

Full wwPDB X-ray Structure Validation Report (i)

Jan 27, 2022 – 03:12 pm GMT

PDB ID	:	7QBS
Title	:	B12-dependent radical SAM methyltransferase, Mmp10 with [4Fe-4S] cluster,
		cobalamin, S-adenosyl-L-methionine, and peptide bound.
Authors	:	Bernardo-Garcia, N.; Fyfe, C.D.; Chavas, L.M.G.; Legrand, P.; Benjdia, A.;
		Berteau, O.
Deposited on		
Resolution	:	2.33 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

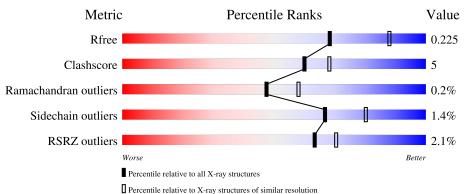
MolProbity		4 02b-467
·		
Mogul	:	1.8.4, CSD as $541be(2020)$
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.33 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	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	5974(2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	А	436	^{2%} 86% 8% • 6%						
2	В	13	46%	15%	38%				



2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 3577 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-arginine methyltransferase Mmp10.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	411	Total 3172	C 2024	N 520	O 608	S 20	0	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	-24	MET	-	initiating methionine	UNP A0A832SFM5
А	-23	ALA	_	expression tag	UNP A0A832SFM5
А	-22	SER	_	expression tag	UNP A0A832SFM5
А	-21	TRP	_	expression tag	UNP A0A832SFM5
А	-20	SER	_	expression tag	UNP A0A832SFM5
А	-19	HIS	-	expression tag	UNP A0A832SFM5
А	-18	PRO	-	expression tag	UNP A0A832SFM5
А	-17	GLN	-	expression tag	UNP A0A832SFM5
А	-16	PHE	-	expression tag	UNP A0A832SFM5
А	-15	GLU	-	expression tag	UNP A0A832SFM5
А	-14	LYS	-	expression tag	UNP A0A832SFM5
А	-13	SER	-	expression tag	UNP A0A832SFM5
А	-12	GLY	-	expression tag	UNP A0A832SFM5
А	-11	GLY	_	expression tag	UNP A0A832SFM5
А	-10	GLY	-	expression tag	UNP A0A832SFM5
А	-9	GLY	-	expression tag	UNP A0A832SFM5
А	-8	GLY	_	expression tag	UNP A0A832SFM5
А	-7	GLU	-	expression tag	UNP A0A832SFM5
А	-6	ASN	-	expression tag	UNP A0A832SFM5
А	-5	LEU	-	expression tag	UNP A0A832SFM5
А	-4	TYR	-	expression tag	UNP A0A832SFM5
А	-3	PHE	-	expression tag	UNP A0A832SFM5
А	-2	GLN	-	expression tag	UNP A0A832SFM5
А	-1	GLY	-	expression tag	UNP A0A832SFM5
А	0	HIS	-	expression tag	UNP A0A832SFM5

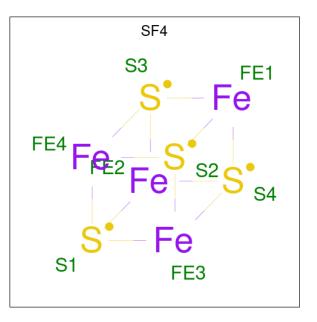
There are 25 discrepancies between the modelled and reference sequences:



• Molecule 2 is a protein called Peptide from Methyl-coenzyme M reductase subunit alpha from Methanosarcina acetivorans.

Mol	Chain	Residues		Ato	\mathbf{ms}			ZeroOcc	AltConf	Trace
2	В	8	Total 66	C 40	N 17	0 8	S 1	0	0	0

• Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



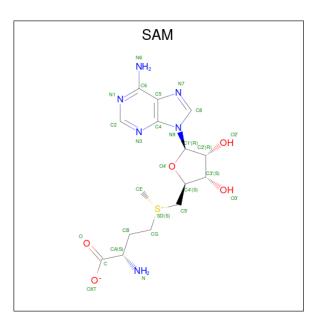
Mo	l Chain	Residues	Atoms			ZeroOcc	AltConf
3	А	1	Total 8	Fe 4	${S \atop 4}$	0	0

• Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Fe 1 1	0	0

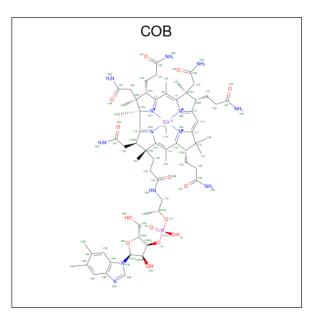
• Molecule 5 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf
5	А	1	Total 27	C 15	N 6	O 5	S 1	0	0

• Molecule 6 is CO-METHYLCOBALAMIN (three-letter code: COB) (formula: $C_{63}H_{91}CoN_{13}O_{14}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	А	1	Total 92		Co 1			Р 1	0	0

• Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	Total Na 1 1	0	0

• Molecule 8 is water.

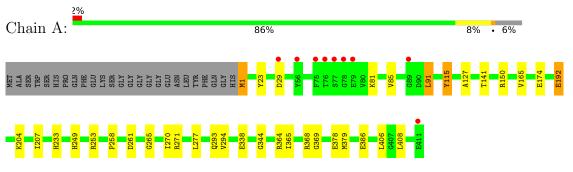
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	208	Total O 208 208	0	0
8	В	2	Total O 2 2	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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-arginine methyltransferase Mmp10



• Molecule 2: Peptide from Methyl-coenzyme M reductase subunit alpha from Methanosarcina acetivorans

Chain B:	46%	15%	38%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	$\begin{array}{cccccccccccccccccccccccccccccccccccc$	Depositor
Resolution (Å)	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	Depositor EDS
% Data completeness	$99.7 \ (45.00-2.33)$	Depositor
(in resolution range)	99.6(45.00-2.33)	EDS
R _{merge}	0.20	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.15 (at 2.32 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.10.4 (16-JUL-2021)	Depositor
D D	0.182 , 0.235	Depositor
R, R_{free}	0.176 , 0.225	DCC
R_{free} test set	1148 reflections (4.80%)	wwPDB-VP
Wilson B-factor $(Å^2)$	56.0	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.040 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3577	wwPDB-VP
Average B, all atoms $(Å^2)$	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, SAM, NA, COB, SF4

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	А	0.41	0/3232	0.61	0/4373	
2	В	0.41	0/66	0.60	0/86	
All	All	0.41	0/3298	0.61	0/4459	

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 (i)

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	А	3172	0	3197	22	0
2	В	66	0	78	3	0
3	А	8	0	0	0	0
4	А	1	0	0	0	0
5	А	27	0	22	3	0
6	А	92	0	86	9	0
7	А	1	0	0	0	0
8	А	208	0	0	1	0
8	В	2	0	0	0	0
All	All	3577	0	3383	31	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.

