



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2014 – 08:56 PM EDT

PDB ID : 4CWZ
Title : Structure of bovine endothelial nitric oxide synthase Y477A mutant heme domain in complex with 4-METHYL-6-(((3R,4R)-4-((5-(4-METHYLPYRIDIN-2-YL)PENTYL)OXY)PYRROLIDIN-3-YL)METHYL)PYRIDIN-2-AMINE
Authors : Li, H.; Poulos, T.L.
Deposited on : 2014-04-03
Resolution : 2.08 Å(reported)

This is a full wwPDB validation 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>

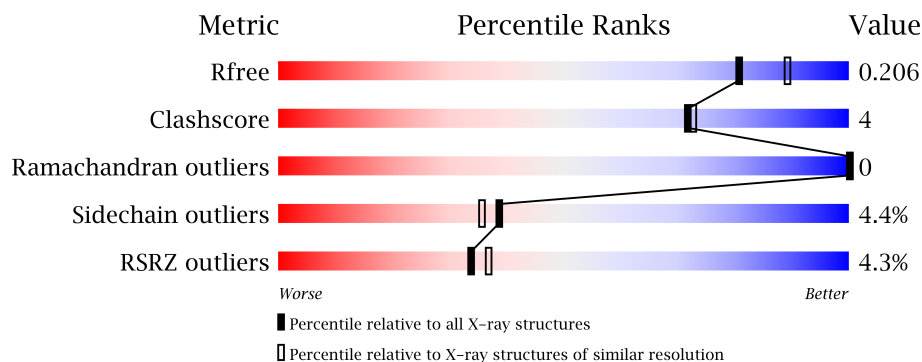
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
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) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 2.08 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}	66092	3396 (2.10-2.06)
Clashscore	79885	4085 (2.10-2.06)
Ramachandran outliers	78287	4045 (2.10-2.06)
Sidechain outliers	78261	4046 (2.10-2.06)
RSRZ outliers	66119	3397 (2.10-2.06)

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	443	
1	B	443	

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

Mol	Type	Chain	Res	Geometry	Electron density
5	ACT	A	860	-	X
5	ACT	B	860	-	X

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 7181 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.

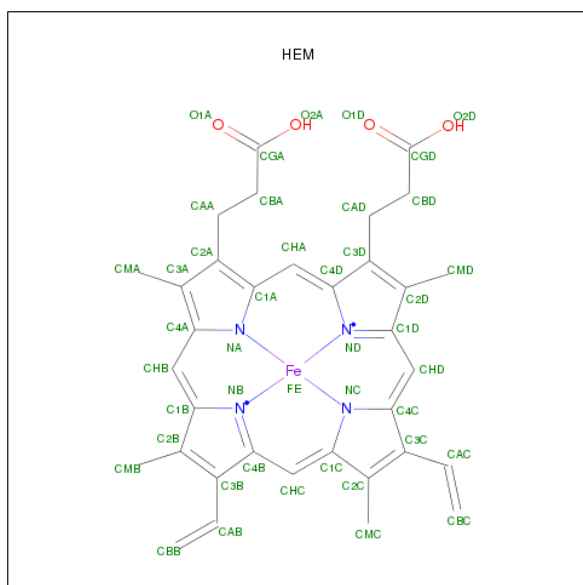
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE, ENDOTHELIAL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	As	C	N	O	S	0	2	0
			3226	1	2051	568	590	16			
1	B	404	Total	As	C	N	O	S	0	2	0
			3227	1	2052	571	587	16			

There are 4 discrepancies between the modelled and reference sequences:

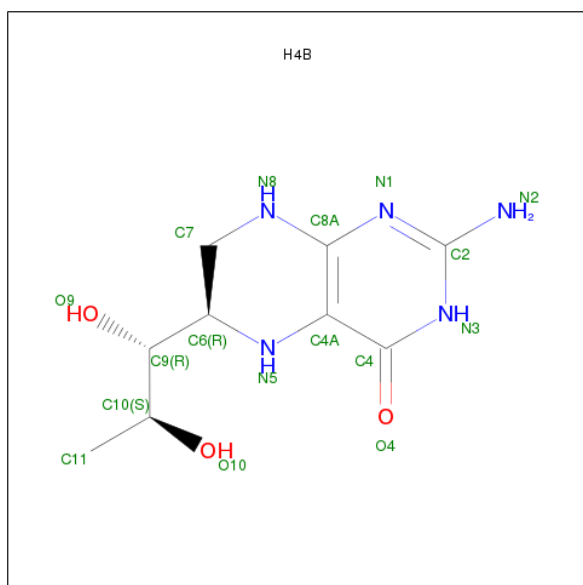
Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	SEE REMARK 999	UNP P29473
A	477	ALA	TYR	ENGINEERED MUTATION	UNP P29473
B	100	ARG	CYS	SEE REMARK 999	UNP P29473
B	477	ALA	TYR	ENGINEERED MUTATION	UNP P29473

