

Full wwPDB X-ray Structure Validation Report (i)

Oct 9, 2023 – 01:32 PM EDT

PDB ID	:	6XK3
Title	:	Nitric Oxide Synthase from Bacillus subtilis in complex with 7-((3-(((pyridin-
		2-ylmethyl)amino)methyl)phenoxy)methyl)quinolin-2-amine
Authors	:	Lewis, M.C.; Poulos, T.L.
Deposited on	:	2020-06-25
Resolution	:	1.95 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 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:

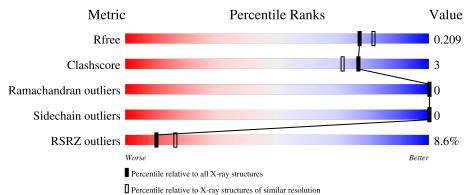
Xtriage (Phenix) EDS buster-report Percentile statistics Refmac CCP4 Ideal geometry (proteins) Ideal geometry (DNA, RNA)	: : : : :	20191225.v01 (using entries in the PDB archive December 25th 2019) 5.8.0158 7.0.044 (Gargrove) Engh & Huber (2001) Parkinson et al. (1996)
Ideal geometry (DNA, RNA) Validation Pipeline (wwPDB-VP)		Parkinson et al. (1996) 2.35.1

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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	٨	262	9%	
	А	363	92%	8%



6XK3

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 3241 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.

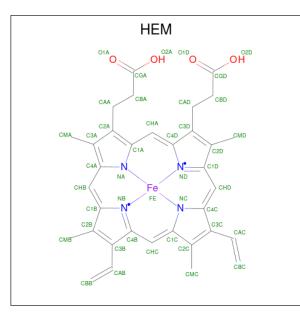
• Molecule 1 is a protein called Nitric oxide synthase oxygenase.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	362	Total 2940	C 1873	N 507	O 552	S 8	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	25	ALA	GLU	conflict	UNP O34453
А	26	ALA	GLU	conflict	UNP O34453
А	316	ALA	GLU	conflict	UNP O34453

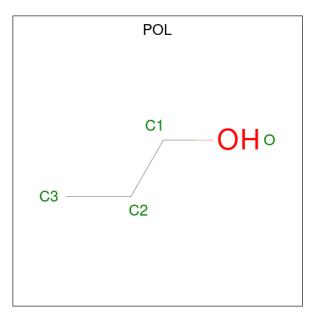
• Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
0	Δ	1	Total	С	Fe	Ν	Ο	0	0
2	A	1	43	34	1	4	4	0	0

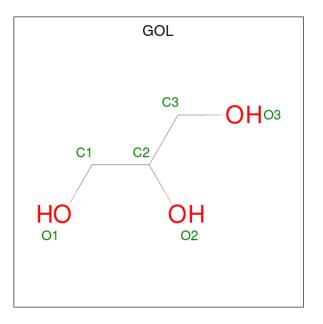


• Molecule 3 is N-PROPANOL (three-letter code: POL) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 3 & 1 \end{array}$	0	0

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

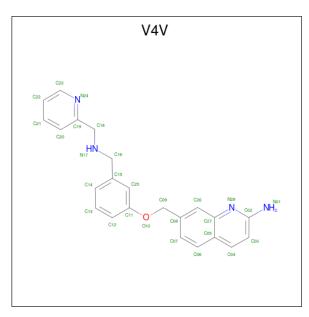


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0



\mathbf{N}	[o]	Chain	Residues	Ate	oms		ZeroOcc	AltConf
	4	А	1	Total 6	С 3	O 3	0	0

• Molecule 5 is 7-{[3-({[(pyridin-2-yl)methyl]amino}methyl)phenoxy]methyl}quinolin-2amine (three-letter code: V4V) (formula: C₂₃H₂₂N₄O) (labeled as "Ligand of Interest" by depositor).



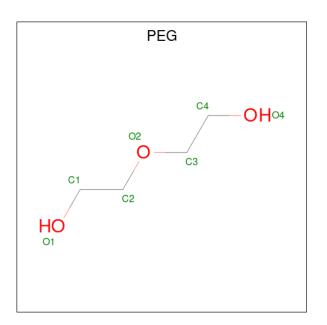
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
5	Δ	1	Total	С	Ν	0	0	0
0	Л	1	28	23	4	1	0	0

• Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	Total Cl 1 1	0	0

• Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).





