, U.; Shima, S.  
Deposited on : 2017-02-07  
Resolution : 2.80 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

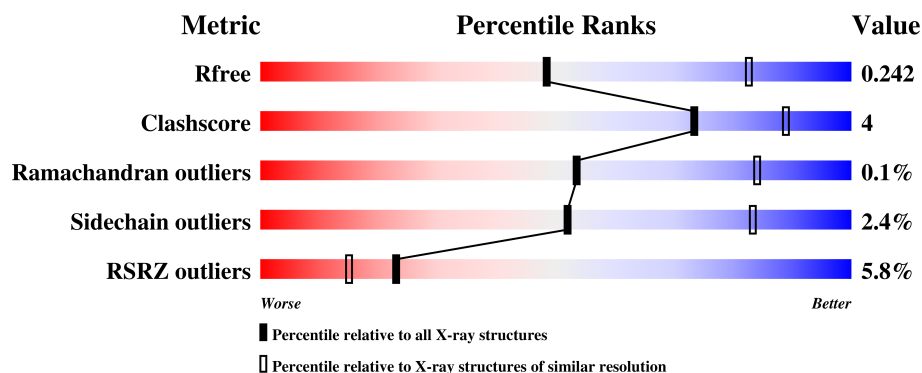
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	111664	2792 (2.80-2.80)
Clashscore	122126	3209 (2.80-2.80)
Ramachandran outliers	120053	3158 (2.80-2.80)
Sidechain outliers	120020	3160 (2.80-2.80)
RSRZ outliers	108989	2726 (2.80-2.80)

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	552	<div> <div>2%</div> <div>89%</div> <div>10% ..</div> </div>
2	B	444	<div> <div>3%</div> <div>91%</div> <div>8%</div> </div>
3	C	260	<div> <div>18%</div> <div>85%</div> <div>13% ..</div> </div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 9806 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 Methyl-coenzyme M reductase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4277	2721	718	816	22			

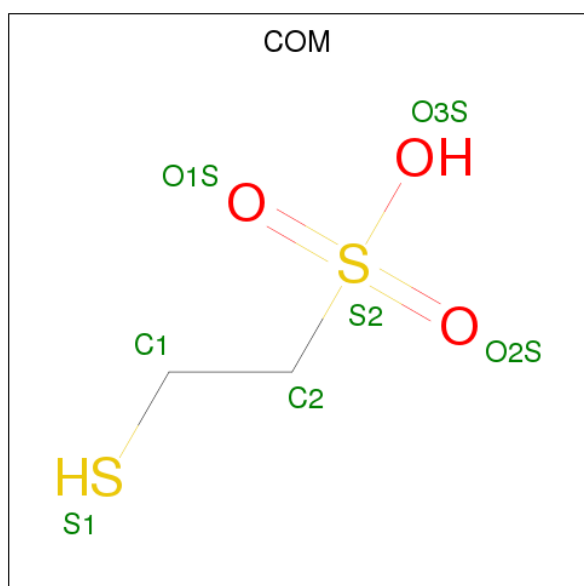
- Molecule 2 is a protein called Methyl-coenzyme M reductase, beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	443	Total	C	N	O	S	0	0	0
			3324	2123	551	630	20			

- Molecule 3 is a protein called Methyl-coenzyme M reductase, gamma subunit.

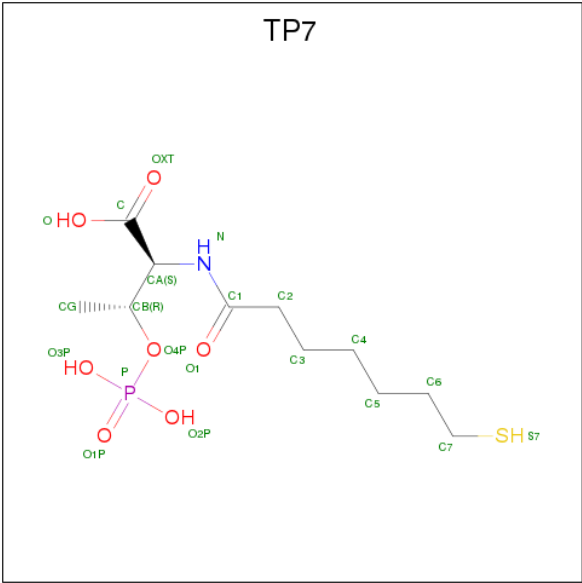
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	258	Total	C	N	O	S	0	0	0
			2113	1331	376	396	10			

- Molecule 4 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula:  $C_2H_6O_3S_2$ ).