All (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

A + a 1	A 4 a	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
6:A:504:COB:H552	6:A:504:COB:H531	1.73	0.69
1:A:192:GLU:OE2	1:A:249:HIS:NE2	2.28	0.66
1:A:338:GLU:HA	1:A:364:ARG:HG2	1.79	0.64
1:A:365:ILE:HD11	1:A:406:LEU:HB3	1.84	0.59
6:A:504:COB:C37	6:A:504:COB:H351	2.33	0.59
1:A:115:TYR:HB3	5:A:503:SAM:HB2	1.85	0.58
6:A:504:COB:H602	6:A:504:COB:H252	1.85	0.58
1:A:127:ALA:HB2	1:A:165:VAL:HG13	1.87	0.55
1:A:207:ILE:HG21	1:A:378:GLU:HG2	1.88	0.55
1:A:270:ILE:HG12	1:A:277:LEU:HD13	1.89	0.54
6:A:504:COB:H351	6:A:504:COB:H371	1.91	0.52
6:A:504:COB:H531	6:A:504:COB:C55	2.37	0.51
1:A:379:MET:HG2	2:B:8:ARG:HA	1.92	0.51
6:A:504:COB:H542	2:B:6:ARG:HG3	1.96	0.48
6:A:504:COB:H533	6:A:504:COB:H482	1.95	0.48
1:A:1:MET:HB2	1:A:81:LYS:H	1.80	0.47
1:A:141:THR:O	1:A:150:ARG:NH2	2.49	0.46
1:A:369:GLY:HA3	6:A:504:COB:HM63	1.98	0.46
1:A:174:GLU:HG3	1:A:204:LYS:HG3	1.97	0.46
1:A:386:GLU:H	1:A:386:GLU:CD	2.19	0.46
1:A:338:GLU:HB2	1:A:408:LEU:HD11	1.98	0.45
1:A:265:GLY:O	1:A:271:ARG:NH1	2.50	0.44
5:A:503:SAM:H4'	2:B:6:ARG:HD3	1.99	0.44
1:A:85:VAL:HG12	1:A:91:LEU:HD21	1.99	0.44
1:A:258:PRO:HB2	1:A:294:VAL:HG11	2.00	0.43
1:A:253:ARG:HH22	1:A:261:ASP:CG	2.23	0.43
6:A:504:COB:H422	6:A:504:COB:H372	2.01	0.42
1:A:233:HIS:HD2	8:A:609:HOH:O	2.02	0.42
1:A:344:GLY:HA2	1:A:368:ARG:HB3	2.02	0.42
1:A:115:TYR:CB	5:A:503:SAM:HB2	2.50	0.41
1:A:293:GLN:H	1:A:293:GLN:HG2	1.74	0.41

There are no symmetry-related clashes.



5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	409/436~(94%)	401 (98%)	7 (2%)	1 (0%)	47	58
2	В	6/13~(46%)	5 (83%)	1 (17%)	0	100	100
All	All	415/449~(92%)	406 (98%)	8 (2%)	1 (0%)	47	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	115	TYR

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	А	356/374~(95%)	351~(99%)	5 (1%)	67 80	
2	В	6/10~(60%)	6 (100%)	0	100 100	
All	All	362/384~(94%)	357~(99%)	5 (1%)	67 80	

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	1	MET
1	А	23	TYR
1	А	29	ASP
1	А	91	LEU
1	А	192	GLU



Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	112	HIS
1	А	172	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 monosaccharides 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		oe Chain Res		Link	Bond lengths			Bond angles		
INIOI	Type	Unam	Res	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
5	SAM	А	503	3	21,29,29	0.71	0	18,42,42	0.92	1 (5%)
3	SF4	А	501	1,5	0,12,12	-	-	-		<u> </u>
6	COB	А	504	-	87,102,102	0.94	5 (5%)	127,170,170	1.43	15 (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
5	SAM	А	503	3	-	3/8/33/33	0/3/3/3
3	SF4	А	501	1,5	-	-	0/6/5/5
6	COB	А	504	-	-	16/52/231/231	0/3/11/11

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	А	504	COB	C8B-C9B	4.16	1.49	1.40
6	А	504	COB	C6B-C5B	3.56	1.49	1.40
6	А	504	COB	O6R-C1R	2.63	1.44	1.41
6	А	504	COB	C10-C9	2.14	1.45	1.39
6	А	504	COB	CO-N24	-2.05	1.88	2.06

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
6	А	504	COB	C12-C11-C10	-5.41	118.60	123.54
6	А	504	COB	C60-C18-C19	4.49	121.13	112.39
6	А	504	COB	C20-C1-C19	-4.34	104.04	109.42
6	А	504	COB	C12-C11-N23	3.88	115.68	111.48
6	А	504	COB	O6R-C1R-C2R	-3.67	101.56	106.93
6	А	504	COB	C37-C7-C6	3.66	118.62	107.12
6	А	504	COB	C3R-C2R-C1R	3.41	107.44	99.89
6	А	504	COB	C55-C17-C18	-3.06	104.80	111.14
6	А	504	COB	C26-C2-C1	3.03	114.73	110.02
6	А	504	COB	C48-C13-C14	2.85	116.25	109.63
5	А	503	SAM	C5-C6-N6	2.44	124.06	120.35
6	А	504	COB	C8-C9-N22	2.23	115.20	110.77
6	А	504	COB	C7-C6-C5	-2.22	124.58	128.07
6	А	504	COB	C7-C37-C38	2.22	120.92	114.25
6	А	504	COB	C26-C2-C3	-2.08	103.73	107.41
6	А	504	COB	C7-C6-N22	2.01	111.61	107.94

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	А	503	SAM	C-CA-CB-CG
6	А	504	COB	C38-C37-C7-C6
6	А	504	COB	C38-C37-C7-C36
6	А	504	COB	C17-C18-C60-C61
6	А	504	COB	C1P-C2P-O3-P

Continued on next page...