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



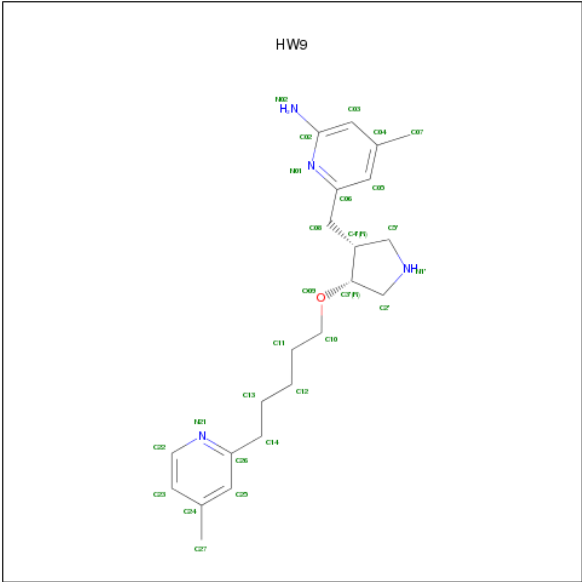
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula: $C_9H_{15}N_5O_3$).



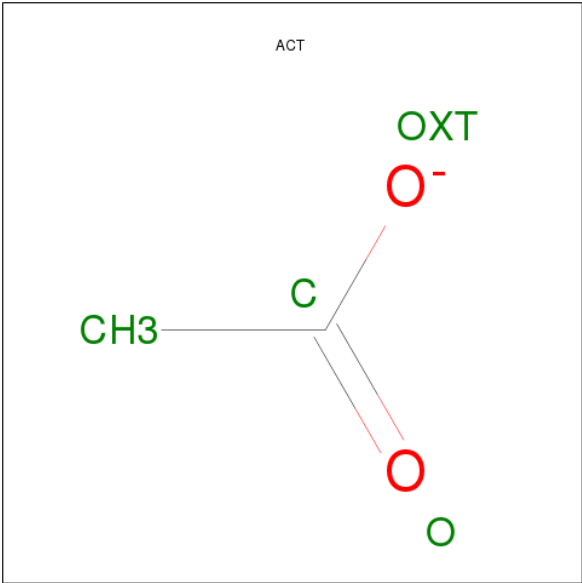
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is 4-METHYL-6-{[(3R,4R)-4-{[5-(4-METHYLPYRIDIN-2-YL)PENTYL]OXY}PYRROLIDIN-3-YL]METHYL}PYRIDIN-2-AMINE (three-letter code: HW9) (formula: $C_{22}H_{32}N_4O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			27	22	4	1		
4	B	1	Total	C	N	O	0	0
			27	22	4	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Zn	0	0
			1	1		

- Molecule 7 is water.

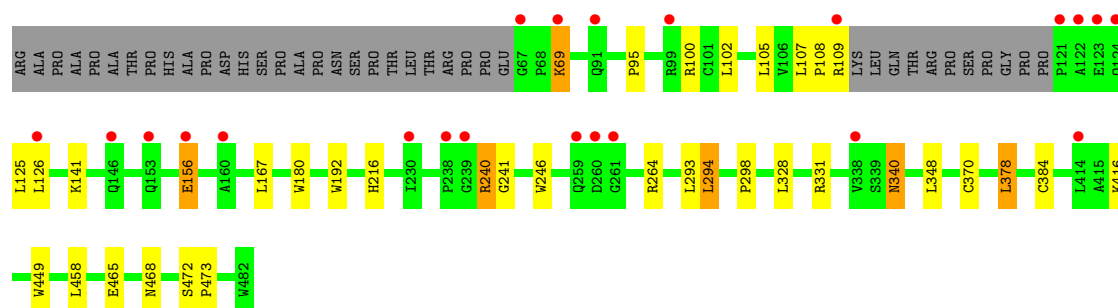
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	288	Total	O	0	0
			288	288		
7	B	249	Total	O	0	0
			249	249		

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.