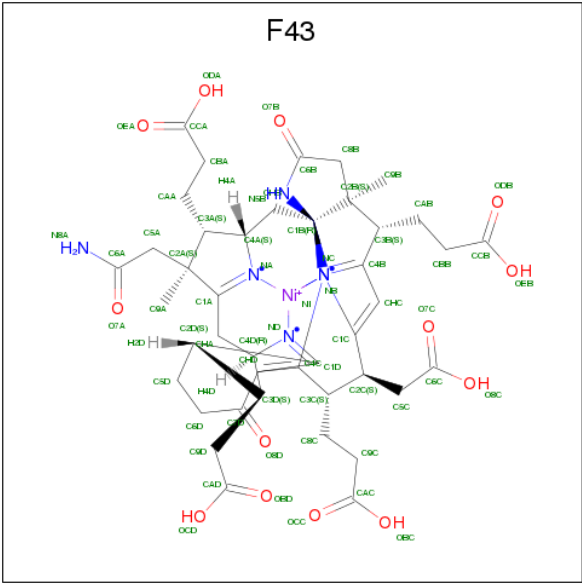
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 5 is Coenzyme B (three-letter code: TP7) (formula:  $C_{11}H_{22}NO_7PS$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
5	A	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		

- Molecule 6 is FACTOR 430 (three-letter code: F43) (formula:  $C_{42}H_{51}N_6NiO_{13}$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	K	0	0
			1	1		

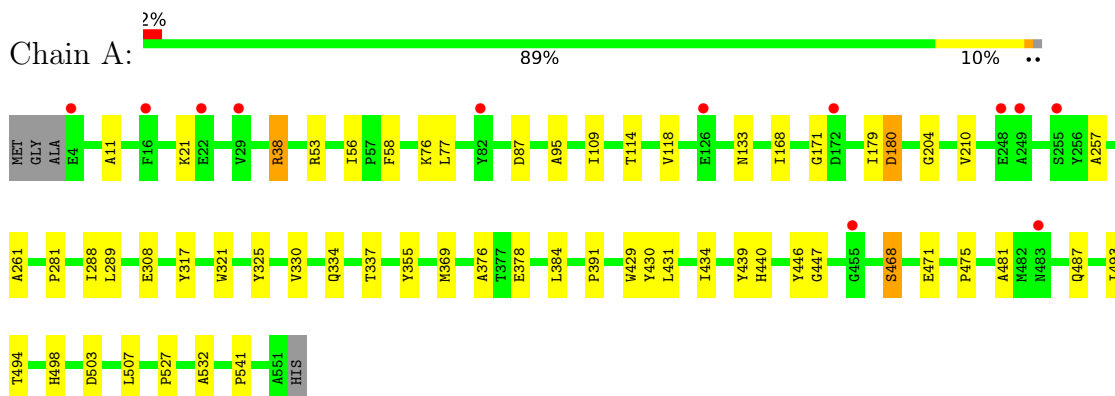
- Molecule 8 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Br	0	0
			1	1		

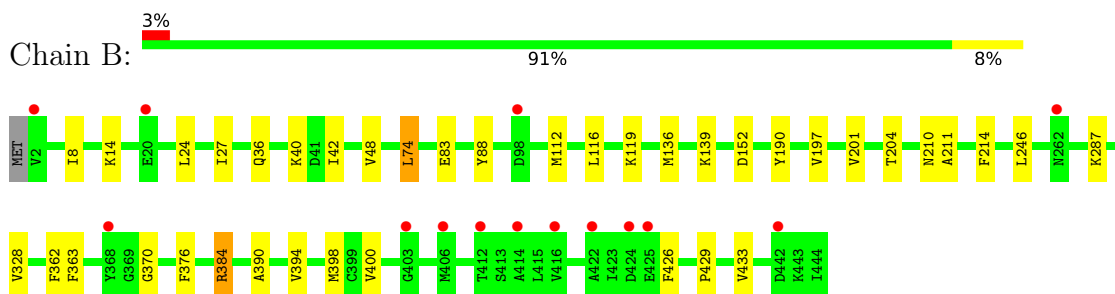
### 3 Residue-property plots [i](#)

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 ( $RSRZ > 2$ ). 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.

