



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2018 – 06:14 pm GMT

PDB ID : 3E7G
Title : Structure of human INOSOX with inhibitor AR-C95791
Authors : Garcin, E.D.; Arvai, A.S.; Rosenfeld, R.J.; Kroeger, M.D.; Crane, B.R.; Andersson, G.; Andrews, G.; Hamley, P.J.; Mallinder, P.R.; Nicholls, D.J.; St-Gallay, S.A.; Tinker, A.C.; Gensmantel, N.P.; Mete, A.; Cheshire, D.R.; Connolly, S.; Stueh, D.J.; Aberg, A.; Wallace, A.V.; Tainer, J.A.; Getzoff, E.D.
Deposited on : 2008-08-18
Resolution : 2.20 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

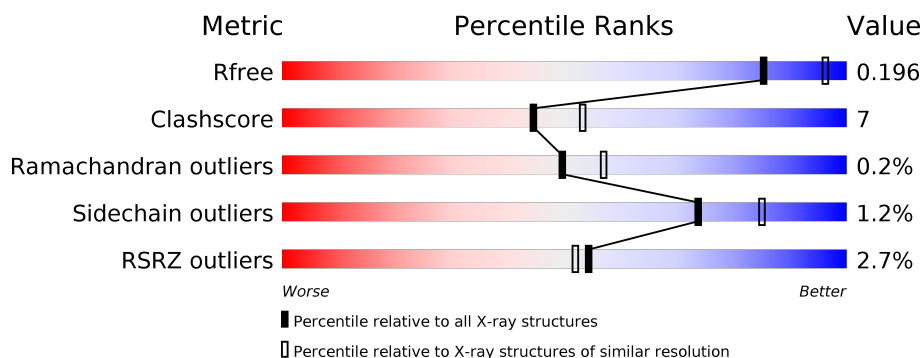
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (2.20-2.20)

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	424	<div> <div>2%</div> <div>82% 17% ..</div> </div>
1	B	424	<div> <div>3%</div> <div>81% 18% .</div> </div>
1	C	424	<div> <div>2%</div> <div>86% 13%</div> </div>
1	D	424	<div> <div>4%</div> <div>79% 20% .</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	H4B	A	902	X	-	-	-
4	H4B	D	3902	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14516 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.

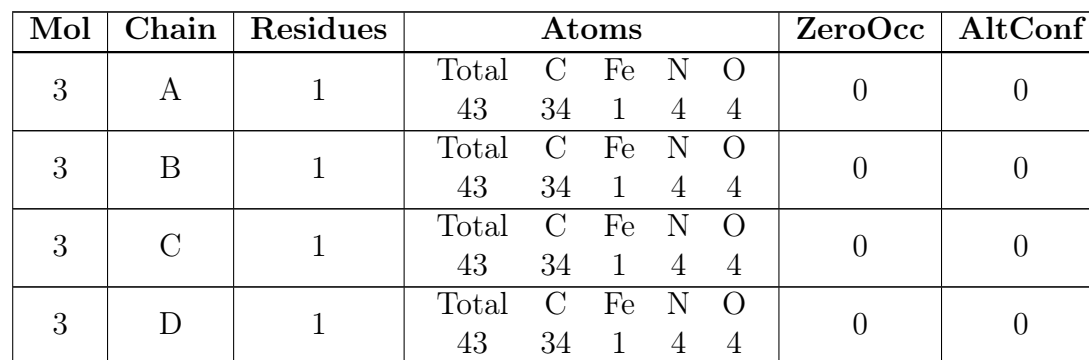
- Molecule 1 is a protein called Nitric oxide synthase, inducible.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3418	2186	597	613	22			
1	B	421	Total	C	N	O	S	0	0	0
			3418	2186	597	613	22			
1	C	423	Total	C	N	O	S	0	0	0
			3440	2198	600	620	22			
1	D	421	Total	C	N	O	S	0	0	0
			3418	2186	597	613	22			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

