



# wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 07:03 AM GMT

PDB ID : 1E6Y  
Title : METHYL-COENZYME M REDUCTASE FROM METHANOSARCINA BARKERI  
Authors : Grabarse, W.; Ermler, U.  
Deposited on : 2000-08-23  
Resolution : 1.60 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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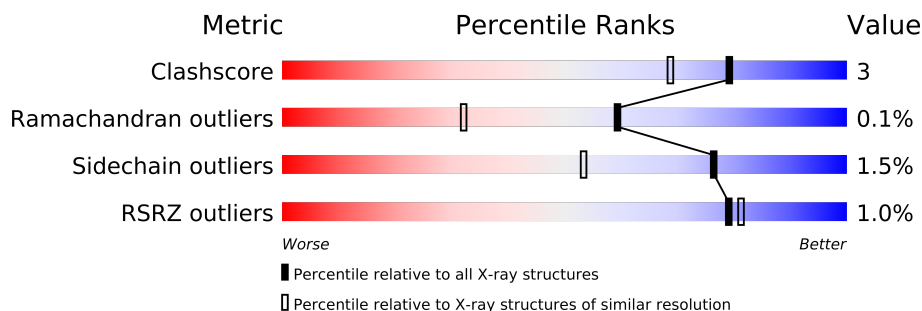
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.60 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))
Clashscore	79885	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)
RSRZ outliers	66119	1872 (1.60-1.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	569	
1	D	569	
2	B	433	
2	E	433	
3	C	247	
3	F	247	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	COM	A	2572	-	X
6	COM	D	5572	-	X
7	GOL	A	2573	-	X
7	GOL	A	2574	-	X
7	GOL	D	5573	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 21340 atoms, of which 0 are hydrogen and 0 are deuterium.

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	568	Total	C	N	O	S	0	4	0
			4346	2735	737	846	28			
1	D	568	Total	C	N	O	S	0	3	0
			4348	2738	740	842	28			

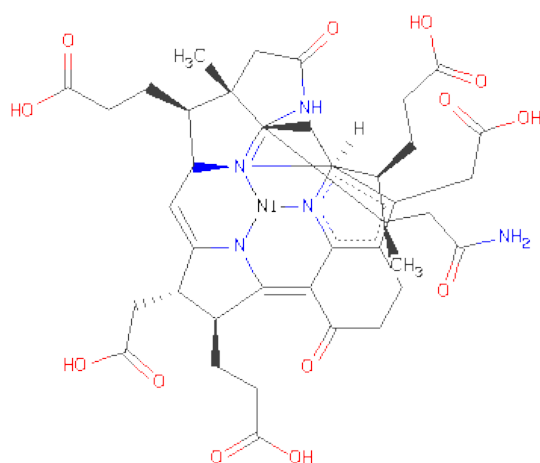
- Molecule 2 is a protein called METHYL-COENZYME M REDUCTASE I BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	432	Total	C	N	O	S	0	4	0
			3176	1987	549	621	19			
2	E	433	Total	C	N	O	S	0	1	0
			3178	1990	550	620	18			

- Molecule 3 is a protein called METHYL-COENZYME M REDUCTASE SUBUNIT GAMMA.

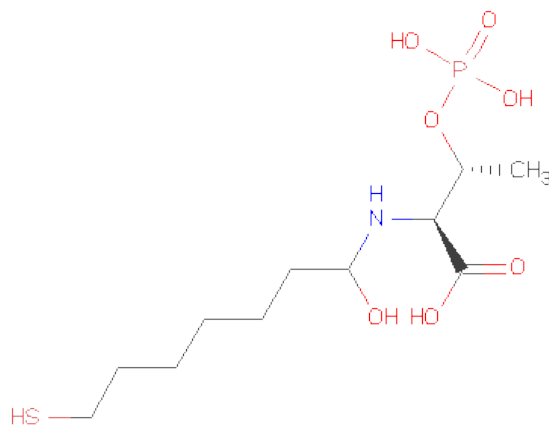
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	247	Total	C	N	O	S	0	0	0
			1947	1202	359	375	11			
3	F	247	Total	C	N	O	S	0	1	0
			1950	1205	359	375	11			

- Molecule 4 is FACTOR 430 (three-letter code: F43) (formula: C<sub>42</sub>H<sub>49</sub>N<sub>6</sub>NiO<sub>13</sub>).



