



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 01:05 PM GMT

PDB ID : 3SQG
Title : Crystal structure of a methyl-coenzyme M reductase purified from Black Sea mats
Authors : Shima, S.; Krueger, M.; Weinert, T.; Demmer, U.; Thauer, R.K.; Ermler, U.
Deposited on : 2011-07-05
Resolution : 2.10 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
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

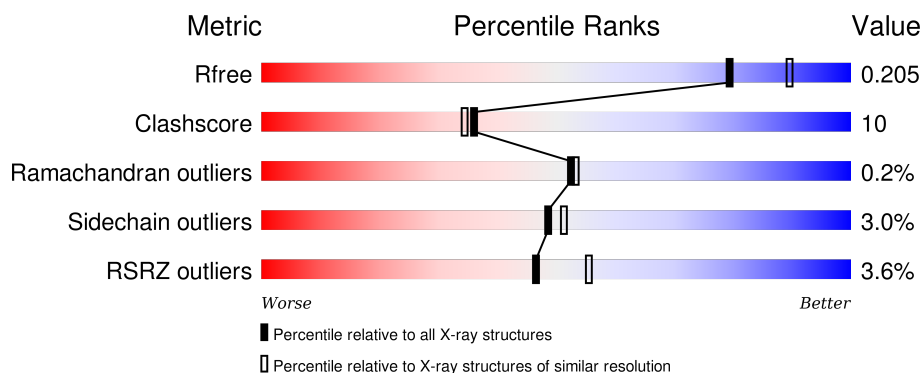
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	579	<div> <div>83%</div> <div>15%</div> <div>•</div> </div>
1	D	579	<div> <div>83%</div> <div>15%</div> <div>•</div> </div>
1	G	579	<div> <div>2%</div> <div>86%</div> <div>13%</div> <div>•</div> </div>
2	B	433	<div> <div>2%</div> <div>81%</div> <div>18%</div> <div>•</div> </div>
2	E	433	<div> <div>8%</div> <div>77%</div> <div>22%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	433	
3	C	279	
3	F	279	
3	I	279	

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
1	GL3	A	464	-	-	X	-
10	CL	A	586	-	-	X	X
12	P6G	B	434	-	-	X	X
13	GOL	C	281	-	-	-	X
13	GOL	E	435	-	-	-	X
5	COM	A	1003	-	-	X	X
5	COM	D	1003	-	-	-	X
5	COM	G	1003	-	-	-	X
6	M43	D	1001	X	-	-	-
6	M43	G	1001	X	-	-	-
7	1PE	A	581	-	-	-	X
7	1PE	D	580	-	-	X	X
7	1PE	G	580	-	-	X	X
7	1PE	H	434	-	-	-	X
8	PGE	A	582	-	-	-	X
8	PGE	A	583	-	-	-	X
8	PGE	D	581	-	-	-	X
8	PGE	G	581	-	-	-	X
9	SO4	D	584	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 32144 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, alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	0	0
			4467	2814	761	855	37			
1	D	578	Total	C	N	O	S	0	1	0
			4475	2819	764	855	37			
1	G	578	Total	C	N	O	S	0	0	0
			4467	2814	761	855	37			

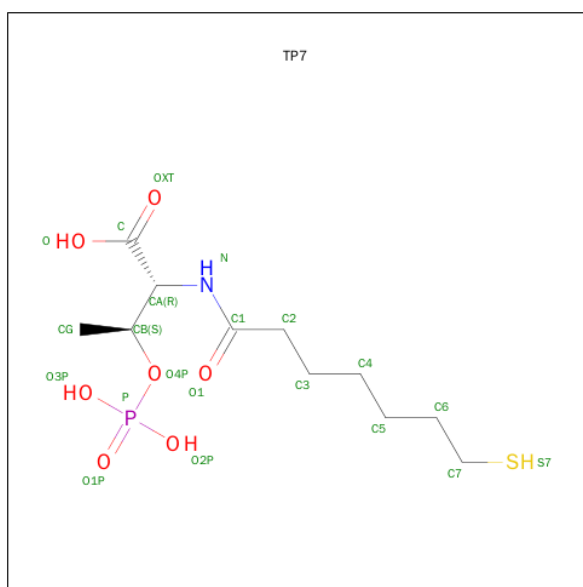
- Molecule 2 is a protein called Methyl-coenzyme M reductase, beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	431	Total	C	N	O	S	0	0	0
			3197	2013	552	600	32			
2	E	431	Total	C	N	O	S	0	0	0
			3197	2013	552	600	32			
2	H	431	Total	C	N	O	S	0	1	0
			3205	2018	555	600	32			

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

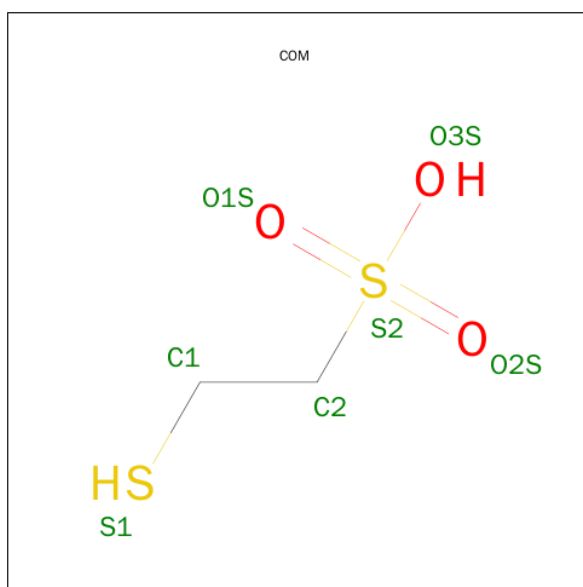
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	278	Total	C	N	O	S	0	0	0
			2205	1379	400	414	12			
3	F	278	Total	C	N	O	S	0	1	0
			2210	1382	401	415	12			
3	I	278	Total	C	N	O	S	0	0	0
			2205	1379	400	414	12			

- Molecule 4 is COENZYME B (three-letter code: TP7) (formula: C₁₁H₂₂NO₇PS).