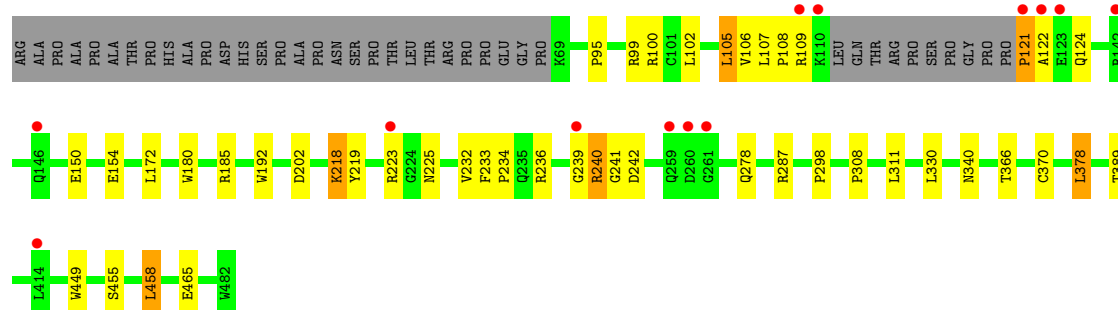
- Molecule 1: NITRIC OXIDE SYNTHASE, ENDOTHELIAL

Chain A: 



- Molecule 1: NITRIC OXIDE SYNTHASE, ENDOTHELIAL

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.82Å 106.41Å 156.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.66 – 2.08 42.63 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.66-2.08) 99.7 (42.63-2.08)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.154 , 0.197 0.165 , 0.206	Depositor DCC
R_{free} test set	2949 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 59003 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7181	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 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: ZN, H4B, CAS, HW9, ACT, 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	0.59	0/3311	0.75	3/4509 (0.1%)
1	B	0.71	2/3311 (0.1%)	0.77	4/4506 (0.1%)
All	All	0.65	2/6622 (0.0%)	0.76	7/9015 (0.1%)

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	121	PRO	C-N	21.57	1.83	1.34
1	B	106	VAL	C-N	5.48	1.46	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	B	240	ARG	NE-CZ-NH1	9.15	124.87	120.30
1	B	106	VAL	O-C-N	-7.29	111.04	122.70
1	A	331	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	B	185	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	A	331	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	240	ARG	NE-CZ-NH1	5.31	122.95	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	239	GLY	Peptide

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	3226	0	3138	27	0
1	B	3227	0	3149	26	0
2	A	43	0	30	1	0
2	B	43	0	30	5	0
3	A	17	0	15	1	0
3	B	17	0	15	2	0
4	A	27	0	32	3	0
4	B	27	0	32	4	0
5	A	8	0	6	0	0
5	B	8	0	6	0	0
6	A	1	0	0	0	0
7	A	288	0	0	3	0
7	B	249	0	0	1	0
All	All	7181	0	6453	57	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 4.