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

- Molecule 5 is PHOSPHORIC ACID N-(1-HYDROXY-7-MERCAPTO-HEPTYL)THREONINEESTER (three-letter code: TP7) (formula:  $C_{11}H_{24}NO_7PS$ ).



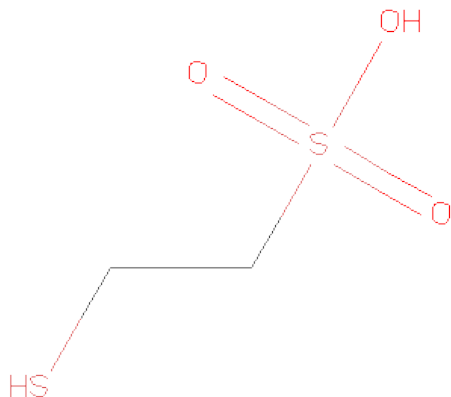
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			21	11	1	7	1	1		

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

- Molecule 6 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula:  $C_2H_6O_3S_2$ ).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

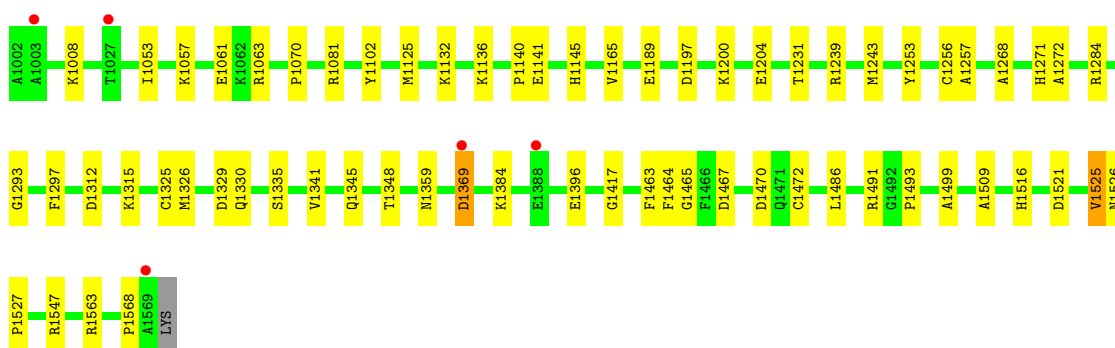
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	489	Total	O	0	0
			489	489		
8	B	340	Total	O	0	2
			342	342		
8	C	241	Total	O	0	0
			241	241		
8	D	522	Total	O	0	0
			522	522		
8	E	339	Total	O	0	0
			339	339		
8	F	264	Total	O	0	0
			264	264		

### 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.

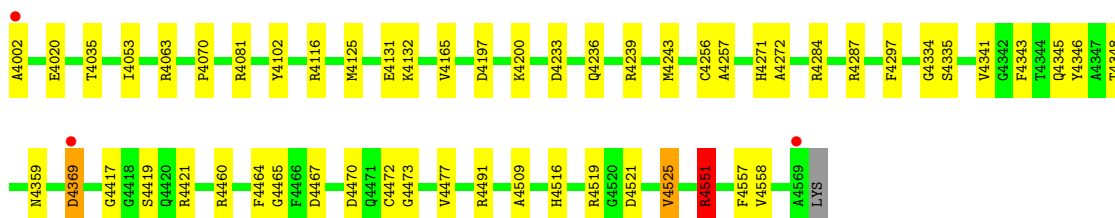
- Molecule 1: METHYL-COENZYME M REDUCTASE SUBUNIT ALPHA