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

- Molecule 5 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: $C_2H_6O_3S_2$).



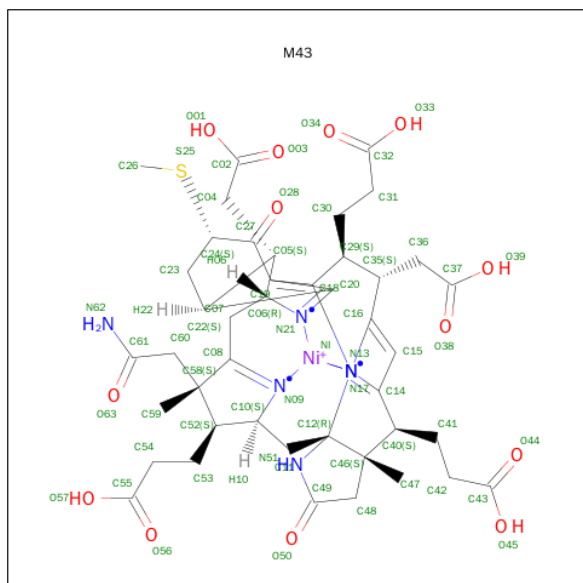
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			7	2	3	2		

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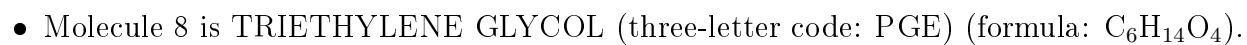
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	O	S	0	0
			7	2	3	2		
5	G	1	Total	C	O	S	0	0
			7	2	3	2		

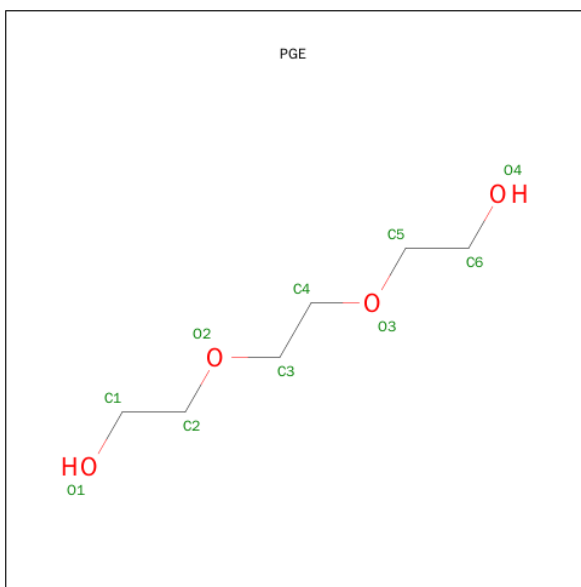
- Molecule 6 is (17[2]S)-17[2]-METHYLTHIO-COENZYME F43 (three-letter code: M43) (formula: $C_{43}H_{53}N_6NiO_{13}S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	Ni	O	S	0	0
			64	43	6	1	13	1		
6	D	1	Total	C	N	Ni	O	S	0	0
			64	43	6	1	13	1		
6	G	1	Total	C	N	Ni	O	S	0	0
			64	43	6	1	13	1		

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		
8	A	1	Total	C	O	0	0
			10	6	4		
8	D	1	Total	C	O	0	0
			10	6	4		
8	D	1	Total	C	O	0	0
			10	6	4		
8	G	1	Total	C	O	0	0
			10	6	4		
8	G	1	Total	C	O	0	0
			10	6	4		

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	H	1	Total	O	S	0	0
			5	4	1		
9	I	1	Total	O	S	0	0
			5	4	1		

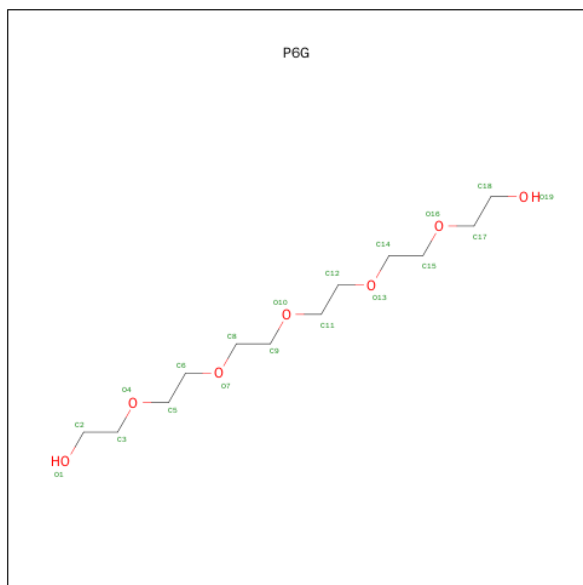
- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Cl	0	0
			1	1		

- Molecule 11 is CALCIUM ION (three-letter code: CA) (formula: Ca).

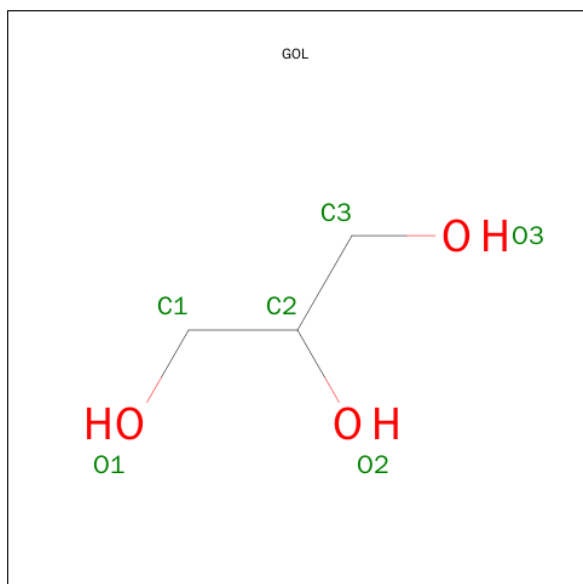
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	G	1	Total	Ca	0	0
			1	1		
11	A	1	Total	Ca	0	0
			1	1		