Mol	Chain	Res	Type	Atoms
6	А	504	COB	C3P-C2P-O3-P
6	А	504	COB	C48-C49-C50-O51
6	А	504	COB	C18-C60-C61-N62
6	А	504	COB	C4-C3-C30-C31
6	А	504	COB	C48-C49-C50-N52
6	А	504	COB	C2-C3-C30-C31
6	А	504	COB	C19-C18-C60-C61
6	А	504	COB	C18-C60-C61-O63
6	А	504	COB	C38-C37-C7-C8
6	А	504	COB	O6R-C4R-C5R-O8R
5	А	503	SAM	N-CA-CB-CG
6	А	504	COB	C3R-O2-P-O3
5	А	503	SAM	O4'-C4'-C5'-SD
6	А	504	COB	C30-C31-C32-N33

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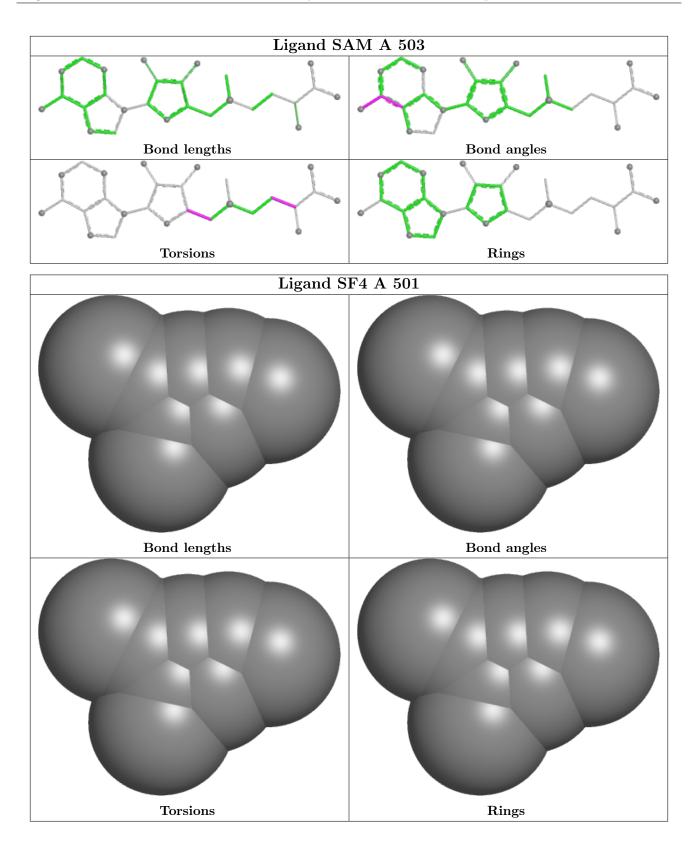
There are no ring outliers.

2 monomers are involved in 12 short contacts:

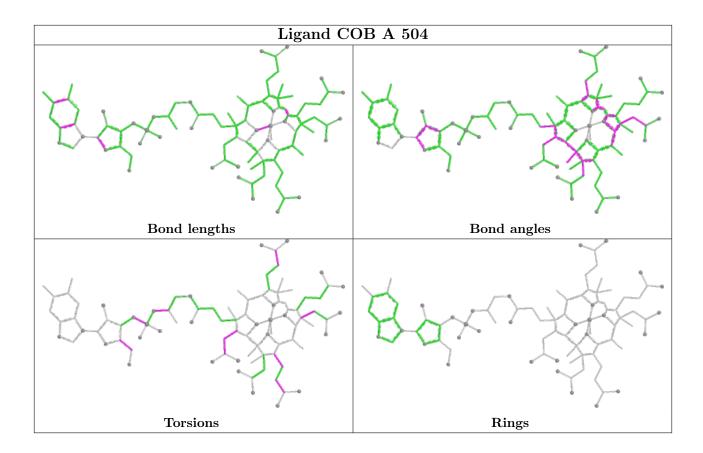
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	А	503	SAM	3	0
6	А	504	COB	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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^{th} 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	А	411/436~(94%)	-0.21	9 (2%) 62 69	43, 59, 84, 105	0
2	В	8/13~(61%)	0.42	0 100 100	69, 73, 88, 91	0
All	All	419/449~(93%)	-0.20	9 (2%) 63 70	43, 60, 84, 105	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	77	SER	4.8
1	А	89	GLY	3.3
1	А	76	THR	3.0
1	А	78	GLY	2.7
1	А	79	GLU	2.6
1	А	29	ASP	2.5
1	А	411	GLU	2.4
1	А	75	PHE	2.2
1	А	56	TYR	2.2

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 monosaccharides in this entry.

6.4 Ligands (i)

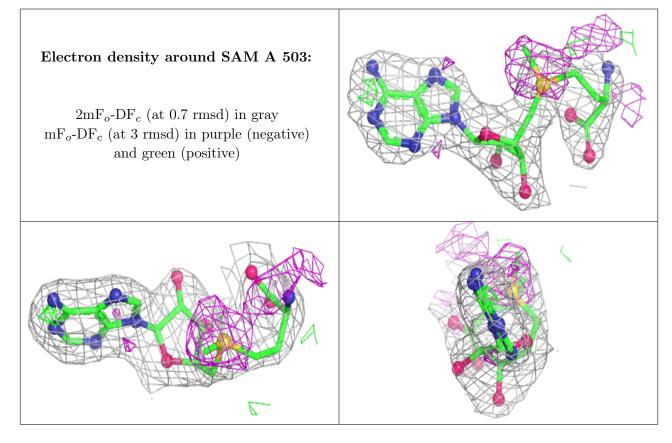
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,



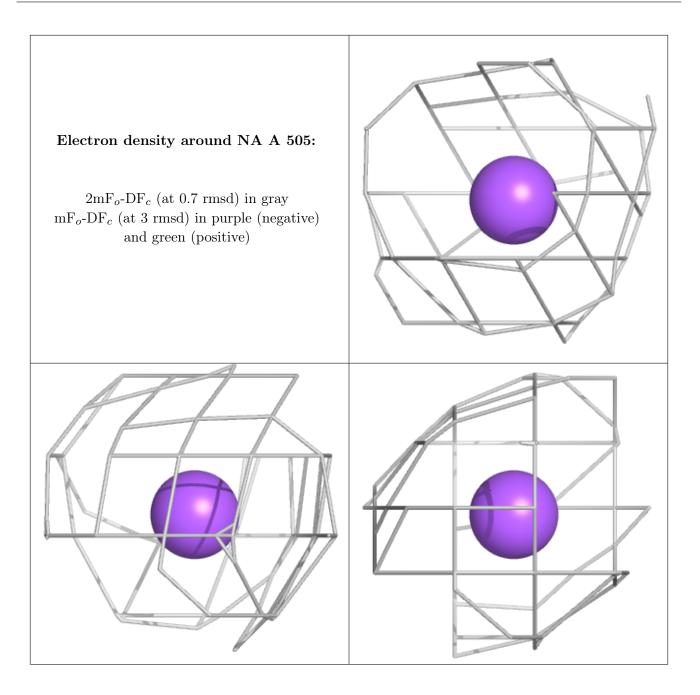
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q < 0.9
5	SAM	А	503	27/27	0.93	0.15	$65,\!69,\!74,\!74$	0
7	NA	А	505	1/1	0.96	0.05	$51,\!51,\!51,\!51$	0
6	COB	А	504	92/92	0.98	0.11	49,51,53,54	0
3	SF4	А	501	8/8	0.99	0.14	$57,\!57,\!58,\!59$	0
4	FE	А	502	1/1	1.00	0.12	64,64,64,64	0

median, 95^{th} 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.