N	Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
	7	А	1	Total 7	$\begin{array}{c} \mathrm{C} \\ 4 \end{array}$	O 3	0	0

• Molecule 8 is water.

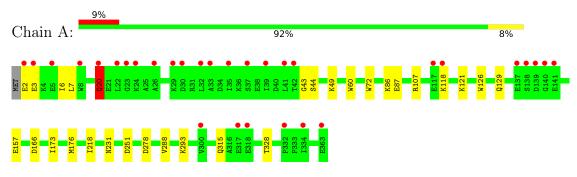
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	А	200	Total O 200 200	0	0



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: Nitric oxide synthase oxygenase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	81.22Å 95.80Å 62.52Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.02 - 1.95	Depositor
Resolution (A)	38.02 - 1.95	EDS
% Data completeness	99.2 (38.02-1.95)	Depositor
(in resolution range)	99.3 (38.02 - 1.95)	EDS
R _{merge}	0.04	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.06 (at 1.95 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.179 , 0.209	Depositor
It, Itfree	0.179 , 0.209	DCC
R_{free} test set	2000 reflections $(5.55%)$	wwPDB-VP
Wilson B-factor ($Å^2$)	30.8	Xtriage
Anisotropy	0.657	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.36 , 46.1	EDS
L-test for twinning ²	$ \langle L \rangle = 0.49, \langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3241	wwPDB-VP
Average B, all atoms $(Å^2)$	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.80% 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: HEM, GOL, POL, PEG, CL, V4V

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).

Mal	Chain	Bo	nd lengths	Bond angles	
Mol	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.92	1/3016~(0.0%)	0.86	7/4088~(0.2%)

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
1	А	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	288	VAL	CB-CG2	6.55	1.66	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	20	GLN	CB-CA-C	-8.99	92.42	110.40
1	А	20	GLN	CA-CB-CG	-7.18	97.60	113.40
1	А	251	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	А	157	GLU	CG-CD-OE2	-6.43	105.43	118.30
1	А	49	LYS	CD-CE-NZ	-5.40	99.29	111.70
1	А	278	ASP	CB-CG-OD1	5.39	123.15	118.30
1	А	166	ASP	CB-CG-OD2	-5.16	113.65	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	А	20	GLN	Sidechain

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	2940	0	2856	16	0
2	А	43	0	30	1	0
3	А	4	0	8	0	0
4	А	18	0	24	0	0
5	А	28	0	0	0	0
6	А	1	0	0	0	0
7	А	7	0	10	2	0
8	А	200	0	0	7	0
All	All	3241	0	2928	18	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 3.

All (18) 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)
1:A:107:ARG:NH1	8:A:1002:HOH:O	2.28	0.65
1:A:3:GLU:HG2	1:A:6:ILE:HD12	1.80	0.61
1:A:328:THR:OG1	7:A:908:PEG:H41	2.02	0.59
1:A:60:TRP:CE3	1:A:72:TRP:HA	2.38	0.58
1:A:43:GLY:HA3	1:A:118:LYS:NZ	2.21	0.55
1:A:293:LYS:NZ	8:A:1003:HOH:O	2.28	0.55
1:A:20:GLN:HG2	1:A:20:GLN:O	2.09	0.52
1:A:86:LYS:HG3	8:A:1131:HOH:O	2.10	0.51
1:A:87:GLU:HG3	8:A:1154:HOH:O	2.12	0.49
1:A:315:GLN:NE2	8:A:1001:HOH:O	1.95	0.49
7:A:908:PEG:H12	8:A:1106:HOH:O	2.17	0.45
2:A:901:HEM:HHC	2:A:901:HEM:HBB2	2.00	0.43
1:A:129:GLN:HG2	1:A:218:ILE:HD13	2.01	0.42
1:A:86:LYS:HG2	1:A:176:MET:HG3	2.00	0.42
1:A:126:TRP:HB2	1:A:173:ILE:HG23	2.01	0.42



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LEU:HD21	1:A:44:SER:HA	2.03	0.41
1:A:121:LYS:HD3	1:A:231:ASN:ND2	2.35	0.41
1:A:2:GLU:N	8:A:1014:HOH:O	2.55	0.40

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		
1	А	360/363~(99%)	351 (98%)	9~(2%)	0	100	100

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.