Chain A: 



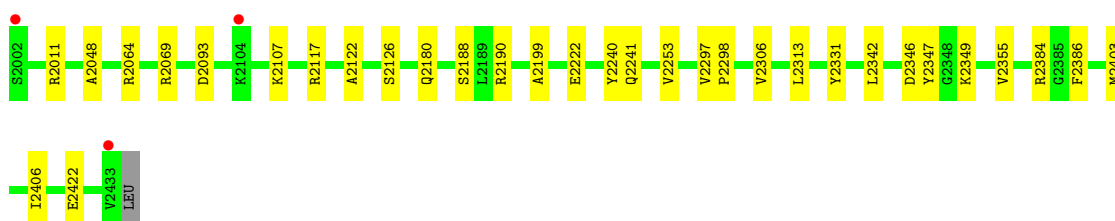
- Molecule 1: METHYL-COENZYME M REDUCTASE SUBUNIT ALPHA

Chain D: 



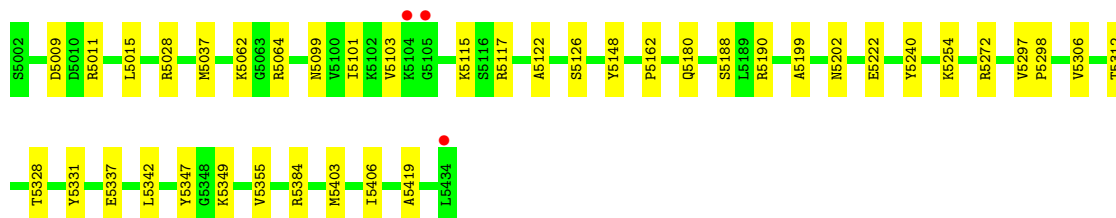
- Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT

Chain B: 



- Molecule 2: METHYL-COENZYME M REDUCTASE I BETA SUBUNIT

Chain E: 



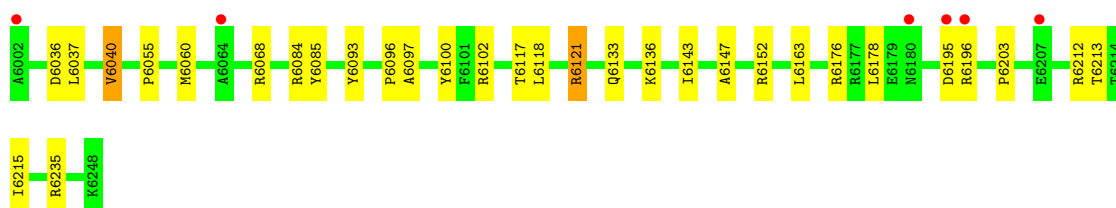
● Molecule 3: METHYL-COENZYME M REDUCTASE SUBUNIT GAMMA

Chain C:



● Molecule 3: METHYL-COENZYME M REDUCTASE SUBUNIT GAMMA

Chain F:





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.68Å 153.10Å 153.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 22.25 – 1.60	Depositor EDS
% Data completeness (in resolution range)	89.0 (30.00-1.60) 89.2 (22.25-1.60)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.98 (at 1.60Å)	Xtriage
Refinement program	CNS 0.3	Depositor
R, $R_{free}$	0.160 , 0.179 0.168 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	11.0	Xtriage
Anisotropy	0.817	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 43.6	EDS
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 326429 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	21340	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.28 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.2047e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, AGM, SMC, F43, TP7, OCS, 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	0.31	0/4423	0.68	9/5988 (0.2%)
1	D	0.64	6/4418 (0.1%)	1.95	26/5979 (0.4%)
2	B	0.29	0/3244	0.61	8/4390 (0.2%)
2	E	0.30	0/3231	0.65	8/4372 (0.2%)
3	C	0.31	0/1976	0.85	17/2666 (0.6%)
3	F	0.32	0/1983	1.85	15/2676 (0.6%)
All	All	0.41	6/19275 (0.0%)	1.24	83/26071 (0.3%)