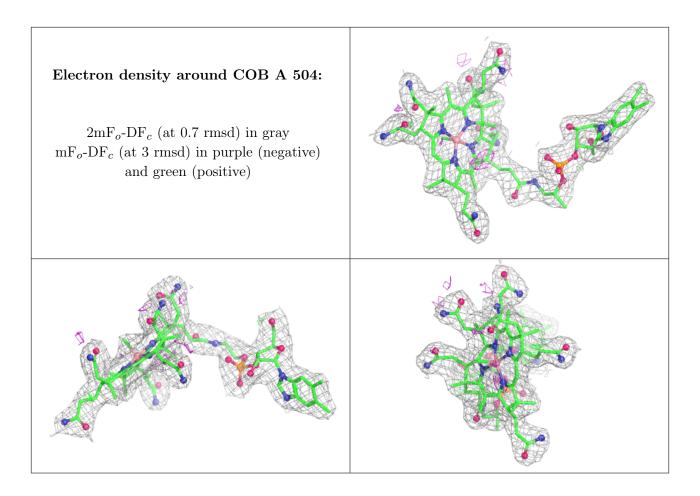
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



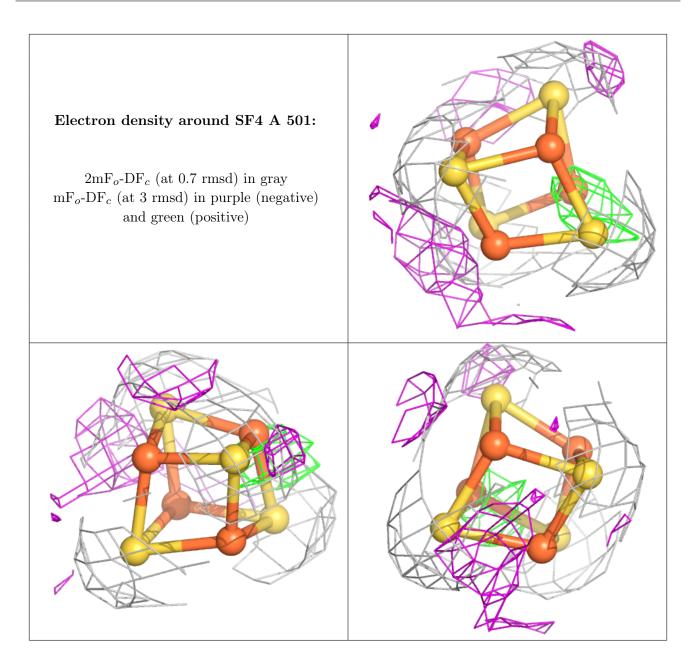




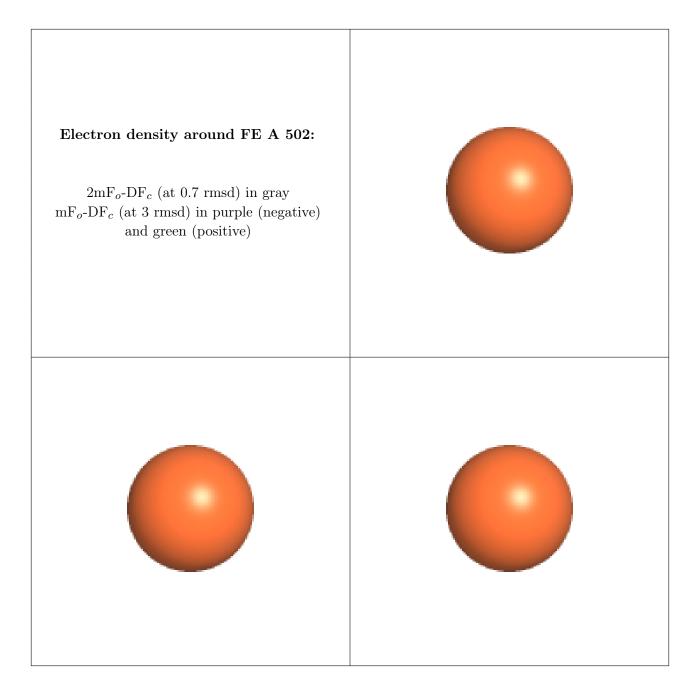












6.5 Other polymers (i)

There are no such residues in this entry.