All (57) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:384:CAS:AS	1:A:384:CAS:SG	2.45	1.34
1:B:121:PRO:C	1:B:122:ALA:N	1.83	1.31
1:B:287[B]:ARG:HG3	1:B:287[B]:ARG:HH11	1.09	1.11
1:B:287[B]:ARG:NH1	1:B:287[B]:ARG:HG3	1.88	0.86
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.71	0.73
1:A:264:ARG:HD3	7:A:2164:HOH:O	1.95	0.67
1:A:384:CAS:CB	1:A:384:CAS:AS	3.06	0.63
1:B:236:ARG:HD2	1:B:242:ASP:OD1	2.00	0.62
1:A:240:ARG:NH2	7:A:2140:HOH:O	2.32	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:107[B]:LEU:HD11	4:B:800:HW9:H5	1.83	0.60
1:A:107[A]:LEU:HD11	4:A:800:HW9:H5	1.82	0.59
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.43	0.59
2:B:500:HEM:HBB2	2:B:500:HEM:HHC	1.89	0.55
1:B:287[B]:ARG:CG	1:B:287[B]:ARG:HH11	1.95	0.55
1:A:126:LEU:HD11	1:A:156:GLU:HA	1.89	0.54
1:B:240:ARG:HD2	1:B:241:GLY:O	2.10	0.52
1:A:378:LEU:HB2	7:A:2219:HOH:O	2.11	0.51
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.39	0.50
1:A:107[A]:LEU:HD11	4:A:800:HW9:C07	2.42	0.50
1:B:449:TRP:HA	3:B:600:H4B:N1	2.27	0.49
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.53	0.49
1:B:150:GLU:O	1:B:154:GLU:HG3	2.13	0.49
1:B:240:ARG:HD3	1:B:298:PRO:HB3	1.95	0.49
2:B:500:HEM:C1C	4:B:800:HW9:H33	2.47	0.49
1:A:449:TRP:HA	3:A:600:H4B:N1	2.29	0.48
2:A:500:HEM:HBB2	2:A:500:HEM:HHC	1.94	0.47
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.44	0.47
1:B:218:LYS:HD3	1:B:219:TYR:N	2.30	0.47
1:B:236:ARG:CD	1:B:242:ASP:OD1	2.63	0.46
1:A:95:PRO:HB3	1:A:108:PRO:HB2	1.98	0.46
1:B:287[B]:ARG:CG	1:B:287[B]:ARG:NH1	2.63	0.45
1:B:172:LEU:HD11	1:B:232:VAL:HG11	1.99	0.44
1:A:105:LEU:HD22	1:B:465:GLU:HB3	1.98	0.44
1:B:455:SER:HB3	1:B:458:LEU:HD22	1.98	0.44
2:B:500:HEM:CMC	2:B:500:HEM:HBC2	2.47	0.44
1:B:107[B]:LEU:HD11	4:B:800:HW9:C07	2.49	0.43
2:B:500:HEM:HMC1	2:B:500:HEM:HBC2	2.00	0.43
1:A:246:TRP:HB2	1:A:294:LEU:HB3	2.00	0.43
1:B:95:PRO:HG3	1:B:108:PRO:HG2	2.00	0.43
1:A:69:LYS:HE2	1:A:69:LYS:HA	2.00	0.43
1:A:240:ARG:HD2	1:A:241:GLY:O	2.19	0.42
1:A:472:SER:HA	1:A:473:PRO:C	2.39	0.42
1:B:107[B]:LEU:HD21	4:B:800:HW9:C04	2.50	0.42
1:A:141:LYS:HD3	1:A:141:LYS:HA	1.92	0.42
1:A:340:ASN:HD22	1:A:340:ASN:H	1.69	0.41
1:B:378:LEU:HB2	7:B:2195:HOH:O	2.20	0.41
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.56	0.41
1:B:366:THR:O	1:B:370:CYS:HB2	2.20	0.41
2:B:500:HEM:O1A	3:B:600:H4B:N3	2.49	0.41
1:A:384:CAS:HB2	1:A:384:CAS:AS	2.80	0.41
1:B:308:PRO:HD2	1:B:311:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:465:GLU:HB3	1:B:105:LEU:HD22	2.03	0.41
1:A:107[A]:LEU:HD21	4:A:800:HW9:C07	2.51	0.41
1:A:180:TRP:CE3	1:A:192:TRP:HA	2.56	0.41
1:A:240:ARG:CD	1:A:241:GLY:O	2.69	0.40
1:A:167:LEU:HG	1:A:348:LEU:HD12	2.01	0.40
1:A:216:HIS:C	1:A:216:HIS:CD2	2.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	402/443 (91%)	393 (98%)	9 (2%)	0	100	100
1	B	401/443 (90%)	389 (97%)	12 (3%)	0	100	100
All	All	803/886 (91%)	782 (97%)	21 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	344/374 (92%)	330 (96%)	14 (4%)	41	40
1	B	344/374 (92%)	328 (95%)	16 (5%)	36	32
All	All	688/748 (92%)	658 (96%)	30 (4%)	39	36

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	100	ARG
1	A	102	LEU
1	A	109	ARG
1	A	125	LEU
1	A	156	GLU
1	A	293	LEU
1	A	294	LEU
1	A	328	LEU
1	A	340	ASN
1	A	378	LEU
1	A	416	LYS
1	A	458	LEU
1	A	468	ASN
1	B	99	ARG
1	B	100	ARG
1	B	102	LEU
1	B	105	LEU
1	B	109	ARG
1	B	124	GLN
1	B	202	ASP
1	B	218	LYS
1	B	223	ARG
1	B	225	ASN
1	B	278	GLN
1	B	330	LEU
1	B	340	ASN
1	B	378	LEU
1	B	389	THR
1	B	458	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	191	GLN
1	A	340	ASN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
1	B	178	GLN