Mol	Chain	Analysed	Analysed Rotameric C			
1	А	309/310~(100%)	309 (100%)	0	100 100	

There are no protein residues with a non-rotameric sidechain to report.

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 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	Bo	ond leng	ths	Bond angles		
10101	Type	Ullaili	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	POL	А	902	-	3,3,3	0.78	0	2,2,2	0.29	0
4	GOL	А	905	-	$5,\!5,\!5$	0.85	0	$5,\!5,\!5$	0.96	0
2	HEM	А	901	1	41,50,50	1.48	7 (17%)	45,82,82	2.34	20 (44%)
5	V4V	А	906	-	31,31,31	1.67	5 (16%)	40,41,41	1.65	6 (15%)
4	GOL	А	903	-	$5,\!5,\!5$	1.23	0	$5,\!5,\!5$	1.50	1 (20%)
4	GOL	А	904	-	$5,\!5,\!5$	0.89	0	$5,\!5,\!5$	0.90	0
7	PEG	А	908	-	$6,\!6,\!6$	0.47	0	$5,\!5,\!5$	1.30	1 (20%)

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
3	POL	A	902	-	-	1/1/1/1	-
4	GOL	А	905	-	-	4/4/4/4	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	А	901	1	-	3/12/54/54	-
5	V4V	А	906	-	-	1/11/11/11	0/4/4/4
4	GOL	А	903	-	-	2/4/4/4	-
4	GOL	А	904	-	-	2/4/4/4	-
7	PEG	А	908	-	-	2/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
5	А	906	V4V	O10-C11	4.04	1.47	1.37
2	А	901	HEM	CHB-C1B	3.46	1.43	1.35
5	А	906	V4V	C02-N01	3.45	1.45	1.35
5	А	906	V4V	C05-C27	-3.21	1.37	1.42
2	А	901	HEM	C1B-NB	-3.14	1.34	1.40
5	А	906	V4V	C18-C19	2.81	1.56	1.51
2	А	901	HEM	FE-NB	2.55	2.09	1.96
2	А	901	HEM	C4D-ND	-2.47	1.36	1.40
2	А	901	HEM	C4D-C3D	2.42	1.49	1.45
2	А	901	HEM	CHA-C4D	2.27	1.40	1.35
2	А	901	HEM	C1A-NA	2.16	1.40	1.36
5	А	906	V4V	C04-C03	2.12	1.41	1.36

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
5	А	906	V4V	C21-C20-C19	4.99	125.14	118.93
2	А	901	HEM	C1B-NB-C4B	4.86	110.09	105.07
2	А	901	HEM	C3B-C2B-C1B	4.59	109.89	106.49
2	А	901	HEM	CHD-C1D-C2D	-4.46	118.01	124.98
2	А	901	HEM	CHD-C1D-ND	4.06	128.84	124.43
2	А	901	HEM	C4B-C3B-C2B	-4.00	103.94	107.11
2	А	901	HEM	CHC-C4B-NB	3.88	128.65	124.43
5	А	906	V4V	C11-C25-C15	3.56	123.65	119.73
2	А	901	HEM	O2D-CGD-CBD	3.47	125.18	114.03
5	А	906	V4V	C20-C19-N24	-3.25	117.49	122.17
5	А	906	V4V	C19-C18-N17	-3.00	107.68	113.27
5	А	906	V4V	C18-C19-N24	2.96	122.01	116.20
2	А	901	HEM	C2C-C3C-C4C	-2.91	104.86	106.90
2	А	901	HEM	O2A-CGA-CBA	2.86	123.22	114.03
2	А	901	HEM	CHA-C4D-C3D	-2.82	120.03	125.33
2	А	901	HEM	CMD-C2D-C1D	2.81	129.32	125.04