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
2	B	0	2
2	E	0	3
3	C	0	1
3	F	0	1
All	All	0	7

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	4551[A]	ARG	CZ-NH2	22.62	1.62	1.33
1	D	4551[B]	ARG	CZ-NH2	22.62	1.62	1.33
1	D	4551[A]	ARG	NE-CZ	10.05	1.46	1.33
1	D	4551[B]	ARG	NE-CZ	10.05	1.46	1.33
1	D	4551[A]	ARG	CG-CD	-8.02	1.31	1.51

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4551[A]	ARG	NH1-CZ-NH2	-85.30	25.57	119.40
1	D	4551[B]	ARG	NH1-CZ-NH2	-85.30	25.57	119.40
3	F	6040[A]	VAL	CG1-CB-CG2	-59.08	16.37	110.90
3	F	6040[B]	VAL	CG1-CB-CG2	-59.08	16.37	110.90
1	D	4551[A]	ARG	NE-CZ-NH2	-44.85	97.87	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	2331	TYR	Sidechain
2	B	2347	TYR	Sidechain
3	C	3093	TYR	Sidechain
2	E	5148	TYR	Sidechain
2	E	5331	TYR	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4346	0	4191	39	0
1	D	4348	0	4205	50	0
2	B	3176	0	3161	17	0
2	E	3178	0	3170	22	0
3	C	1947	0	1888	9	0
3	F	1950	0	1894	13	0
4	A	62	0	43	6	0
4	D	62	0	43	5	0
5	A	21	0	19	2	0
5	D	21	0	19	1	0
6	A	7	0	5	1	0
6	D	7	0	5	0	0
7	A	12	0	16	0	0
7	D	6	0	8	0	0
8	A	489	0	0	5	0
8	B	342	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	241	0	0	1	0
8	D	522	0	0	4	0
8	E	339	0	0	4	0
8	F	264	0	0	2	0
All	All	21340	0	18667	131	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

The worst 5 of 131 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:4551[B]:ARG:CZ	1:D:4551[B]:ARG:NH2	1.69	1.56
1:D:4551[B]:ARG:CG	1:D:4551[B]:ARG:CD	1.76	1.55
1:D:4551[B]:ARG:CG	1:D:4551[B]:ARG:NE	1.87	1.38
1:D:4551[B]:ARG:CB	1:D:4551[B]:ARG:CD	2.38	1.01
1:D:4551[B]:ARG:HG2	1:D:4551[B]:ARG:HE	1.24	1.01

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	566/569 (100%)	546 (96%)	19 (3%)	1 (0%)	56	29
1	D	565/569 (99%)	546 (97%)	18 (3%)	1 (0%)	56	29
2	B	434/433 (100%)	428 (99%)	6 (1%)	0	100	100
2	E	432/433 (100%)	426 (99%)	6 (1%)	0	100	100
3	C	244/247 (99%)	239 (98%)	5 (2%)	0	100	100
3	F	245/247 (99%)	237 (97%)	8 (3%)	0	100	100
All	All	2486/2498 (100%)	2422 (97%)	62 (2%)	2 (0%)	59	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1525	VAL
1	D	4525	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	446/443 (101%)	436 (98%)	10 (2%)	64	34
1	D	445/443 (100%)	436 (98%)	9 (2%)	68	38
2	B	335/332 (101%)	333 (99%)	2 (1%)	92	84
2	E	333/332 (100%)	331 (99%)	2 (1%)	92	84
3	C	201/201 (100%)	197 (98%)	4 (2%)	68	38
3	F	202/201 (100%)	198 (98%)	4 (2%)	68	38
All	All	1962/1952 (100%)	1931 (98%)	31 (2%)	76	50

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	3178	LEU
1	D	4131	GLU
3	F	6178	LEU
3	C	3196	ARG
1	D	4335	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	3070	ASN
3	C	3122	GLN
2	E	5402	GLN
2	B	2402	GLN
1	D	4019	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