- Molecule 12 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	B	1	Total	C	O	0	0
			19	12	7		

- Molecule 13 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	C	O	0	0
			6	3	3		
13	E	1	Total	C	O	0	0
			6	3	3		

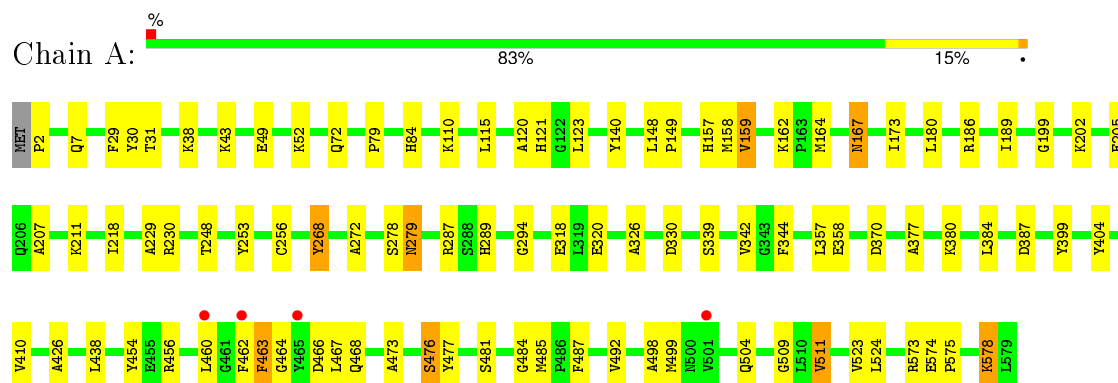
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	391	Total	O	0	0
			391	391		
14	B	173	Total	O	0	0
			173	173		
14	C	178	Total	O	0	0
			178	178		
14	D	341	Total	O	0	0
			341	341		
14	E	142	Total	O	0	0
			142	142		
14	F	120	Total	O	0	0
			120	120		
14	G	364	Total	O	0	0
			364	364		
14	H	140	Total	O	0	0
			140	140		
14	I	156	Total	O	0	0
			156	156		

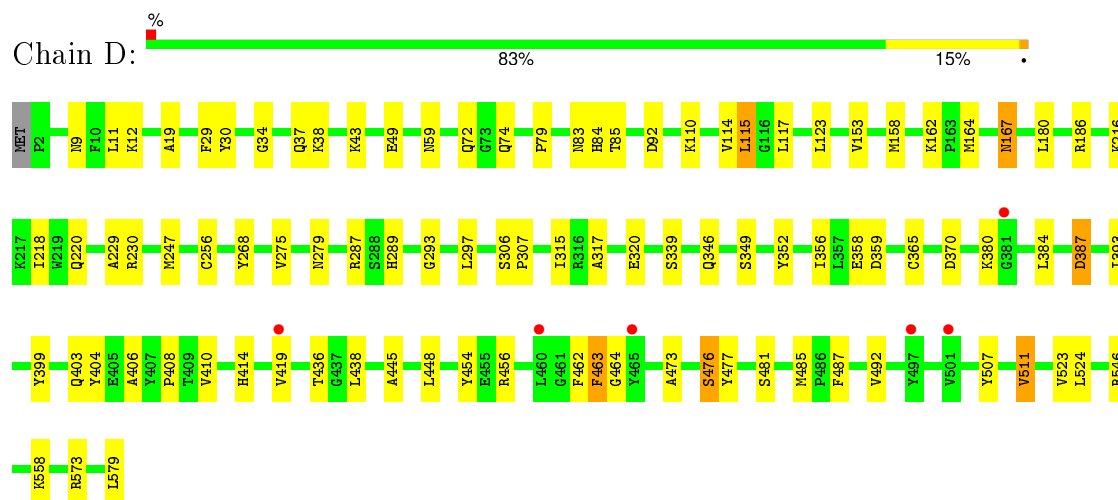
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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.

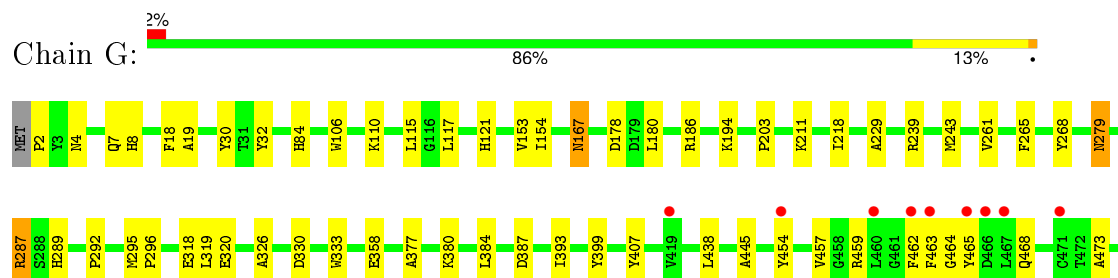
- Molecule 1: Methyl coenzyme M reductase, alpha subunit

