

# wwPDB X-ray Structure Validation Summary Report (i)

Nov 15, 2023 – 03:25 pm GMT

PDB ID	:	8QMK
Title	:	Enzymatically-produced complex-B bound TmHydE structure
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Deposited on		
Resolution	:	1.30  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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

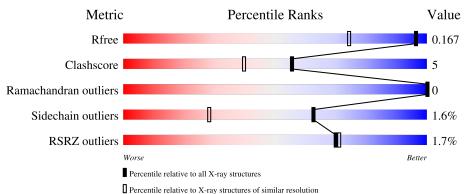
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 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 1.30 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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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		
			2%		
1	А	358	87%	11%	••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CMO	А	502[C]	-	-	Х	-

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Continued	from	previous	page
		1	1 0

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CMO	А	503[C]	-	-	Х	-
4	CYN	A	504	_	_	Х	-



#### 8QMK

# 2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 3991 atoms, of which 332 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 [FeFe] hydrogenase maturase subunit HydE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	А	356	Total 3415	C 1987	Н 328	N 526	O 553	S 21	0	43	0

Chain Residue Modelled Reference Actual Comment UNP Q9X0Z6 А -9 MET initiating methionine \_ А -8 TRP expression tag UNP Q9X0Z6 \_ А -7 SER expression tag UNP Q9X0Z6 -Α HIS UNP Q9X0Z6 expression tag -6 \_ UNP Q9X0Z6 А -5 PRO expression tag -UNP Q9X0Z6 А -4 GLN expression tag \_ А -3 PHE expression tag UNP Q9X0Z6 \_ А -2 GLU expression tag UNP Q9X0Z6 \_ А LYS expression tag UNP Q9X0Z6 -1 \_ А 0 ALA expression tag UNP Q9X0Z6 -А 1 SER expression tag UNP Q9X0Z6 \_ А 291ILE MET engineered mutation UNP Q9X0Z6 Α CYS UNP Q9X0Z6 311 SER engineered mutation CYS SER engineered mutation UNP Q9X0Z6 А 319 А SER CYS UNP Q9X0Z6 322 engineered mutation

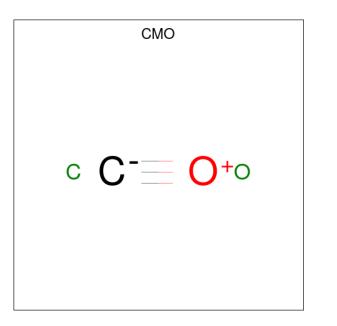
There are 15 discrepancies between the modelled and reference sequences:

• Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	1

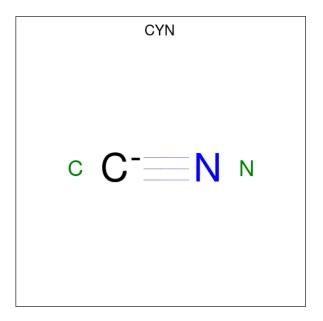
• Molecule 3 is CARBON MONOXIDE (three-letter code: CMO) (formula: CO) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 2 & 1 & 1 \end{array}$	0	1
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 2  1  1 \end{array}$	0	1

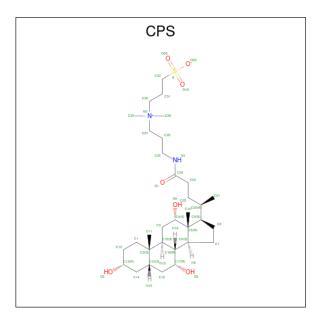
• Molecule 4 is CYANIDE ION (three-letter code: CYN) (formula: CN) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	А	1	Total 2	C 1	N 1	0	0

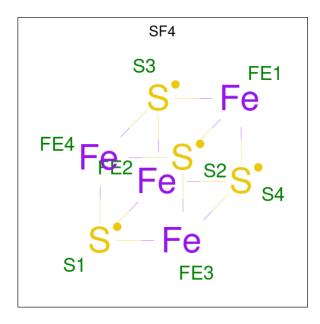


• Molecule 5 is 3-[(3-CHOLAMIDOPROPYL)DIMETHYLAMMONIO]-1-PROPANESULFO NATE (three-letter code: CPS) (formula:  $C_{32}H_{58}N_2O_7S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	А	1	Total 23	C 20	0 3	0	1

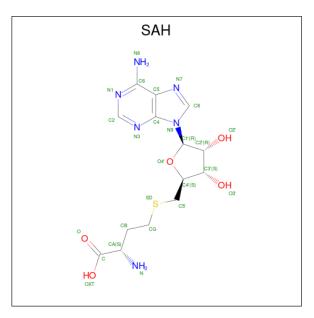
• Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $Fe_4S_4$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
6	А	1	Total 8	Fe 4	$\frac{S}{4}$	0	0



• Molecule 7 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula:  $C_{14}H_{20}N_6O_5S$ ).