10 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	1271	1	11,11,12	6.31	2 (18%)	12,14,16	1.19	0
1	AGM	A	1285	1	11,11,12	5.46	2 (18%)	11,13,15	1.50	2 (18%)
1	GL3	A	1465	1	1,3,4	0.03	0	0,2,4	0.00	-
1	SMC	A	1472	1	6,6,7	7.37	2 (33%)	4,6,8	1.58	1 (25%)
3	OCS	C	3065	3	8,8,9	6.45	3 (37%)	9,11,13	2.09	2 (22%)
1	MHS	D	4271	1	11,11,12	6.05	3 (27%)	12,14,16	1.53	2 (16%)
1	AGM	D	4285	1	11,11,12	5.41	2 (18%)	11,13,15	1.47	2 (18%)
1	GL3	D	4465	1	1,3,4	0.01	0	0,2,4	0.00	-
1	SMC	D	4472	1	6,6,7	7.34	2 (33%)	4,6,8	1.66	1 (25%)
3	OCS	F	6065	3	8,8,9	6.46	2 (25%)	9,11,13	1.59	1 (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
1	MHS	A	1271	1	-	0/4/6/8	0/1/1/1
1	AGM	A	1285	1	-	0/9/11/13	0/0/0/0
1	GL3	A	1465	1	-	0/0/1/2	0/0/0/0
1	SMC	A	1472	1	-	0/3/5/7	0/0/0/0
3	OCS	C	3065	3	-	0/5/7/9	0/0/0/0
1	MHS	D	4271	1	-	0/4/6/8	0/1/1/1
1	AGM	D	4285	1	-	0/9/11/13	0/0/0/0
1	GL3	D	4465	1	-	0/0/1/2	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SMC	D	4472	1	-	0/3/5/7	0/0/0/0
3	OCS	F	6065	3	-	0/5/7/9	0/0/0/0

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1271	MHS	O-C	20.26	1.25	1.11
1	D	4271	MHS	O-C	19.32	1.24	1.11
1	A	1472	SMC	O-C	17.86	1.23	1.11
1	A	1285	AGM	O-C	17.86	1.23	1.11
1	D	4472	SMC	O-C	17.78	1.23	1.11

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3065	OCS	C-CA-N	-4.70	109.14	113.83
1	A	1285	AGM	C-CA-N	-4.43	109.40	113.83
1	D	4285	AGM	C-CA-N	-4.26	109.58	113.83
1	D	4271	MHS	C-CA-N	-3.46	110.37	113.83
1	D	4472	SMC	C-CA-N	-3.16	110.67	113.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

9 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	F43	A	2570	1,6	71,71,71	4.04	27 (38%)	103,118,118	2.96	38 (36%)
5	TP7	A	2571	-	20,20,20	2.57	5 (25%)	26,26,26	2.09	6 (23%)
6	COM	A	2572	4	6,6,6	1.66	2 (33%)	8,8,8	1.66	2 (25%)
7	GOL	A	2573	-	5,5,5	0.92	0	5,5,5	0.52	0
7	GOL	A	2574	-	5,5,5	0.79	0	5,5,5	0.53	0
4	F43	D	5570	1,6	71,71,71	4.02	27 (38%)	103,118,118	2.97	40 (38%)
5	TP7	D	5571	-	20,20,20	2.60	5 (25%)	26,26,26	2.09	6 (23%)
6	COM	D	5572	4	6,6,6	1.58	1 (16%)	8,8,8	1.72	2 (25%)
7	GOL	D	5573	-	5,5,5	0.94	0	5,5,5	0.57	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
4	F43	A	2570	1,6	2/2/25/27	0/28/165/165	0/0/10/10
5	TP7	A	2571	-	1/1/5/6	0/23/24/24	0/0/0/0
6	COM	A	2572	4	-	0/4/4/4	0/0/0/0
7	GOL	A	2573	-	-	0/4/4/4	0/0/0/0
7	GOL	A	2574	-	-	0/4/4/4	0/0/0/0
4	F43	D	5570	1,6	2/2/25/27	0/28/165/165	0/0/10/10
5	TP7	D	5571	-	1/1/5/6	0/23/24/24	0/0/0/0
6	COM	D	5572	4	-	0/4/4/4	0/0/0/0
7	GOL	D	5573	-	-	0/4/4/4	0/0/0/0