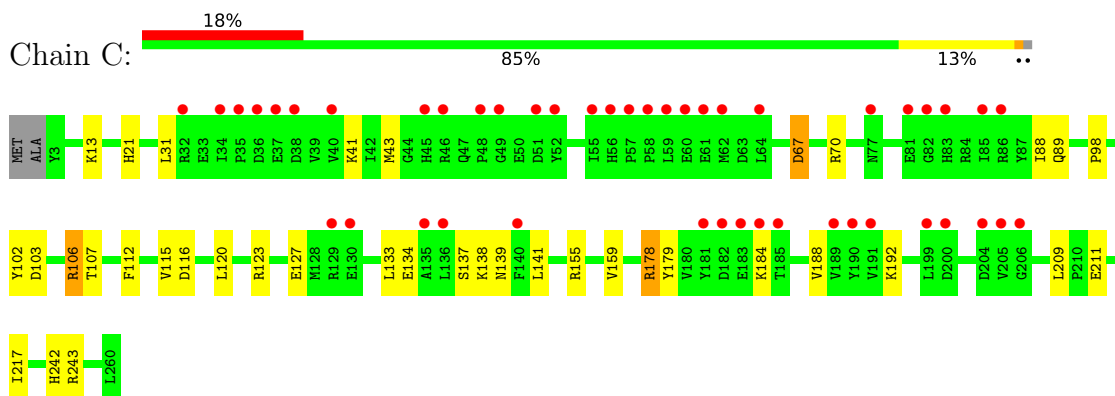
- Molecule 1: Methyl-coenzyme M reductase subunit alpha



- Molecule 2: Methyl-coenzyme M reductase, beta subunit



- Molecule 3: Methyl-coenzyme M reductase, gamma subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.70Å 127.70Å 160.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.85 – 2.80 45.52 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.85-2.80) 99.9 (45.52-2.80)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.96 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, $R_{free}$	0.198 , 0.221 0.218 , 0.242	Depositor DCC
$R_{free}$ test set	1901 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.2	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 57.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9806	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: AGM, K, F43, MGN, TP7, TRX, BR, GL3, COM, MHS

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	0/4319	0.58	0/5844
2	B	0.41	0/3382	0.61	0/4590
3	C	0.39	0/2161	0.60	0/2919
All	All	0.40	0/9862	0.60	0/13353

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	4277	0	4140	32	0
2	B	3324	0	3372	18	0
3	C	2113	0	2073	22	0
4	A	7	0	6	1	0
5	A	21	0	19	0	0
6	A	62	0	43	3	0
7	A	1	0	0	0	0
8	C	1	0	0	0	0
All	All	9806	0	9653	70	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 4.

The worst 5 of 70 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)
3:C:89:GLN:HB2	3:C:155:ARG:O	1.84	0.76
1:A:308:GLU:HG3	1:A:527:PRO:HD2	1.73	0.70
3:C:103:ASP:O	3:C:107:THR:HG23	1.92	0.69
2:B:328:VAL:HG21	2:B:394:VAL:HA	1.75	0.67
3:C:137:SER:HA	3:C:141:LEU:HB2	1.80	0.64

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	541/552 (98%)	513 (95%)	27 (5%)	1 (0%)	49	81
2	B	441/444 (99%)	430 (98%)	11 (2%)	0	100	100
3	C	256/260 (98%)	245 (96%)	11 (4%)	0	100	100
All	All	1238/1256 (99%)	1188 (96%)	49 (4%)	1 (0%)	53	84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	468	SER

### 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	436/438 (100%)	428 (98%)	8 (2%)	62	88
2	B	350/351 (100%)	341 (97%)	9 (3%)	49	81
3	C	228/229 (100%)	221 (97%)	7 (3%)	43	77
All	All	1014/1018 (100%)	990 (98%)	24 (2%)	52	83

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	74	LEU
2	B	116	LEU
3	C	184	LYS
2	B	83	GLU
2	B	88	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	487	GLN
2	B	36	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