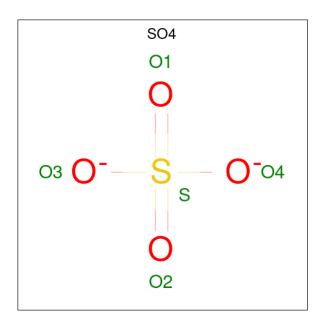
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
7	Λ	1	Total	С	Ν	0	$\mathbf{S}$	0	0
(	A	1	26	14	6	5	1	0	0

• Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

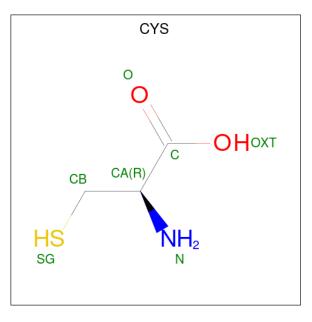
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	2	Total Cl 2 2	0	2

• Molecule 9 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).





Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
9	А	1	Total 10	O 8	${ m S} { m 2}$	0	1



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf			
10	А	1	Total 11	С 3	Н 4	N 1	0 2	S 1	0	0

• Molecule 11 is water.



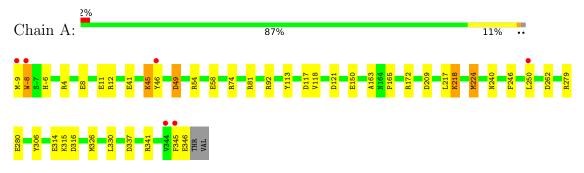
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	А	482	Total O 489 489	0	28



# 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: [FeFe] hydrogenase maturase subunit HydE





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	63.83Å 83.56Å 70.84Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	34.96 - 1.30	Depositor
Resolution (A)	47.42 - 1.30	EDS
% Data completeness	99.8 (34.96-1.30)	Depositor
(in resolution range)	$100.0 \ (47.42 - 1.30)$	EDS
R <sub>merge</sub>	(Not available)	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.21 (at 1.30 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
$R, R_{free}$	0.143 , $0.168$	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.142 , $0.167$	DCC
$R_{free}$ test set	4685 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	13.6	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.32 , $52.7$	EDS
L-test for $twinning^2$	$ L  > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	3991	wwPDB-VP
Average B, all atoms $(Å^2)$	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.37% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: CL, SAH, CYN, CMO, SF4, FE2, CPS, SO4

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	Bo	nd lengths	Bond angles		
		RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	1.05	7/3269~(0.2%)	1.10	16/4408~(0.4%)	

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
1	А	45[A]	LYS	CE-NZ	-6.02	1.33	1.49
1	А	45[B]	LYS	CE-NZ	-6.02	1.33	1.49
1	А	58	GLU	CD-OE2	5.75	1.31	1.25
1	А	306	TYR	CE1-CZ	-5.33	1.31	1.38
1	А	49[A]	ASP	CG-OD1	5.14	1.37	1.25

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	49[A]	ASP	CB-CG-OD1	10.02	127.32	118.30
1	А	49[B]	ASP	CB-CG-OD1	10.02	127.32	118.30
1	А	337	ASP	CB-CG-OD1	7.30	124.87	118.30
1	А	117	ASP	CB-CG-OD1	7.27	124.84	118.30
1	А	49[A]	ASP	CB-CG-OD2	-7.22	111.81	118.30