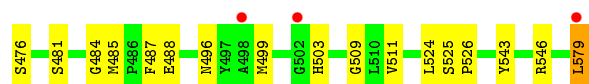


- Molecule 1: Methyl coenzyme M reductase, alpha subunit

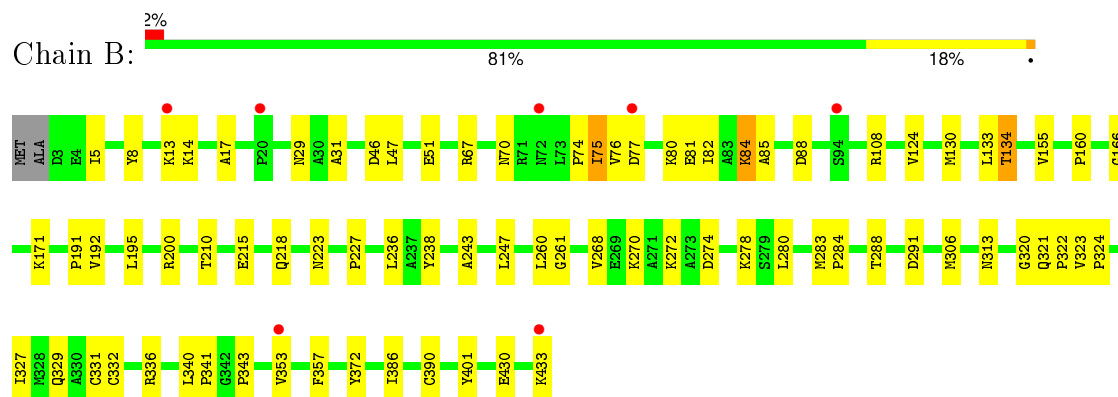


- Molecule 1: Methyl coenzyme M reductase, alpha subunit

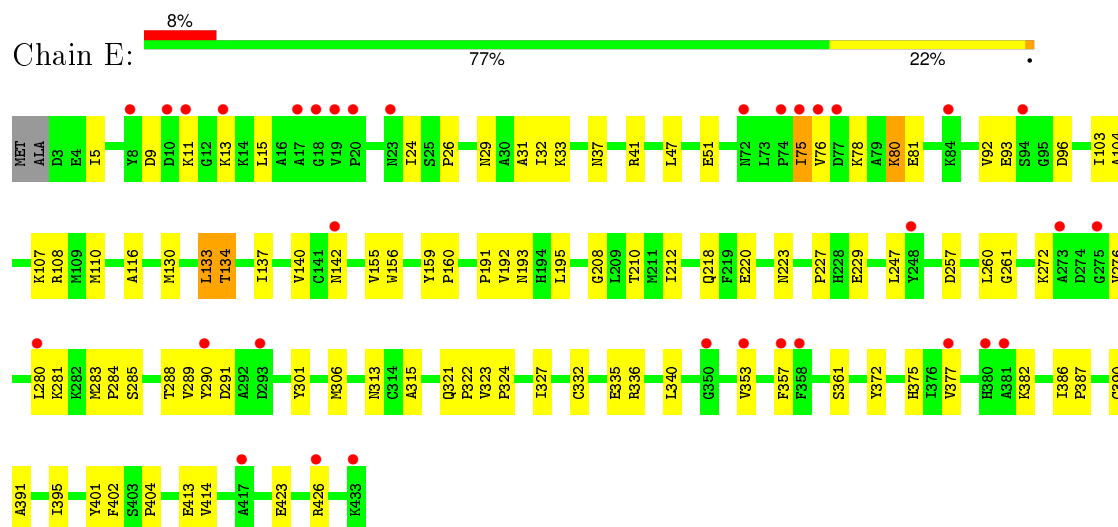




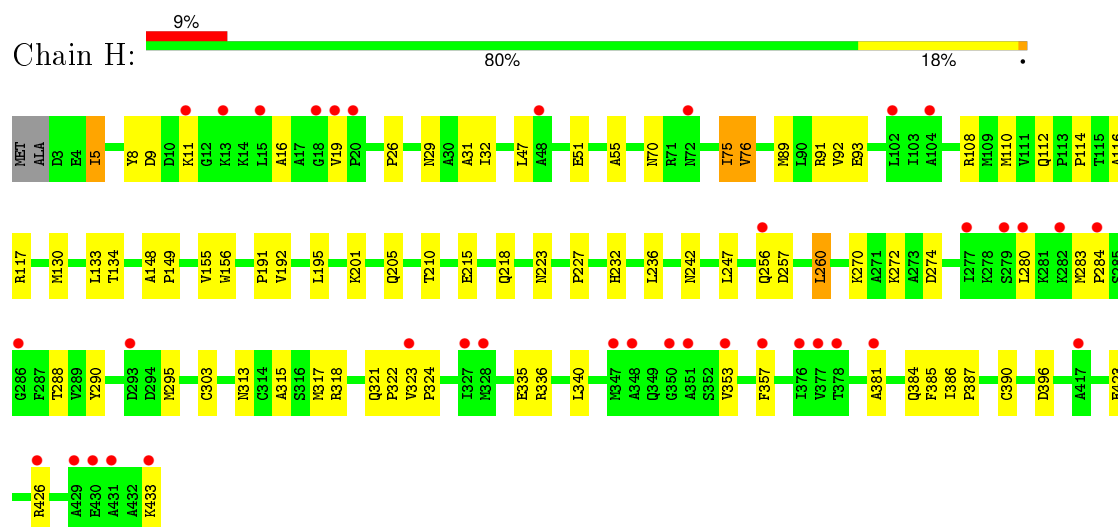
- Molecule 2: Methyl-coenzyme M reductase, beta subunit



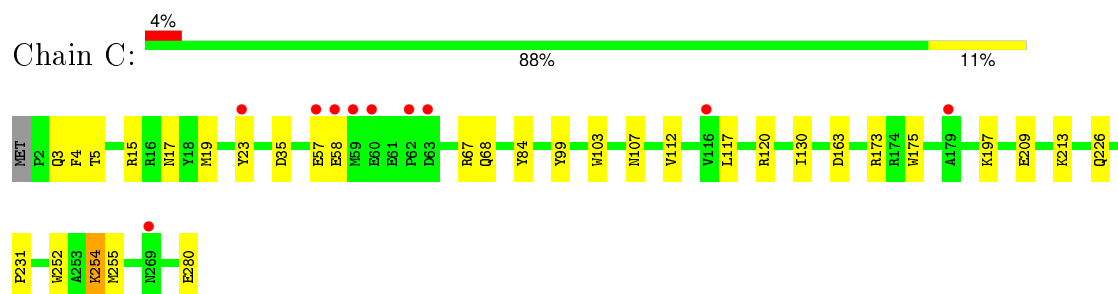
- Molecule 2: Methyl-coenzyme M reductase, beta subunit



