wwPDB X-ray Structure Validation Summary Report (i)

Feb 28, 2014 – 12:18 PM GMT

PDB ID : 1RS9

Title : Bovine endothelial NOS heme domain with D-phenylalanine-D-nitroarginin eamide bound

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Deposited on : 2003-12-09

Resolution : 2.22 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html

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

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1   Overall quality at a glance ⓘ

The reported resolution of this entry is 2.22 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.
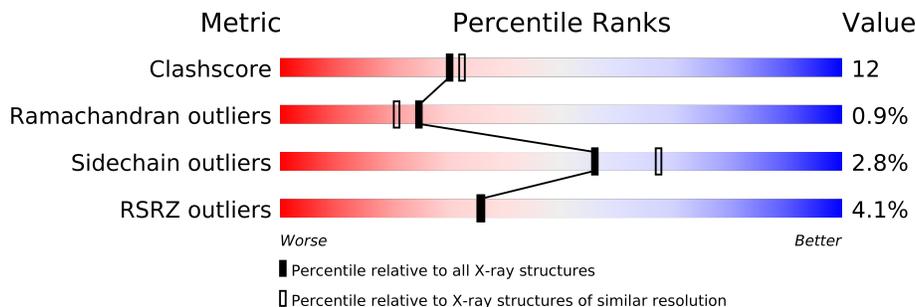
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	4208 (2.24-2.20)
Ramachandran outliers	78287	4135 (2.24-2.20)
Sidechain outliers	78261	4136 (2.24-2.20)
RSRZ outliers	66119	3341 (2.24-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	416	
1	B	416	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	ACT	B	861	-	X

2   Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 7008 atoms, of which 0 are hydrogen and 0 are deuterium.

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, endothelial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	406	Total 3227	C 2052	N 569	O 590	S 16	0	0	0
1	B	404	Total 3216	C 2045	N 567	O 588	S 16	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29473
B	100	ARG	CYS	SEE REMARK 999	UNP P29473

- Molecule 2 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).
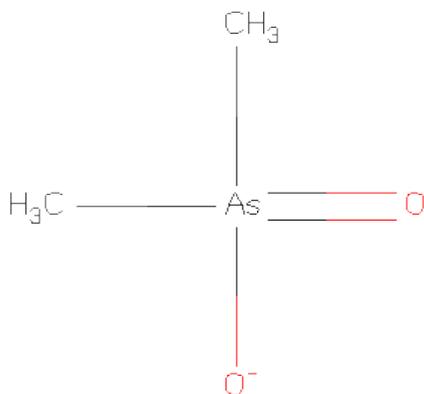
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 3	As 1	C 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 3	As 1	C 2	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
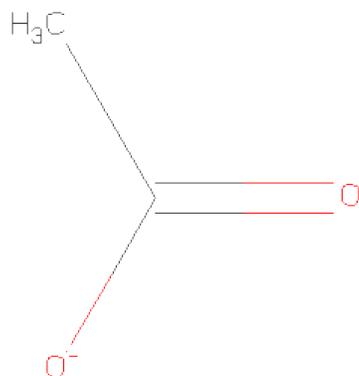
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Zn 1	0	0

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
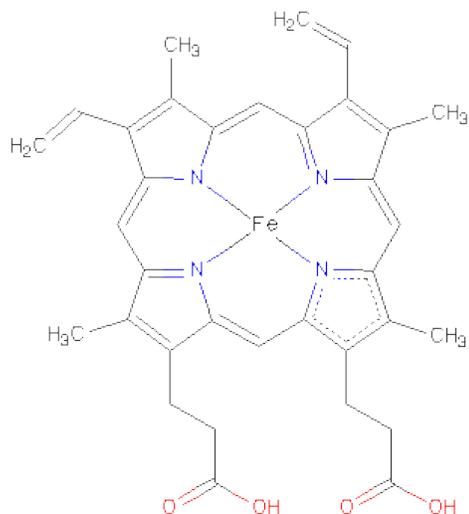
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).
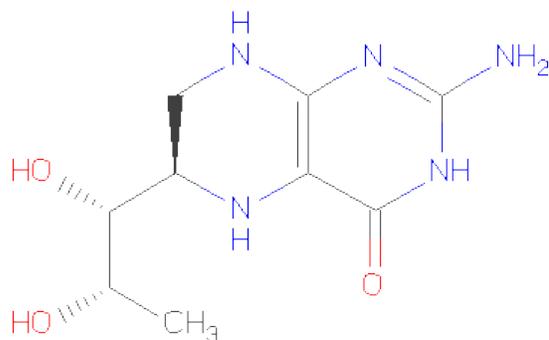
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			17	9	5	3		