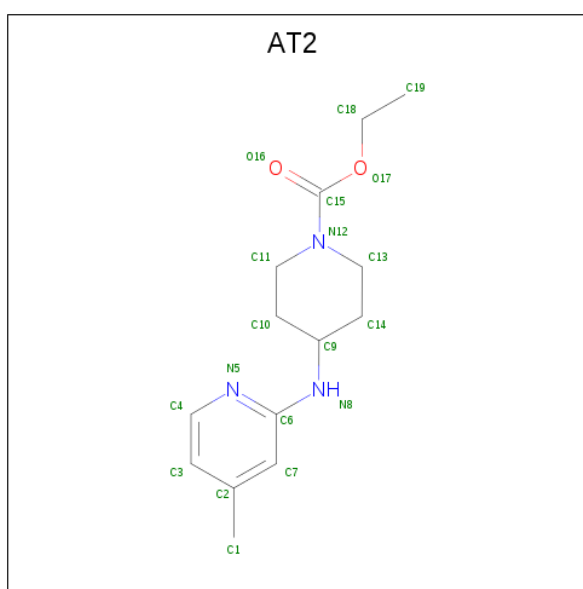
- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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- The chemical structure of H4B (Hydroxybenzoyl-CoA) is shown. It consists of a benzoyl group (a benzene ring with a carboxyl group) attached to the CoA moiety. The benzoyl group is shown in green, and the CoA moiety is shown in blue. The attachment point is labeled C10(S). The carboxyl group is labeled O9 and O10. The benzene ring is labeled C6(P) and C9(R). The CoA moiety is labeled N1, N3, N5, N8, and N2. The benzoyl group is shown in green, and the CoA moiety is shown in blue.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	9	5	3		
4	B	1	Total	C	N	O	0	0
			17	9	5	3		
4	C	1	Total	C	N	O	0	0
			17	9	5	3		
4	D	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 5 is ETHYL 4-[(4-METHYLPYRIDIN-2-YL)AMINO]PIPERIDINE-1-CARBOXYLATE (three-letter code: AT2) (formula: C₁₄H₂₁N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			19	14	3	2		
5	B	1	Total	C	N	O	0	0
			19	14	3	2		
5	C	1	Total	C	N	O	0	0
			19	14	3	2		
5	D	1	Total	C	N	O	0	0
			19	14	3	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	121	Total	O	0	0
			121	121		

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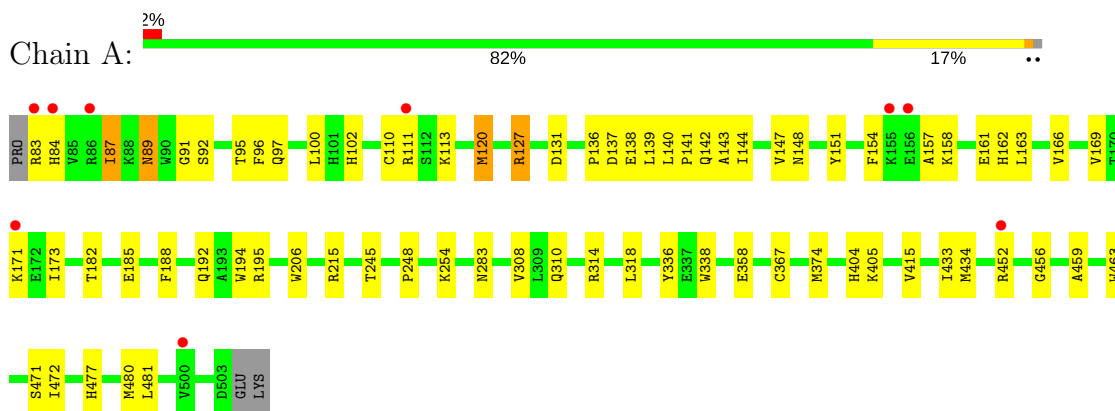
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	110	Total 110	O 110	0	0
6	C	137	Total 137	O 137	0	0
6	D	136	Total 136	O 136	0	0