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	3087	328	3185	26	1
2	А	1	0	0	0	0
3	А	4	0	0	5	0
4	А	2	0	0	2	0
5	А	23	0	31	2	0
6	А	8	0	0	0	0
7	А	26	0	19	0	0
8	А	2	0	0	0	0
9	А	10	0	0	0	0
10	А	7	4	3	2	0
11	А	489	0	0	12	2
All	All	3659	332	3238	33	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 33 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:A:502[C]:CMO:C	3:A:503[C]:CMO:C	2.54	0.86
1:A:49[B]:ASP:OD1	11:A:601:HOH:O	1.96	0.82
1:A:218:LYS:NZ	11:A:862[B]:HOH:O	2.14	0.80
3:A:503[C]:CMO:C	4:A:504:CYN:C	2.61	0.79
1:A:41:GLU:O	1:A:45[B]:LYS:HD3	1.93	0.69

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:GLU:O	11:A:1058:HOH:O[4_555]	2.12	0.08
11:A:971:HOH:O	11:A:1077:HOH:O[4_554]	2.14	0.06

### 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



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	А	394/358~(110%)	383~(97%)	11 (3%)	0	100 100

analysed, and the total number of residues.

There are no Ramachandran outliers to report.

#### 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.

Ι	Mol	Chain	Analysed	Analysed Rotameric		Percentiles	
	1	А	347/313~(111%)	338~(97%)	9~(3%)	46 10	

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	А	224[D]	MET
1	А	341	ARG
1	А	11	GLU
1	А	224[A]	MET
1	А	224[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

#### 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 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	Turne	Chain	Res	Link	Bo	ond leng	ths	B	ond ang	gles
IVIOI	Type	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	CYN	А	504	-	$0,\!1,\!1$	-	-	-		
6	SF4	А	506	7,1	$0,\!12,\!12$	-	-	-		
10	CYS	А	511	2	$5,\!6,\!6$	1.65	2 (40%)	5,7,7	2.14	3 (60%)
3	CMO	А	502[C]	-	$0,\!1,\!1$	-	-	-		
7	SAH	А	507	6	24,28,28	1.25	2 (8%)	$25,\!40,\!40$	1.68	<u>6 (24%)</u>
9	SO4	А	510[B]	-	4,4,4	0.10	0	$6,\!6,\!6$	0.13	0
3	CMO	А	503[C]	-	0,1,1	-	-	-		
9	SO4	А	510[A]	-	4,4,4	0.23	0	6,6,6	0.19	0
5	CPS	А	505[A]	-	$26,\!26,\!45$	1.00	0	40,43,70	1.82	10 (25%)

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	$\mathbf{Res}$	Link	Chirals	Torsions	Rings
7	SAH	А	507	6	-	2/11/31/31	0/3/3/3
10	CYS	А	511	2	-	1/6/6/6	-
5	CPS	А	505[A]	-	-	-	0/4/4/4
6	SF4	А	506	7,1	-	-	0/6/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$\operatorname{Observed}(\operatorname{\AA})$	$\mathrm{Ideal}(\mathrm{\AA})$
10	А	511	CYS	OXT-C	-2.64	1.21	1.30
7	А	507	SAH	O4'-C1'	2.30	1.44	1.41
7	А	507	SAH	C2-N3	2.20	1.35	1.32
10	А	511	CYS	O-C	2.09	1.28	1.22

The worst 5 of 19 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$\mathbf{Ideal}(^{o})$
7	А	507	SAH	C5-C6-N6	4.11	126.59	120.35
5	А	505[A]	CPS	C11-C2-C19	-4.04	105.61	111.18
5	А	505[A]	CPS	C5-C6-C18	-3.71	110.00	114.74
5	А	505[A]	CPS	C3-C19-C2	-3.61	110.00	113.73
5	А	505[A]	CPS	C19-C2-C15	3.42	113.38	108.58

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	А	507	SAH	C-CA-CB-CG
7	А	507	SAH	N-CA-CB-CG
10	А	511	CYS	N-CA-CB-SG