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

- Molecule 7 is D-PHENYLALANYL-N 5 -[(2,2-DIHYDROXYHYDRAZINO)(IMINO)METHYL]-D-ORNITHINAMIDE (three-letter code: D7P) (formula: $C_{15}H_{25}N_7O_4$).
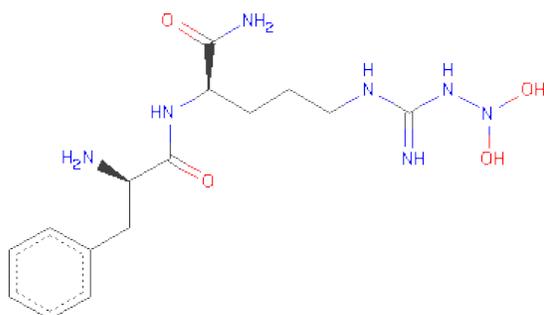
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 26	C 15	N 7	O 4	0	0
7	B	1	Total 26	C 15	N 7	O 4	0	0

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
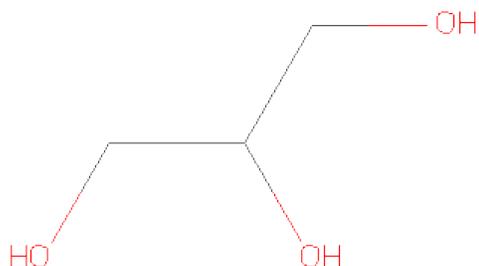
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 6	C 3	O 3	0	0
8	B	1	Total 6	C 3	O 3	0	0

• Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	182	Total 182	O 182	0	0
9	B	184	Total 184	O 184	0	0

3 Residue-property plots ⓘ

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: Nitric-oxide synthase, endothelial

Chain A:
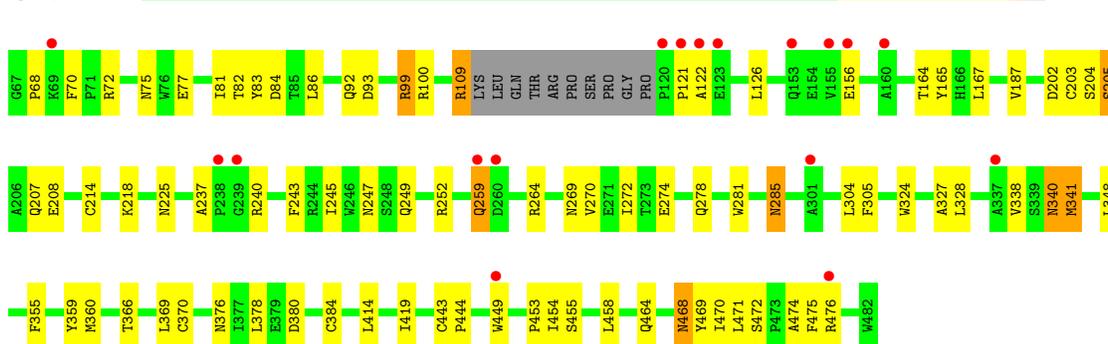
- Molecule 1: Nitric-oxide synthase, endothelial