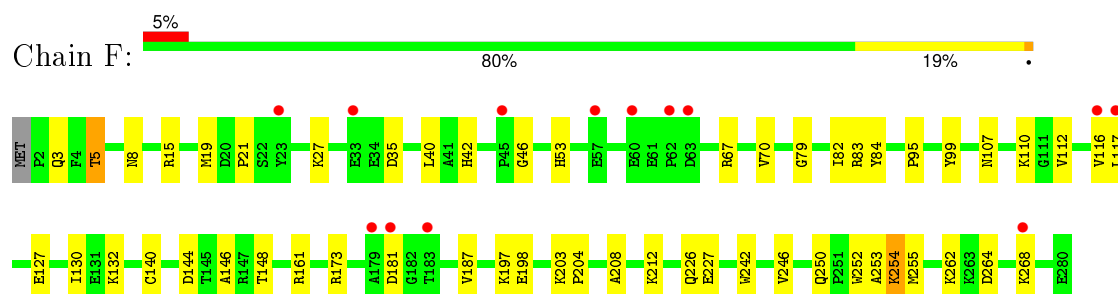
- Molecule 2: Methyl-coenzyme M reductase, beta subunit



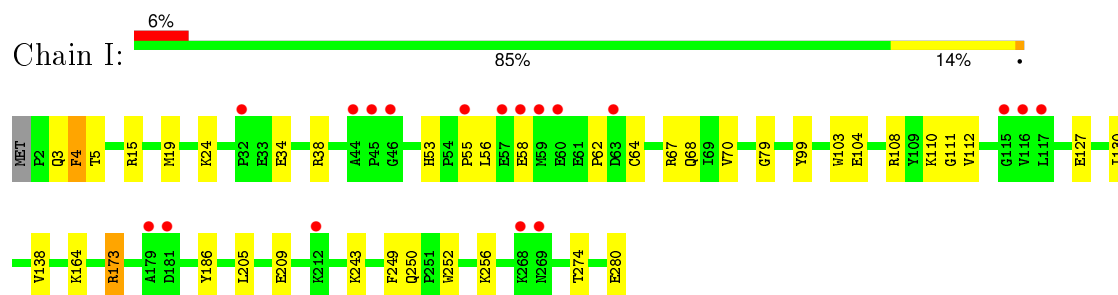
- Molecule 3: Methyl-coenzyme M reductase, gamma subunit



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	128.86Å 412.49Å 165.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.58 – 2.10 47.58 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.2 (47.58-2.10) 95.3 (47.58-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.161 , 0.206 0.162 , 0.205	Depositor DCC
R_{free} test set	12184 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 242974 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	32144	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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: MHO, PGE, P6G, GOL, M43, CA, CL, 1PE, TP7, SO4, 0AF, 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	0.44	0/4528	0.55	0/6126
1	D	0.41	0/4539	0.53	0/6140
1	G	0.41	0/4528	0.54	0/6126
2	B	0.35	0/3258	0.49	0/4410
2	E	0.32	0/3258	0.49	0/4410
2	H	0.34	0/3269	0.50	0/4424
3	C	0.40	0/2251	0.55	0/3034
3	F	0.31	0/2259	0.49	0/3045
3	I	0.38	0/2251	0.52	0/3034
All	All	0.38	0/30141	0.52	0/40749

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	4467	0	4266	89	0
1	D	4475	0	4279	101	0
1	G	4467	0	4266	72	0
2	B	3197	0	3195	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3197	0	3195	96	0
2	H	3205	0	3208	92	0
3	C	2205	0	2187	35	0
3	F	2210	0	2193	55	0
3	I	2205	0	2187	42	0
4	A	42	0	38	1	0
4	G	21	0	19	1	0
5	A	7	0	5	4	0
5	D	7	0	5	3	0
5	G	7	0	5	3	0
6	A	64	0	48	3	0
6	D	64	0	48	1	0
6	G	64	0	48	3	0
7	A	16	0	22	5	0
7	D	16	0	22	8	0
7	E	16	0	22	2	0
7	F	16	0	22	4	0
7	G	16	0	22	9	0
7	H	16	0	22	5	0
8	A	20	0	28	5	0
8	D	20	0	28	5	0
8	G	20	0	28	1	0
9	A	10	0	0	0	0
9	B	10	0	0	0	0
9	C	5	0	0	0	0
9	D	10	0	0	0	0
9	H	5	0	0	0	0
9	I	5	0	0	0	0
10	A	1	0	0	3	0
11	A	1	0	0	0	0
11	G	1	0	0	0	0
12	B	19	0	26	11	0
13	C	6	0	8	0	0
13	E	6	0	8	0	0
14	A	391	0	0	5	0
14	B	173	0	0	7	0
14	C	178	0	0	4	0
14	D	341	0	0	8	0
14	E	142	0	0	8	0
14	F	120	0	0	4	0
14	G	364	0	0	2	0
14	H	140	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	I	156	0	0	1	0
All	All	32144	0	29450	572	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 10.