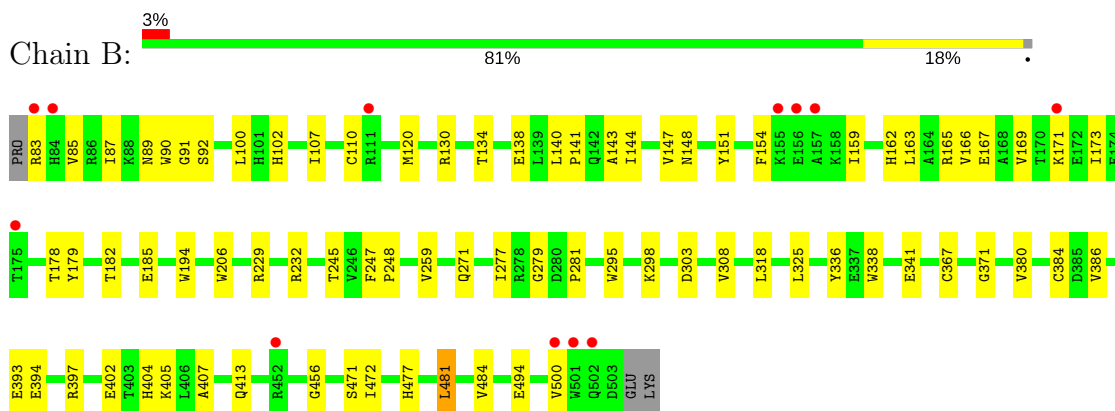
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

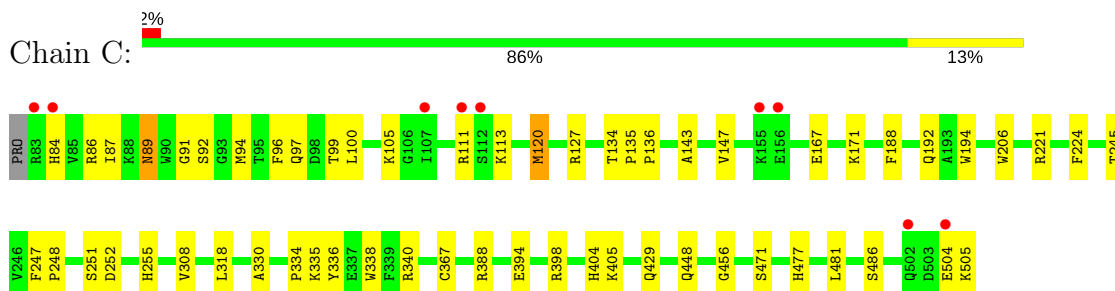
- Molecule 1: Nitric oxide synthase, inducible



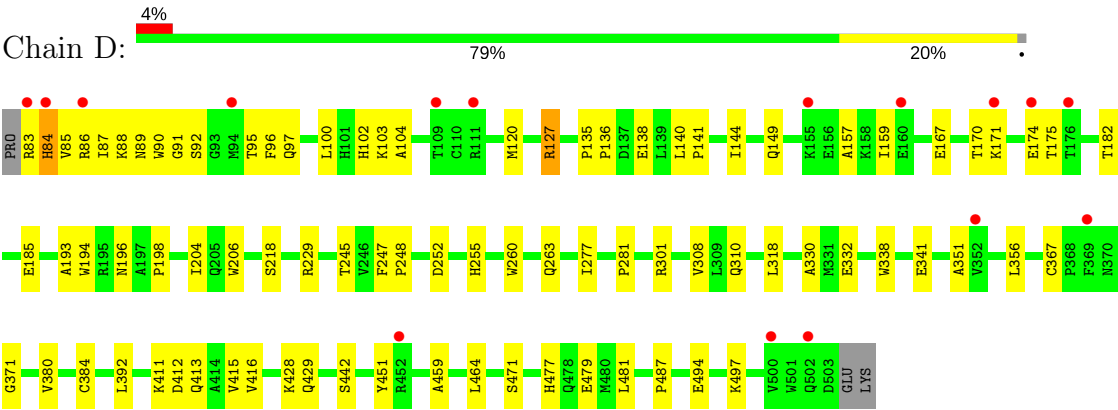
- Molecule 1: Nitric oxide synthase, inducible



- Molecule 1: Nitric oxide synthase, inducible



● Molecule 1: Nitric oxide synthase, inducible



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.21Å 158.67Å 191.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.51 – 2.20 39.50 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.2 (39.51-2.20) 84.8 (39.50-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.10Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.182 , 0.213 0.171 , 0.196	Depositor DCC
R_{free} test set	7159 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.367	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14516	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: HEM, ZN, AT2, H4B