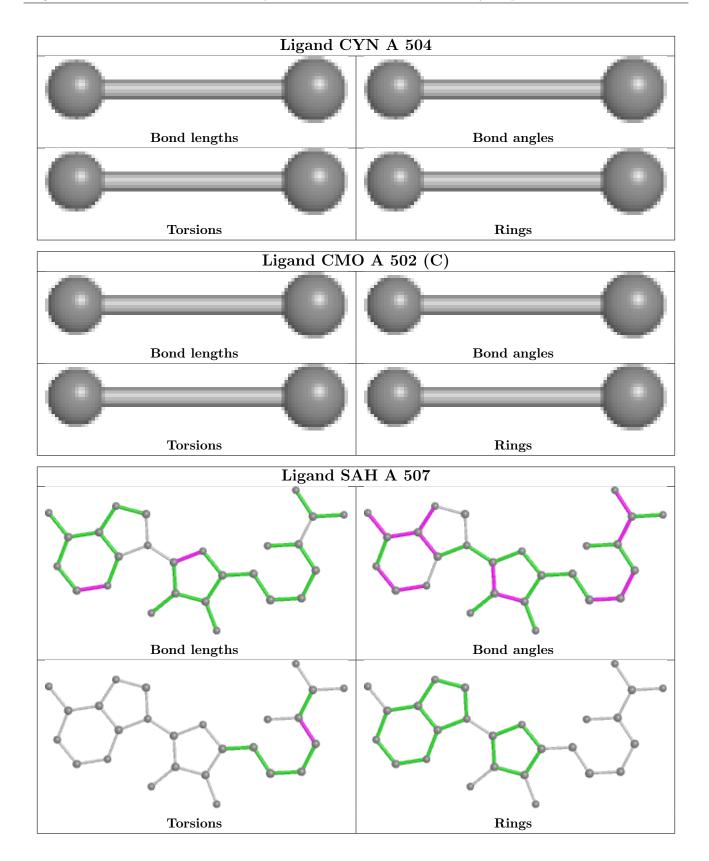
There are no ring outliers.

5 monomers are involved in 7 short contacts:

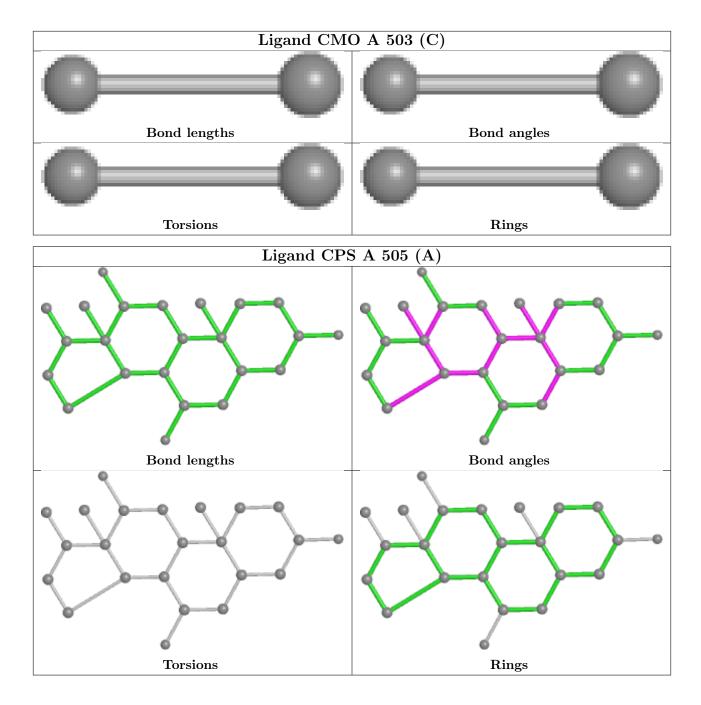
Mol	Chain	$\mathbf{Res}$	Type	Clashes	Symm-Clashes
4	А	504	CYN	2	0
10	А	511	CYS	2	0
3	А	502[C]	CMO	3	0
3	А	503[C]	CMO	3	0
5	А	505[A]	CPS	2	0

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 $>$	# <b>R</b> \$	SRZ>	>2	$OWAB(Å^2)$	Q<0.9
1	А	356/358~(99%)	0.05	6 (1%)	70	71	10, 16, 34, 67	1 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	-8[A]	TRP	5.8
1	А	-9[A]	MET	5.5
1	А	345[A]	PHE	3.5
1	А	344	VAL	2.7
1	А	46[A]	TYR	2.6

#### 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, 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	${f B} ext{-factors}({ m \AA}^2)$	Q<0.9
9	SO4	А	510[A]	5/5	0.52	0.40	87,87,89,89	5
9	SO4	А	510[B]	5/5	0.52	0.40	45,48,48,50	5