The worst 5 of 572 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)
2:B:51:GLU:HB2	2:B:75:ILE:CD1	1.77	1.15
1:D:186:ARG:HH12	7:G:580:1PE:H221	1.16	1.10
2:B:14:LYS:CE	2:B:17:ALA:HB2	1.86	1.06
1:A:186:ARG:HH12	7:A:581:1PE:H121	1.20	1.03
7:D:580:1PE:H141	1:G:186:ARG:HH11	1.25	1.02

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	572/579 (99%)	547 (96%)	23 (4%)	2 (0%)	46	45
1	D	573/579 (99%)	545 (95%)	26 (4%)	2 (0%)	46	45
1	G	572/579 (99%)	547 (96%)	24 (4%)	1 (0%)	52	53
2	B	429/433 (99%)	421 (98%)	8 (2%)	0	100	100
2	E	429/433 (99%)	418 (97%)	11 (3%)	0	100	100
2	H	430/433 (99%)	417 (97%)	13 (3%)	0	100	100
3	C	276/279 (99%)	267 (97%)	8 (3%)	1 (0%)	39	37
3	F	277/279 (99%)	269 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	276/279 (99%)	267 (97%)	8 (3%)	1 (0%)	39	37
All	All	3834/3873 (99%)	3698 (96%)	129 (3%)	7 (0%)	52	53

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	481	SER
1	A	481	SER
1	D	481	SER
3	I	4	PHE
1	A	339	SER

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	453/454 (100%)	435 (96%)	18 (4%)	38	38
1	D	454/454 (100%)	437 (96%)	17 (4%)	41	41
1	G	453/454 (100%)	438 (97%)	15 (3%)	45	47
2	B	331/332 (100%)	320 (97%)	11 (3%)	45	47
2	E	331/332 (100%)	323 (98%)	8 (2%)	57	61
2	H	332/332 (100%)	324 (98%)	8 (2%)	57	61
3	C	231/232 (100%)	226 (98%)	5 (2%)	60	64
3	F	232/232 (100%)	228 (98%)	4 (2%)	68	74
3	I	231/232 (100%)	226 (98%)	5 (2%)	60	64
All	All	3048/3054 (100%)	2957 (97%)	91 (3%)	48	51

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	384	LEU
1	D	579	LEU

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Mol	Chain	Res	Type
2	H	257	ASP
1	D	387	ASP
1	D	476	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	279	ASN
2	E	326	ASN
3	I	3	GLN
1	D	289	HIS
2	E	218	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	271	1	8,11,12	0.70	0	7,14,16	1.73	2 (28%)
1	0AF	A	333	1	13,16,17	1.13	1 (7%)	10,22,24	1.44	1 (10%)
1	GL3	A	464	1	3,3,4	2.91	1 (33%)	2,2,4	1.02	0
1	MHO	A	499	1	7,8,9	0.60	0	6,9,11	2.17	3 (50%)
1	MHS	D	271	1	8,11,12	0.93	0	7,14,16	1.36	2 (28%)
1	0AF	D	333	1	13,16,17	1.24	1 (7%)	10,22,24	1.48	1 (10%)
1	GL3	D	464	1	3,3,4	2.72	1 (33%)	2,2,4	1.34	0
1	MHO	D	499	1	7,8,9	0.63	0	6,9,11	2.13	3 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MHS	G	271	1	8,11,12	0.98	0	7,14,16	1.28	1 (14%)
1	0AF	G	333	1	13,16,17	1.14	0	10,22,24	1.31	1 (10%)
1	GL3	G	464	1	3,3,4	2.53	1 (33%)	2,2,4	1.14	0
1	MHO	G	499	1	7,8,9	0.87	0	6,9,11	2.49	4 (66%)

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	271	1	-	0/4/6/8	0/1/1/1
1	0AF	A	333	1	-	0/3/6/8	0/2/2/2
1	GL3	A	464	1	-	0/1/1/2	0/0/0/0
1	MHO	A	499	1	-	0/5/7/9	0/0/0/0
1	MHS	D	271	1	-	0/4/6/8	0/1/1/1
1	0AF	D	333	1	-	0/3/6/8	0/2/2/2
1	GL3	D	464	1	-	0/1/1/2	0/0/0/0
1	MHO	D	499	1	-	0/5/7/9	0/0/0/0
1	MHS	G	271	1	-	0/4/6/8	0/1/1/1
1	0AF	G	333	1	-	0/3/6/8	0/2/2/2
1	GL3	G	464	1	-	0/1/1/2	0/0/0/0
1	MHO	G	499	1	-	0/5/7/9	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	464	GL3	C-S	-5.00	1.63	1.80
1	D	464	GL3	C-S	-4.67	1.64	1.80
1	G	464	GL3	C-S	-4.29	1.66	1.80
1	A	333	0AF	CD1-NE1	2.04	1.40	1.36
1	D	333	0AF	CD1-NE1	2.35	1.41	1.36