Chain B:
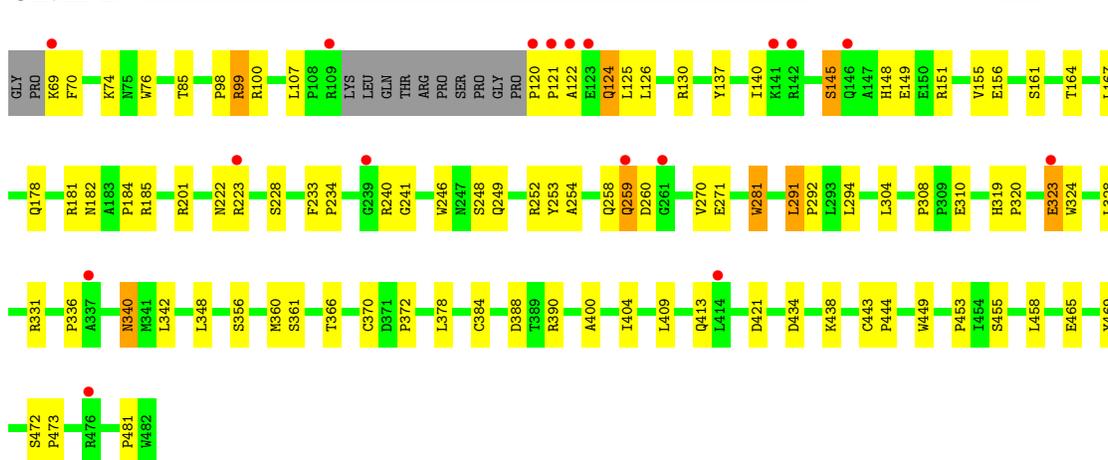
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.79Å 106.65Å 157.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.50 – 2.22 39.50 – 2.22	Depositor EDS
% Data completeness (in resolution range)	98.3 (39.50-2.22) 88.4 (39.50-2.22)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	4.19 (at 2.22Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.264 0.207 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	38.9	Xtriage
Anisotropy	0.963	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Outliers	2 of 49041 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7008	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, H4B, D7P, ACT, CAC, HEM

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	0.40	0/3318	0.65	2/4520 (0.0%)
1	B	0.39	0/3306	0.64	1/4503 (0.0%)
All	All	0.39	0/6624	0.64	3/9023 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	360	MET	N-CA-C	-5.88	95.14	111.00
1	B	360	MET	N-CA-C	-5.40	96.43	111.00
1	A	243	PHE	N-CA-C	-5.31	96.65	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3227	0	3135	74	0
1	B	3216	0	3125	80	0
2	A	3	0	0	3	0
2	B	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	4	0	3	1	0
3	B	4	0	3	0	0
4	B	1	0	0	0	0
5	A	43	0	30	2	0
5	B	43	0	30	2	0
6	A	17	0	15	1	0
6	B	17	0	15	1	0
7	A	26	0	24	1	0
7	B	26	0	24	0	0
8	A	6	0	8	2	0
8	B	6	0	8	0	0
9	A	182	0	0	10	0
9	B	184	0	0	12	0
All	All	7008	0	6420	157	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

The worst 5 of 157 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:109:ARG:HH11	1:A:109:ARG:HA	1.01	1.14
1:A:99:ARG:HH11	1:A:99:ARG:HB2	1.23	0.97
1:B:281:TRP:HB2	1:B:304:LEU:HD11	1.48	0.94
1:A:109:ARG:HA	1:A:109:ARG:NH1	1.82	0.93
1:A:249:GLN:HE21	1:A:252:ARG:HE	1.12	0.92

There are no symmetry-related clashes.

5.3 Torsion angles

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	402/416 (97%)	380 (94%)	20 (5%)	2 (0%)	38	38
1	B	400/416 (96%)	375 (94%)	20 (5%)	5 (1%)	18	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	802/832 (96%)	755 (94%)	40 (5%)	7 (1%)	25	21

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	GLN
1	B	281	TRP
1	A	205	SER
1	B	124	GLN
1	B	145	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	345/354 (98%)	333 (96%)	12 (4%)	48	57
1	B	344/354 (97%)	337 (98%)	7 (2%)	68	79
All	All	689/708 (97%)	670 (97%)	19 (3%)	56	67