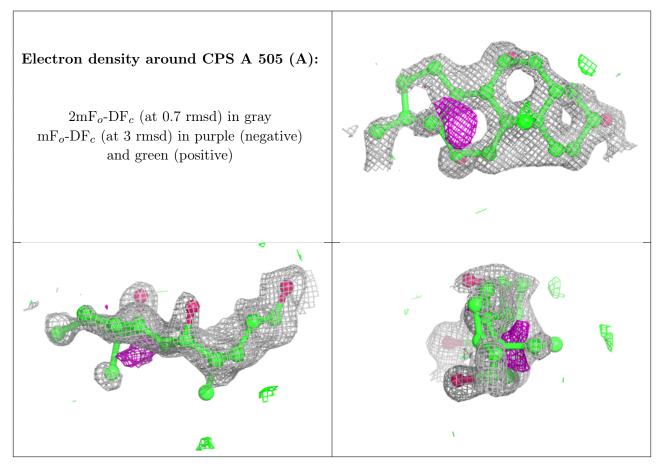
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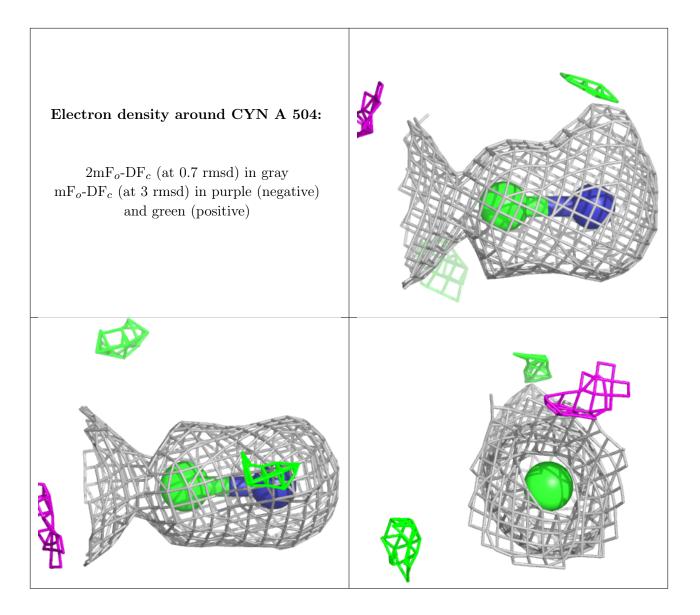
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
5	CPS	А	505[A]	23/42	0.73	0.17	38,41,46,49	23
4	CYN	А	504	2/2	0.96	0.08	15,15,15,16	0
3	CMO	А	503[C]	2/2	0.96	0.11	13,13,13,14	0
7	SAH	А	507	26/26	0.97	0.07	10,12,14,15	0
10	CYS	А	511	7/7	0.97	0.12	15,18,20,22	0
6	SF4	А	506	8/8	0.99	0.06	11,11,12,12	0
3	CMO	А	502[C]	2/2	0.99	0.07	13,13,13,15	0
8	CL	А	509[A]	1/1	0.99	0.09	16,16,16,16	1
2	FE2	А	501[A]	1/1	1.00	0.06	12,12,12,12	1
8	CL	А	508[A]	1/1	1.00	0.06	$15,\!15,\!15,\!15$	1