5 non-standard protein/DNA/RNA residues 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
1	MHS	A	260	1	8,11,12	1.13	1 (12%)	8,14,16	1.80	3 (37%)
1	AGM	A	274	1	11,11,12	1.03	1 (9%)	7,13,15	0.80	0
1	MGN	A	402	1	6,9,10	0.61	0	5,12,14	0.61	0
1	TRX	A	429	1	15,16,17	1.35	2 (13%)	15,22,24	1.40	2 (13%)
1	GL3	A	447	1	2,3,4	3.35	1 (50%)	1,2,4	0.08	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
1	MHS	A	260	1	-	0/4/6/8	0/1/1/1
1	AGM	A	274	1	-	0/9/11/13	0/0/0/0
1	MGN	A	402	1	-	0/7/9/12	0/0/0/0
1	TRX	A	429	1	-	0/3/6/8	0/2/2/2
1	GL3	A	447	1	-	0/1/1/2	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	447	GL3	C-S	-4.74	1.64	1.80
1	A	429	TRX	CD2-CE2	2.31	1.48	1.42
1	A	260	MHS	CA-C	2.52	1.53	1.50
1	A	429	TRX	CA-C	2.82	1.54	1.50
1	A	274	AGM	CA-C	3.06	1.54	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	429	TRX	CZ3-CE3-CD2	-2.60	117.58	121.17
1	A	260	MHS	O-C-CA	-2.24	118.98	124.98
1	A	260	MHS	NE2-CE1-ND1	-2.23	108.95	112.26
1	A	429	TRX	CE3-CD2-CE2	2.35	121.29	118.17
1	A	260	MHS	CM-ND1-CG	2.97	128.39	124.44

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
1	A	429	TRX	2	0
1	A	447	GL3	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are 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$
4	COM	A	601	-	6,6,6	1.36	2 (33%)	7,8,8	3.16	4 (57%)
5	TP7	A	602	-	16,20,20	0.47	0	20,26,26	0.65	0
6	F43	A	603	1	47,71,71	2.22	6 (12%)	44,118,118	1.20	5 (11%)

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	COM	A	601	-	-	0/4/4/4	0/0/0/0
5	TP7	A	602	-	-	0/20/24/24	0/0/0/0
6	F43	A	603	1	-	0/18/185/185	0/0/10/10

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	F43	CHD-C1D	-5.92	1.35	1.43
6	A	603	F43	C4D-ND	-2.17	1.45	1.49
4	A	601	COM	O2S-S2	2.06	1.51	1.45
4	A	601	COM	O1S-S2	2.20	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	603	F43	CHC-C4B	2.77	1.47	1.39

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	COM	O2S-S2-O1S	-4.30	99.08	113.95
6	A	603	F43	C9D-C3D-C4D	-2.25	108.74	114.67
6	A	603	F43	O8D-C7D-C6D	-2.23	117.15	120.85
6	A	603	F43	O7B-C6B-C8B	-2.04	124.10	126.60
6	A	603	F43	C2B-C1B-NB	2.20	105.13	101.84

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
4	A	601	COM	1	0
6	A	603	F43	3	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<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	543/552 (98%)	-0.10	12 (2%) 62 52	30, 49, 83, 102	0
2	B	443/444 (99%)	0.04	14 (3%) 47 37	37, 55, 84, 94	1 (0%)
3	C	258/260 (99%)	0.80	46 (17%) 1 1	35, 76, 121, 132	0
All	All	1244/1256 (99%)	0.14	72 (5%) 23 15	30, 55, 101, 132	1 (0%)

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	200	ASP	5.0
3	C	49	GLY	5.0
3	C	52	TYR	4.8
3	C	34	ILE	4.6
3	C	56	HIS	4.4

### 6.2 Non-standard residues in protein, DNA, RNA chains

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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	MHS	A	260	11/12	0.88	0.29	70,72,74,74	0
1	MGN	A	402	10/11	0.96	0.16	40,42,46,47	0
1	GL3	A	447	4/5	0.96	0.23	40,40,44,45	0
1	AGM	A	274	12/13	0.96	0.18	43,45,47,47	0
1	TRX	A	429	15/16	0.97	0.20	39,42,44,45	0

### 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
5	TP7	A	602	21/21	0.82	0.32	80,82,89,90	0
4	COM	A	601	7/7	0.91	0.27	70,77,81,82	0
7	K	A	604	1/1	0.94	0.41	89,89,89,89	1
6	F43	A	603	62/62	0.94	0.22	55,59,67,72	0
8	BR	C	301	1/1	0.96	0.09	94,94,94,94	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.