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	0/3517	0.65	1/4774 (0.0%)
1	B	0.43	0/3517	0.64	1/4774 (0.0%)
1	C	0.45	0/3539	0.66	0/4801
1	D	0.45	0/3517	0.64	1/4774 (0.0%)
All	All	0.44	0/14090	0.65	3/19123 (0.0%)

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	D	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	374	MET	N-CA-C	-5.66	95.72	111.00
1	D	371	GLY	N-CA-C	-5.14	100.25	113.10
1	B	371	GLY	N-CA-C	-5.06	100.45	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	451	TYR	Sidechain

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	3418	0	3318	50	0
1	B	3418	0	3317	51	0
1	C	3440	0	3339	44	0
1	D	3418	0	3317	58	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
3	A	43	0	30	0	0
3	B	43	0	30	0	0
3	C	43	0	30	1	0
3	D	43	0	30	0	0
4	A	17	0	14	1	0
4	B	17	0	14	2	0
4	C	17	0	15	1	0
4	D	17	0	14	0	0
5	A	19	0	21	0	0
5	B	19	0	21	0	0
5	C	19	0	21	0	0
5	D	19	0	21	0	0
6	A	121	0	0	0	0
6	B	110	0	0	1	0
6	C	137	0	0	1	0
6	D	136	0	0	5	0
All	All	14516	0	13552	196	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 7.

The worst 5 of 196 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:D:260:TRP:HE1	1:D:310:GLN:HE21	1.07	1.00
1:D:260:TRP:HE1	1:D:310:GLN:NE2	1.65	0.93
1:A:192:GLN:HE22	1:A:195:ARG:HH11	1.22	0.86
1:C:505:LYS:HG2	1:C:505:LYS:O	1.79	0.82
1:C:505:LYS:CG	1:C:505:LYS:O	2.33	0.77

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	419/424 (99%)	402 (96%)	16 (4%)	1 (0%)	49	57
1	B	419/424 (99%)	398 (95%)	21 (5%)	0	100	100
1	C	421/424 (99%)	400 (95%)	21 (5%)	0	100	100
1	D	419/424 (99%)	401 (96%)	15 (4%)	3 (1%)	24	23
All	All	1678/1696 (99%)	1601 (95%)	73 (4%)	4 (0%)	49	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	84	HIS
1	D	104	ALA
1	D	157	ALA
1	A	157	ALA

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	A	365/370 (99%)	359 (98%)	6 (2%)	65	79
1	B	365/370 (99%)	361 (99%)	4 (1%)	76	87
1	C	368/370 (100%)	364 (99%)	4 (1%)	76	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	365/370 (99%)	362 (99%)	3 (1%)	83	91
All	All	1463/1480 (99%)	1446 (99%)	17 (1%)	74	85

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	413	GLN
1	B	481	LEU
1	C	136	PRO
1	B	259	VAL
1	D	120	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	288	GLN
1	C	97	GLN
1	D	429	GLN
1	B	413	GLN
1	B	477	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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
3	HEM	A	901	1	27,50,50	1.59	3 (11%)	17,82,82	1.61	4 (23%)
4	H4B	A	902	-	15,18,18	2.04	2 (13%)	11,26,26	1.97	5 (45%)
5	AT2	A	906	-	20,20,20	1.76	5 (25%)	26,26,26	1.57	4 (15%)
3	HEM	B	1901	1	27,50,50	1.38	4 (14%)	17,82,82	1.27	2 (11%)
4	H4B	B	1902	-	15,18,18	1.88	2 (13%)	11,26,26	2.03	5 (45%)
5	AT2	B	1906	-	20,20,20	1.77	5 (25%)	26,26,26	1.55	6 (23%)
3	HEM	C	2901	1	27,50,50	1.73	5 (18%)	17,82,82	1.45	4 (23%)
4	H4B	C	2902	-	15,18,18	1.64	2 (13%)	11,26,26	1.99	4 (36%)
5	AT2	C	2906	-	20,20,20	1.88	5 (25%)	26,26,26	1.43	5 (19%)
3	HEM	D	3901	1	27,50,50	1.38	3 (11%)	17,82,82	1.62	4 (23%)
4	H4B	D	3902	-	15,18,18	2.04	2 (13%)	11,26,26	2.15	5 (45%)
5	AT2	D	3906	-	20,20,20	1.84	5 (25%)	26,26,26	1.58	6 (23%)