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	340	ASN
1	A	376	ASN
1	B	222	ASN
1	A	328	LEU
1	B	291	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	376	ASN
1	A	464	GLN
1	B	340	ASN
1	A	413	GLN
1	A	468	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 1 is 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	#$|Z| > 2$
5	HEM	A	500	1	49,50,50	2.85	13 (26%)	46,82,82	1.60	9 (19%)
6	H4B	A	760	-	18,18,18	1.58	4 (22%)	24,26,26	2.50	10 (41%)
7	D7P	A	797	-	23,26,26	1.71	3 (13%)	29,33,33	1.22	4 (13%)
2	CAC	A	850	-	2,2,4	0.44	0	0,1,6	0.00	-
3	ACT	A	860	-	1,3,3	3.41	1 (100%)	0,3,3	0.00	-
8	GOL	A	880	-	5,5,5	0.17	0	5,5,5	0.28	0
5	HEM	B	500	1	49,50,50	2.05	14 (28%)	46,82,82	1.56	8 (17%)
6	H4B	B	761	-	18,18,18	1.44	4 (22%)	24,26,26	2.50	10 (41%)
7	D7P	B	798	-	23,26,26	1.54	4 (17%)	29,33,33	1.33	3 (10%)
2	CAC	B	852	-	2,2,4	0.45	0	0,1,6	0.00	-
3	ACT	B	861	-	1,3,3	3.42	1 (100%)	0,3,3	0.00	-
8	GOL	B	882	-	5,5,5	0.20	0	5,5,5	0.32	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
5	HEM	A	500	1	-	0/14/114/114	0/0/8/8
6	H4B	A	760	-	-	0/8/17/17	0/0/2/2
7	D7P	A	797	-	-	0/23/27/27	0/1/1/1
2	CAC	A	850	-	-	0/0/0/0	0/0/0/0
3	ACT	A	860	-	-	0/0/0/0	0/0/0/0
8	GOL	A	880	-	-	0/4/4/4	0/0/0/0
5	HEM	B	500	1	-	0/14/114/114	0/0/8/8
6	H4B	B	761	-	-	0/8/17/17	0/0/2/2
7	D7P	B	798	-	-	0/23/27/27	0/1/1/1
2	CAC	B	852	-	-	0/0/0/0	0/0/0/0
3	ACT	B	861	-	-	0/0/0/0	0/0/0/0
8	GOL	B	882	-	-	0/4/4/4	0/0/0/0

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	500	HEM	C2D-C1D	11.42	1.47	1.44
5	A	500	HEM	C3D-C4D	8.75	1.46	1.44
5	A	500	HEM	C3D-C2D	-5.91	1.33	1.43
5	A	500	HEM	C3B-C2B	-5.32	1.34	1.43
5	B	500	HEM	C2B-C1B	-5.27	1.43	1.44

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	760	H4B	C4-C4A-C8A	8.42	122.36	114.56
6	B	761	H4B	C4-C4A-C8A	8.21	122.16	114.56
5	B	500	HEM	C3B-C4B-NB	-4.34	110.90	114.00
5	A	500	HEM	C3A-C4A-NA	4.32	112.67	109.41
7	B	798	D7P	CD-NE-CZ	4.19	131.39	124.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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(Å²)	Q<0.9
1	A	406/416 (97%)	0.20	17 (4%)	35	35	30, 49, 71, 91	0
1	B	404/416 (97%)	0.14	17 (4%)	35	35	31, 51, 72, 92	0
All	All	810/832 (97%)	0.17	34 (4%)	35	35	30, 51, 72, 92	0

The worst 5 of 34 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	PRO	7.7
1	B	122	ALA	6.2
1	A	122	ALA	5.1
1	A	239	GLY	4.8
1	A	121	PRO	4.6

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ACT	B	861	4/4	0.14	2.51	62,63,63,64	0
8	GOL	B	882	6/6	0.20	1.49	43,49,50,51	0
6	H4B	B	761	17/17	0.22	1.37	29,33,35,38	0
6	H4B	A	760	17/17	0.21	1.08	34,35,37,38	0
3	ACT	A	860	4/4	0.13	1.04	60,60,60,60	0
7	D7P	A	797	26/26	0.20	0.83	35,39,42,44	0
7	D7P	B	798	26/26	0.21	0.70	31,37,44,47	0
5	HEM	B	500	43/43	0.17	0.68	29,32,35,38	0
5	HEM	A	500	43/43	0.18	0.62	30,32,39,42	0
8	GOL	A	880	6/6	0.18	0.58	42,45,45,45	0
2	CAC	A	850	3/5	0.12	0.21	85,85,87,88	0
2	CAC	B	852	3/5	0.14	-1.05	112,112,112,112	0
4	ZN	B	900	1/1	0.09	-1.10	40,40,40,40	0

6.5   Other polymers ⓘ

There are no such residues in this entry.