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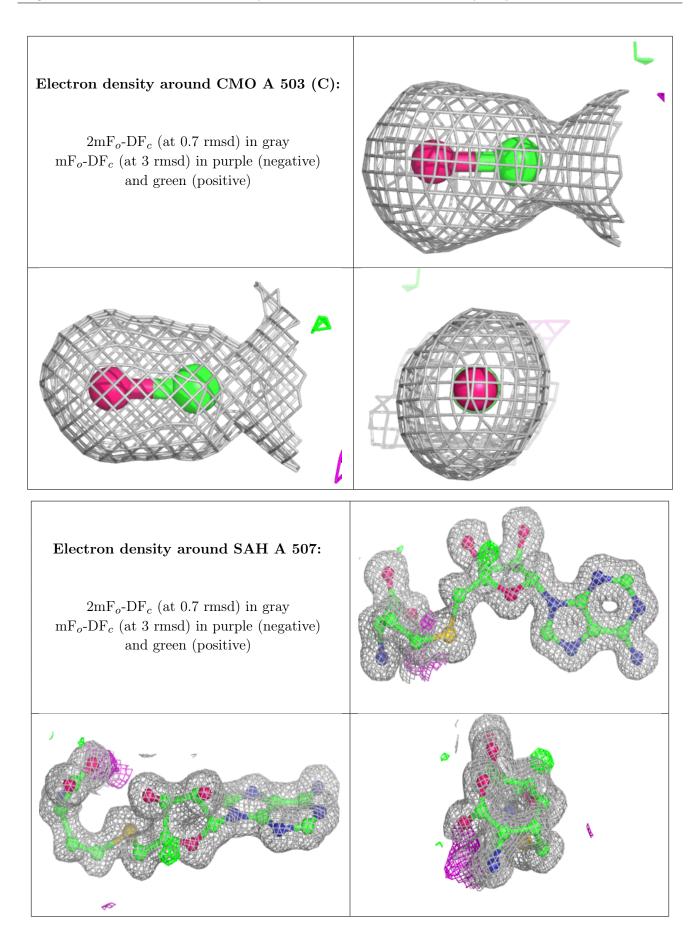
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



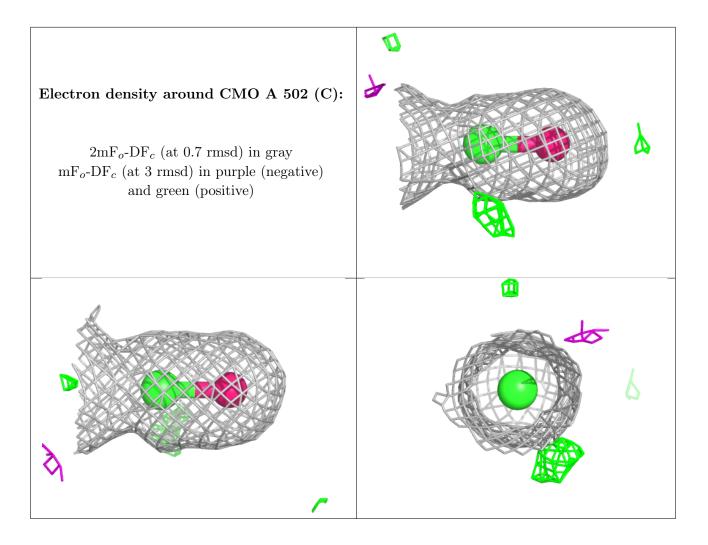




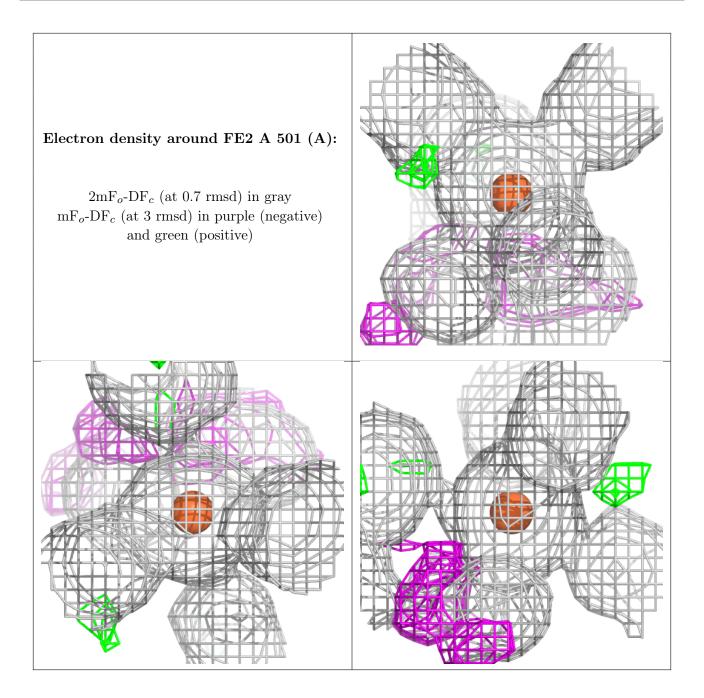












### 6.5 Other polymers (i)

There are no such residues in this entry.