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	903	GOL	O2-C2-C3	2.74	121.19	109.12
2	А	901	HEM	C2D-C1D-ND	2.66	113.07	109.88
2	А	901	HEM	O1A-CGA-CBA	-2.64	114.61	123.08
2	А	901	HEM	C4A-C3A-C2A	2.56	108.78	107.00
7	А	908	PEG	C3-O2-C2	-2.54	102.28	113.29
2	А	901	HEM	CHA-C4D-ND	2.52	127.50	124.38
5	А	906	V4V	C22-C21-C20	-2.46	116.45	120.19
2	А	901	HEM	CAD-C3D-C4D	2.44	128.92	124.66
2	А	901	HEM	O2D-CGD-O1D	-2.32	117.52	123.30
2	А	901	HEM	C3D-C4D-ND	2.07	112.47	110.17
2	А	901	HEM	CMC-C2C-C3C	2.06	128.53	124.68
2	А	901	HEM	CBA-CAA-C2A	-2.02	109.18	112.62

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	А	903	GOL	O1-C1-C2-O2
4	А	903	GOL	O1-C1-C2-C3
4	А	905	GOL	O1-C1-C2-C3
4	А	905	GOL	C1-C2-C3-O3
4	А	905	GOL	O2-C2-C3-O3
7	А	908	PEG	O1-C1-C2-O2
4	А	904	GOL	C1-C2-C3-O3
4	А	905	GOL	O1-C1-C2-O2
2	А	901	HEM	C2A-CAA-CBA-CGA
3	А	902	POL	O-C1-C2-C3
5	А	906	V4V	C15-C16-N17-C18
4	А	904	GOL	O2-C2-C3-O3
2	А	901	HEM	CAD-CBD-CGD-O1D
2	А	901	HEM	CAA-CBA-CGA-O1A
7	А	908	PEG	C1-C2-O2-C3

There are no ring outliers.

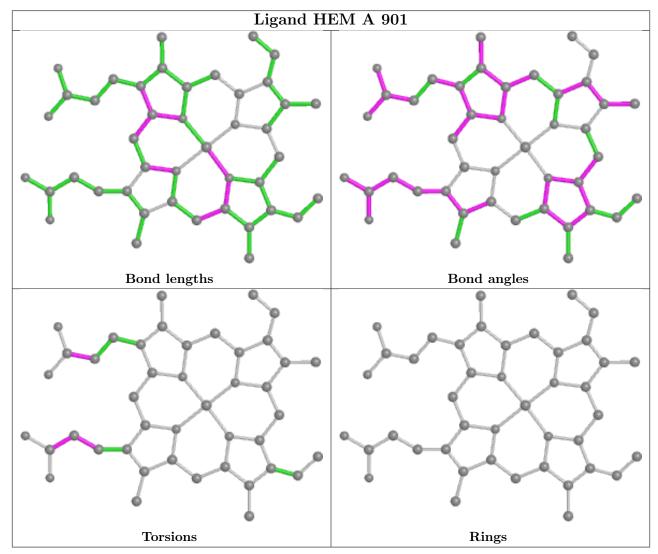
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	901	HEM	1	0
7	А	908	PEG	2	0

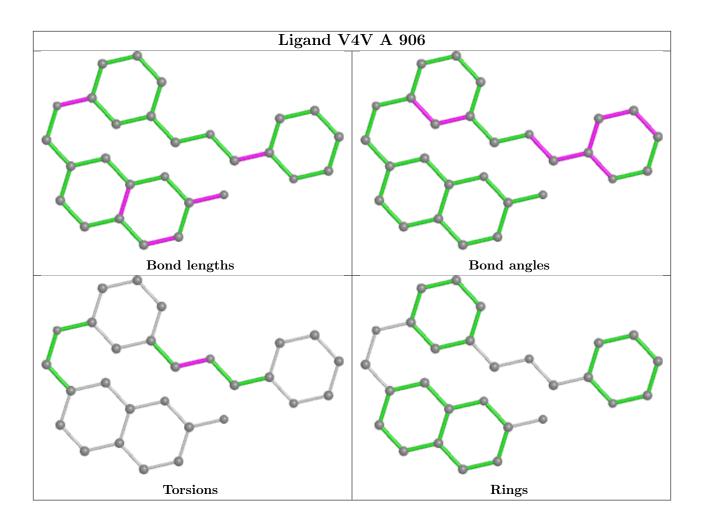
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,