The worst 5 of 67 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5570	F43	C4B-NB	-14.77	1.19	1.47
4	A	2570	F43	C4B-NB	-14.61	1.20	1.47
4	D	5570	F43	CHB-C1B	-11.10	1.41	1.52
4	A	2570	F43	CHB-C1B	-10.86	1.41	1.52
4	D	5570	F43	NI-NA	9.30	2.15	1.88

The worst 5 of 94 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5570	F43	C3B-C4B-NB	12.54	124.48	103.42
4	A	2570	F43	C3B-C4B-NB	12.52	124.45	103.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	5570	F43	CHA-C4D-C3D	-9.30	111.00	129.63
4	A	2570	F43	CHA-C4D-C3D	-9.29	111.01	129.63
4	A	2570	F43	C2D-C1D-ND	8.71	120.39	109.62

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	D	5571	TP7	C1
4	D	5570	F43	C4B
4	D	5570	F43	C4A
5	A	2571	TP7	C1
4	A	2570	F43	C4B

There are no torsion outliers.

There are no ring outliers.

## 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, 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	568/569 (99%)	-0.48	5 (0%) 81 83	7, 12, 22, 36	0
1	D	568/569 (99%)	-0.52	3 (0%) 88 90	7, 11, 20, 36	0
2	B	432/433 (99%)	-0.44	3 (0%) 84 87	8, 12, 24, 42	0
2	E	433/433 (100%)	-0.48	3 (0%) 84 87	8, 12, 22, 37	0
3	C	247/247 (100%)	-0.33	4 (1%) 68 68	9, 15, 24, 35	0
3	F	247/247 (100%)	-0.38	6 (2%) 56 56	10, 14, 24, 39	0
All	All	2495/2498 (99%)	-0.46	24 (0%) 79 81	7, 12, 23, 42	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4569	ALA	8.7
1	A	1569	ALA	8.3
3	C	3002	ALA	5.1
2	B	2433	VAL	4.3
3	C	3064	ALA	4.2

### 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. 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	AGM	A	1285	12/13	0.07	1.53	6,7,8,8	0
1	AGM	D	4285	12/13	0.07	1.19	6,7,8,8	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MHS	D	4271	11/12	0.06	-0.01	10,11,12,13	0
3	OCS	C	3065	9/10	0.09	-0.19	19,24,26,26	0
3	OCS	F	6065	9/10	0.07	-0.62	18,22,25,25	0
1	MHS	A	1271	11/12	0.05	-0.68	9,10,12,12	0
1	SMC	A	1472	7/8	0.05	-0.71	9,9,10,11	0
1	SMC	D	4472	7/8	0.05	-0.89	9,10,10,10	0
1	GL3	A	1465	4/5	0.04	-1.79	9,9,9,9	0
1	GL3	D	4465	4/5	0.05	-2.44	8,8,8,8	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	GOL	D	5573	6/6	0.24	12.41	30,32,33,35	0
7	GOL	A	2573	6/6	0.20	10.98	33,34,35,37	0
7	GOL	A	2574	6/6	0.26	7.96	36,38,39,40	0
6	COM	D	5572	7/7	0.10	6.81	16,17,17,18	0
6	COM	A	2572	7/7	0.10	5.59	15,16,17,18	0
4	F43	D	5570	62/62	0.07	1.50	8,10,12,13	0
4	F43	A	2570	62/62	0.07	1.38	8,10,11,14	0
5	TP7	A	2571	21/21	0.06	0.00	8,8,10,12	0
5	TP7	D	5571	21/21	0.06	-0.03	7,9,10,12	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.