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	MHO	O-C-CA	-3.37	116.71	125.49
1	D	499	MHO	O-C-CA	-3.31	116.86	125.49
1	G	499	MHO	O-C-CA	-3.22	117.11	125.49
1	G	499	MHO	CE-SD-CG	-3.11	90.04	97.59
1	D	333	0AF	O-C-CA	-3.04	117.58	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	464	GL3	4	0
1	A	499	MHO	1	0
1	D	464	GL3	3	0
1	G	333	0AF	1	0
1	G	464	GL3	3	0
1	G	499	MHO	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 3 are monoatomic - leaving 33 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	$\# Z > 2$
6	M43	A	1001	1,5	46,73,73	4.04	21 (45%)	46,121,121	3.02	11 (23%)
4	TP7	A	1002	-	16,20,20	2.75	2 (12%)	16,26,26	2.89	3 (18%)
5	COM	A	1003	6	5,6,6	0.70	0	5,8,8	5.83	2 (40%)
4	TP7	A	580	-	16,20,20	2.82	2 (12%)	16,26,26	2.94	5 (31%)
7	1PE	A	581	-	15,15,15	0.65	0	14,14,14	1.51	0
8	PGE	A	582	-	9,9,9	0.41	0	8,8,8	0.44	0
8	PGE	A	583	-	9,9,9	0.54	0	8,8,8	0.36	0
9	SO4	A	584	-	4,4,4	0.18	0	6,6,6	0.13	0
9	SO4	A	585	-	4,4,4	0.19	0	6,6,6	0.07	0
12	P6G	B	434	-	18,18,18	0.71	0	17,17,17	1.52	0
9	SO4	B	435	-	4,4,4	0.20	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	SO4	B	436	-	4,4,4	0.23	0	6,6,6	0.27	0
13	GOL	C	281	-	5,5,5	0.37	0	5,5,5	0.55	0
9	SO4	C	282	-	4,4,4	0.19	0	6,6,6	0.18	0
6	M43	D	1001	1,5	46,73,73	4.21	19 (41%)	46,121,121	2.69	11 (23%)
5	COM	D	1003	6	5,6,6	0.75	0	5,8,8	1.63	1 (20%)
7	1PE	D	580	-	15,15,15	0.67	0	14,14,14	1.55	2 (14%)
8	PGE	D	581	-	9,9,9	0.52	0	8,8,8	0.28	0
8	PGE	D	582	-	9,9,9	0.54	0	8,8,8	0.23	0
9	SO4	D	583	-	4,4,4	0.21	0	6,6,6	0.08	0
9	SO4	D	584	-	4,4,4	0.19	0	6,6,6	0.10	0
7	1PE	E	434	-	15,15,15	0.69	0	14,14,14	1.50	2 (14%)
13	GOL	E	435	-	5,5,5	0.38	0	5,5,5	0.17	0
7	1PE	F	281	-	15,15,15	0.64	0	14,14,14	1.58	3 (21%)
6	M43	G	1001	5	46,73,73	3.78	21 (45%)	46,121,121	2.59	9 (19%)
4	TP7	G	1002	-	16,20,20	2.88	2 (12%)	16,26,26	2.85	5 (31%)
5	COM	G	1003	6	5,6,6	0.79	0	5,8,8	2.35	2 (40%)
7	1PE	G	580	-	15,15,15	0.58	0	14,14,14	1.64	3 (21%)
8	PGE	G	581	-	9,9,9	0.51	0	8,8,8	0.23	0
8	PGE	G	582	-	9,9,9	0.51	0	8,8,8	0.19	0
7	1PE	H	434	-	15,15,15	0.68	0	14,14,14	1.58	3 (21%)
9	SO4	H	435	-	4,4,4	0.21	0	6,6,6	0.07	0
9	SO4	I	281	-	4,4,4	0.21	0	6,6,6	0.12	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
6	M43	A	1001	1,5	-	0/18/190/190	0/0/10/10
4	TP7	A	1002	-	-	0/20/24/24	0/0/0/0
5	COM	A	1003	6	-	0/4/4/4	0/0/0/0
4	TP7	A	580	-	-	0/20/24/24	0/0/0/0
7	1PE	A	581	-	-	0/13/13/13	0/0/0/0
8	PGE	A	582	-	-	0/7/7/7	0/0/0/0
8	PGE	A	583	-	-	0/7/7/7	0/0/0/0
9	SO4	A	584	-	-	0/0/0/0	0/0/0/0
9	SO4	A	585	-	-	0/0/0/0	0/0/0/0
12	P6G	B	434	-	-	0/16/16/16	0/0/0/0
9	SO4	B	435	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	SO4	B	436	-	-	0/0/0/0	0/0/0/0
13	GOL	C	281	-	-	0/4/4/4	0/0/0/0
9	SO4	C	282	-	-	0/0/0/0	0/0/0/0
6	M43	D	1001	1,5	1/1/31/33	0/18/190/190	0/0/10/10
5	COM	D	1003	6	-	0/4/4/4	0/0/0/0
7	1PE	D	580	-	-	0/13/13/13	0/0/0/0
8	PGE	D	581	-	-	0/7/7/7	0/0/0/0
8	PGE	D	582	-	-	0/7/7/7	0/0/0/0
9	SO4	D	583	-	-	0/0/0/0	0/0/0/0
9	SO4	D	584	-	-	0/0/0/0	0/0/0/0
7	1PE	E	434	-	-	0/13/13/13	0/0/0/0
13	GOL	E	435	-	-	0/4/4/4	0/0/0/0
7	1PE	F	281	-	-	0/13/13/13	0/0/0/0
6	M43	G	1001	5	1/1/31/33	0/18/190/190	0/0/10/10
4	TP7	G	1002	-	-	0/20/24/24	0/0/0/0
5	COM	G	1003	6	-	0/4/4/4	0/0/0/0
7	1PE	G	580	-	-	0/13/13/13	0/0/0/0
8	PGE	G	581	-	-	0/7/7/7	0/0/0/0
8	PGE	G	582	-	-	0/7/7/7	0/0/0/0
7	1PE	H	434	-	-	0/13/13/13	0/0/0/0
9	SO4	H	435	-	-	0/0/0/0	0/0/0/0
9	SO4	I	281	-	-	0/0/0/0	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)
6	D	1001	M43	C06-N21	-7.22	1.36	1.49
6	A	1001	M43	C06-N21	-6.85	1.37	1.49
6	D	1001	M43	C48-C49	-5.53	1.39	1.50
6	G	1001	M43	C06-N21	-5.51	1.39	1.49
6	G	1001	M43	C48-C49	-4.92	1.40	1.50

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	580	TP7	O1-C1-N	-8.90	107.90	123.01
4	A	1002	TP7	O1-C1-N	-8.72	108.21	123.01
4	G	1002	TP7	O1-C1-N	-7.57	110.17	123.01
6	D	1001	M43	C16-N17-C18	-7.45	99.96	107.93
4	G	1002	TP7	O1-C1-C2	-6.87	110.12	121.98

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	G	1001	M43	N17
6	D	1001	M43	N17

There are no torsion outliers.

There are no ring outliers.