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 $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	362/363~(99%)	0.43	31 (8%) 10 16	24, 34, 72, 102	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	41	LEU	6.0
1	А	139	ASP	5.7
1	А	138	SER	4.8
1	А	140	GLY	4.2
1	А	141	GLU	3.9
1	А	3	GLU	3.6
1	А	29	LYS	3.5
1	А	363	GLU	3.4
1	А	118	LYS	3.2
1	А	117	GLU	3.1
1	А	137	GLU	3.1
1	А	23	GLY	3.1
1	А	5	GLU	2.9
1	А	20	GLN	2.8
1	А	32	LEU	2.7
1	А	300	VAL	2.6
1	А	30	ASP	2.6
1	А	318	GLU	2.5
1	А	317	GLU	2.5
1	А	8	TRP	2.4
1	А	42	THR	2.4
1	А	37	SER	2.4
1	А	2	GLU	2.3
1	А	24	LYS	2.3
1	А	33	ALA	2.3
1	А	35	ILE	2.3
1	А	39	ILE	2.2



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Mol	Chain	Res	Type	RSRZ
1	А	334	ILE	2.1
1	А	332	PRO	2.1
1	А	26	ALA	2.0
1	А	22	LEU	2.0

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.

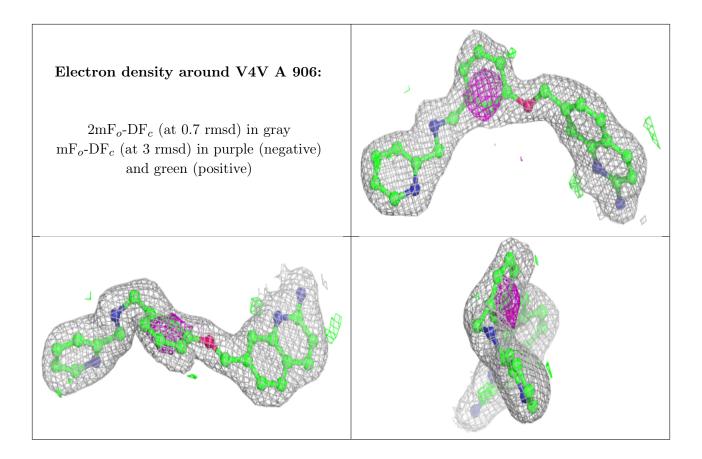
6.4 Ligands (i)

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.

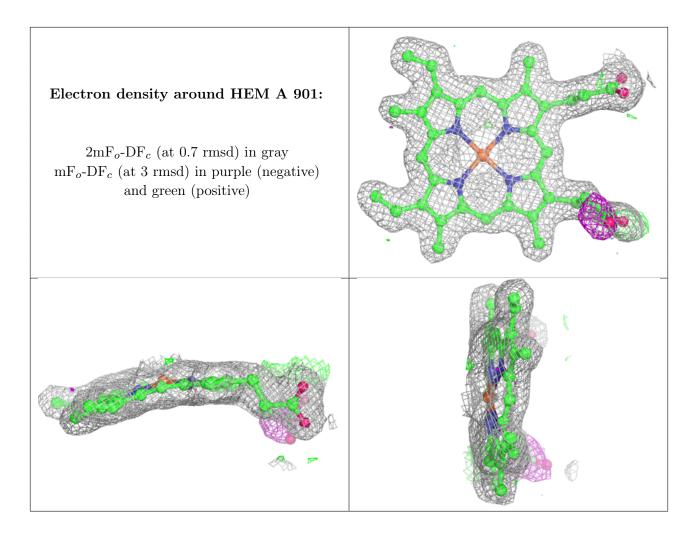
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q < 0.9
4	GOL	А	903	6/6	0.74	0.25	37,42,47,52	0
4	GOL	А	904	6/6	0.81	0.17	$36,\!45,\!50,\!56$	0
4	GOL	А	905	6/6	0.81	0.17	42,46,52,56	0
7	PEG	А	908	7/7	0.86	0.27	46,48,60,72	0
3	POL	А	902	4/4	0.87	0.20	$26,\!37,\!40,\!45$	0
5	V4V	А	906	28/28	0.89	0.18	25,34,46,51	0
2	HEM	А	901	43/43	0.97	0.19	23,26,36,70	0
6	CL	А	907	1/1	0.99	0.11	35,35,35,35	0

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.