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	HEM	A	901	1	-	0/6/54/54	0/0/8/8
4	H4B	A	902	-	1/1/3/5	0/8/17/17	0/2/2/2
5	AT2	A	906	-	-	0/11/21/21	0/2/2/2
3	HEM	B	1901	1	-	0/6/54/54	0/0/8/8
4	H4B	B	1902	-	-	0/8/17/17	0/2/2/2
5	AT2	B	1906	-	-	0/11/21/21	0/2/2/2
3	HEM	C	2901	1	-	0/6/54/54	0/0/8/8
4	H4B	C	2902	-	-	0/8/17/17	0/2/2/2
5	AT2	C	2906	-	-	0/11/21/21	0/2/2/2
3	HEM	D	3901	1	-	0/6/54/54	0/0/8/8
4	H4B	D	3902	-	1/1/3/5	0/8/17/17	0/2/2/2
5	AT2	D	3906	-	-	0/11/21/21	0/2/2/2

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902	H4B	C7-C6	-7.26	1.45	1.52
4	D	3902	H4B	C7-C6	-7.24	1.45	1.52
4	B	1902	H4B	C7-C6	-6.59	1.45	1.52
4	C	2902	H4B	C7-C6	-5.66	1.46	1.52
3	C	2901	HEM	C3B-C2B	-5.11	1.33	1.40

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2901	HEM	CBD-CAD-C3D	-3.62	105.57	112.47
3	A	901	HEM	CBD-CAD-C3D	-3.57	105.66	112.47
5	A	906	AT2	C3-C4-N5	-2.92	120.37	123.92
3	D	3901	HEM	C4A-C3A-C2A	-2.89	104.98	107.00
5	B	1906	AT2	C3-C4-N5	-2.88	120.42	123.92

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	D	3902	H4B	C6
4	A	902	H4B	C6

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	H4B	1	0
4	B	1902	H4B	2	0
3	C	2901	HEM	1	0
4	C	2902	H4B	1	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 [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, 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	421/424 (99%)	-0.21	9 (2%) 63 61	29, 46, 79, 95	0
1	B	421/424 (99%)	-0.17	12 (2%) 51 49	30, 48, 80, 101	0
1	C	423/424 (99%)	-0.35	9 (2%) 63 61	25, 43, 73, 92	0
1	D	421/424 (99%)	-0.15	16 (3%) 40 38	29, 45, 75, 93	0
All	All	1686/1696 (99%)	-0.22	46 (2%) 54 52	25, 45, 77, 101	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	111	ARG	4.4
1	C	155	LYS	4.1
1	B	155	LYS	4.0
1	C	504	GLU	3.9
1	B	156	GLU	3.7

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 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. 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	B-factors(\AA^2)	Q<0.9
4	H4B	D	3902	17/17	0.91	0.23	57,59,65,66	0
4	H4B	B	1902	17/17	0.92	0.19	58,59,65,65	0
4	H4B	C	2902	17/17	0.92	0.15	61,63,67,67	0
4	H4B	A	902	17/17	0.94	0.20	53,55,62,63	0
5	AT2	B	1906	19/19	0.97	0.16	27,30,37,37	0
3	HEM	D	3901	43/43	0.98	0.23	30,32,39,43	0
2	ZN	C	3002	1/1	0.98	0.07	73,73,73,73	0
5	AT2	D	3906	19/19	0.98	0.23	27,31,37,38	0
5	AT2	C	2906	19/19	0.98	0.17	24,27,34,34	0
5	AT2	A	906	19/19	0.98	0.19	27,29,31,31	0
3	HEM	A	901	43/43	0.98	0.19	29,31,34,39	0
3	HEM	B	1901	43/43	0.98	0.17	32,34,37,39	0
3	HEM	C	2901	43/43	0.99	0.15	25,29,34,38	0
2	ZN	A	3001	1/1	0.99	0.10	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.