20 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1001	M43	3	0
4	A	1002	TP7	1	0
5	A	1003	COM	4	0
7	A	581	1PE	5	0
8	A	582	PGE	1	0
8	A	583	PGE	4	0
12	B	434	P6G	11	0
6	D	1001	M43	1	0
5	D	1003	COM	3	0
7	D	580	1PE	8	0
8	D	581	PGE	3	0
8	D	582	PGE	2	0
7	E	434	1PE	2	0
7	F	281	1PE	4	0
6	G	1001	M43	3	0
4	G	1002	TP7	1	0
5	G	1003	COM	3	0
7	G	580	1PE	9	0
8	G	582	PGE	1	0
7	H	434	1PE	5	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, 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	574/579 (99%)	-0.35	4 (0%) 89 91	16, 24, 36, 58	0
1	D	574/579 (99%)	-0.33	6 (1%) 84 87	17, 27, 40, 61	0
1	G	574/579 (99%)	-0.28	12 (2%) 67 72	20, 28, 41, 68	0
2	B	431/433 (99%)	-0.07	7 (1%) 74 79	21, 37, 55, 79	0
2	E	431/433 (99%)	0.29	33 (7%) 16 22	26, 42, 61, 83	0
2	H	431/433 (99%)	0.31	37 (8%) 13 18	29, 41, 58, 70	1 (0%)
3	C	278/279 (99%)	-0.30	10 (3%) 46 55	20, 31, 48, 72	0
3	F	278/279 (99%)	0.11	13 (4%) 35 44	27, 42, 59, 96	0
3	I	278/279 (99%)	0.16	18 (6%) 22 29	24, 38, 54, 96	0
All	All	3849/3873 (99%)	-0.08	140 (3%) 46 55	16, 33, 54, 96	1 (0%)

The worst 5 of 140 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	59	MET	5.0
3	F	60	GLU	4.8
1	G	460	LEU	4.4
2	H	353	VAL	4.3
3	I	63	ASP	4.3

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, 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(\AA^2)	Q<0.9
1	MHS	A	271	11/12	0.98	0.09	-	28,29,32,32	0
1	MHS	G	271	11/12	0.96	0.08	-	30,32,34,34	0
1	GL3	G	464	4/5	0.98	0.21	-	27,28,28,29	0
1	GL3	A	464	4/5	0.99	0.19	-	21,22,24,24	0
1	MHO	D	499	9/10	0.97	0.21	-	23,29,30,30	0
1	OAF	D	333	15/16	0.97	0.14	-	19,22,24,26	0
1	OAF	A	333	15/16	0.98	0.18	-	17,22,23,24	0
1	MHO	A	499	9/10	0.99	0.20	-	18,22,24,24	0
1	MHO	G	499	9/10	0.97	0.21	-	21,26,31,32	0
1	OAF	G	333	15/16	0.96	0.13	-	21,25,26,27	0
1	GL3	D	464	4/5	0.99	0.16	-	29,32,32,34	0
1	MHS	D	271	11/12	0.98	0.07	-	24,26,27,27	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. 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(\AA^2)	Q<0.9
13	GOL	E	435	6/6	0.79	0.19	9.78	65,67,68,68	0
8	PGE	G	581	10/10	0.93	0.14	9.63	41,43,52,52	0
8	PGE	D	581	10/10	0.89	0.15	8.83	40,42,45,47	0
13	GOL	C	281	6/6	0.61	0.20	7.32	37,44,45,46	0
9	SO4	D	584	5/5	0.94	0.34	7.23	98,98,99,99	0
5	COM	A	1003	7/7	0.93	0.33	5.80	14,18,28,29	7
5	COM	D	1003	7/7	0.84	0.46	5.55	17,23,45,46	7
8	PGE	A	583	10/10	0.90	0.14	4.18	42,45,50,53	0
7	1PE	D	580	16/16	0.84	0.16	4.08	42,61,62,63	0
10	CL	A	586	1/1	0.99	0.13	3.92	47,47,47,47	0
7	1PE	A	581	16/16	0.80	0.15	3.41	33,58,61,61	0
12	P6G	B	434	19/19	0.88	0.18	3.27	41,44,58,60	0
7	1PE	G	580	16/16	0.83	0.14	3.17	34,55,59,59	0
5	COM	G	1003	7/7	0.84	0.38	3.01	17,28,33,35	7

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	1PE	H	434	16/16	0.90	0.16	2.59	43,47,51,52	0
8	PGE	A	582	10/10	0.88	0.18	2.05	58,61,70,70	0
7	1PE	E	434	16/16	0.91	0.18	1.96	40,45,47,49	0
8	PGE	D	582	10/10	0.68	0.20	1.69	58,62,68,69	0
4	TP7	A	580	21/21	0.97	0.20	0.53	24,29,30,31	0
8	PGE	G	582	10/10	0.88	0.13	0.36	49,51,57,58	0
6	M43	G	1001	64/64	0.98	0.16	0.34	16,26,31,33	0
6	M43	A	1001	64/64	0.97	0.15	0.25	20,28,33,36	0
7	1PE	F	281	16/16	0.67	0.20	0.12	56,63,68,68	0
6	M43	D	1001	64/64	0.98	0.14	0.11	13,20,25,27	0
4	TP7	A	1002	21/21	0.98	0.16	-0.26	18,22,27,27	0
4	TP7	G	1002	21/21	0.97	0.17	-0.33	21,26,33,37	0
11	CA	A	587	1/1	0.99	0.05	-2.88	24,24,24,24	0
11	CA	G	583	1/1	1.00	0.03	-3.43	22,22,22,22	1
9	SO4	C	282	5/5	0.91	0.15	-	62,63,63,66	0
9	SO4	A	584	5/5	0.92	0.17	-	53,54,56,58	5
9	SO4	D	583	5/5	0.94	0.13	-	85,85,86,86	0
9	SO4	B	436	5/5	0.89	0.16	-	71,72,72,73	5
9	SO4	H	435	5/5	0.92	0.16	-	65,66,67,68	5
9	SO4	A	585	5/5	0.89	0.20	-	110,110,110,110	0
9	SO4	B	435	5/5	0.93	0.22	-	63,64,64,65	5
9	SO4	I	281	5/5	0.92	0.24	-	64,64,65,67	5

6.5 Other polymers [i](#)

There are no such residues in this entry.