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Mol	Chain	Res	Type
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	340	ASN
1	B	376	ASN
1	B	405	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
1	CAS	A	384	1	8,8,9	11.67	3 (37%)	7,9,11	5.82	3 (42%)
1	CAS	B	384	1	8,8,9	11.25	4 (50%)	7,9,11	4.11	4 (57%)

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
1	CAS	A	384	1	-	0/2/7/9	0/0/0/0
1	CAS	B	384	1	-	0/2/7/9	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	CAS	AS-SG	30.24	2.45	2.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	384	CAS	AS-SG	27.11	2.43	2.26
1	B	384	CAS	O-C	16.23	1.22	1.11
1	A	384	CAS	O-C	12.70	1.20	1.11
1	A	384	CAS	CA-C	2.83	1.55	1.49
1	B	384	CAS	CA-C	2.11	1.53	1.49
1	B	384	CAS	AS-CE1	2.09	2.01	1.96

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	CAS	CE2-AS-CE1	13.15	117.27	96.77
1	B	384	CAS	CE2-AS-CE1	8.84	110.56	96.77
1	A	384	CAS	AS-SG-CB	-7.11	90.38	102.24
1	B	384	CAS	AS-SG-CB	-4.80	94.25	102.24
1	A	384	CAS	C-CA-N	-3.23	110.60	113.83
1	B	384	CAS	C-CA-N	-2.84	110.99	113.83
1	B	384	CAS	CE2-AS-SG	-2.79	86.03	96.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\# Z > 2$
2	HEM	A	500	1	42,50,50	2.57	11 (26%)	27,82,82	1.47	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	H4B	A	600	-	18,18,18	0.91	0	24,26,26	1.80	6 (25%)
4	HW9	A	800	-	29,29,29	0.59	0	38,38,38	1.53	8 (21%)
5	ACT	A	860	-	1,3,3	0.73	0	0,3,3	0.00	-
5	ACT	A	861	-	1,3,3	0.96	0	0,3,3	0.00	-
2	HEM	B	500	1	42,50,50	2.66	12 (28%)	27,82,82	1.53	4 (14%)
3	H4B	B	600	-	18,18,18	1.00	2 (11%)	24,26,26	1.71	5 (20%)
4	HW9	B	800	-	29,29,29	0.52	0	38,38,38	1.62	11 (28%)
5	ACT	B	860	-	1,3,3	1.62	0	0,3,3	0.00	-
5	ACT	B	861	-	1,3,3	1.91	0	0,3,3	0.00	-

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
2	HEM	A	500	1	-	0/14/114/114	0/0/8/8
3	H4B	A	600	-	-	0/8/17/17	0/2/2/2
4	HW9	A	800	-	-	0/13/23/23	0/3/3/3
5	ACT	A	860	-	-	0/0/0/0	0/0/0/0
5	ACT	A	861	-	-	0/0/0/0	0/0/0/0
2	HEM	B	500	1	-	0/14/114/114	0/0/8/8
3	H4B	B	600	-	-	0/8/17/17	0/2/2/2
4	HW9	B	800	-	-	0/13/23/23	0/3/3/3
5	ACT	B	860	-	-	0/0/0/0	0/0/0/0
5	ACT	B	861	-	-	0/0/0/0	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3B-C2B	-10.22	1.35	1.45
2	A	500	HEM	C3B-C2B	-10.05	1.35	1.45
2	B	500	HEM	C3C-C2C	-7.18	1.39	1.45
2	A	500	HEM	C3C-C2C	-5.96	1.40	1.45
2	A	500	HEM	CMC-C2C	4.42	1.52	1.45
2	B	500	HEM	CMB-C2B	4.16	1.52	1.45
2	A	500	HEM	C3D-C2D	-4.15	1.32	1.43
2	A	500	HEM	CMD-C2D	4.12	1.52	1.45
2	B	500	HEM	CMD-C2D	3.85	1.51	1.45
2	B	500	HEM	FE-NB	3.68	2.08	1.95
2	A	500	HEM	CMB-C2B	3.64	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	CMC-C2C	3.64	1.51	1.45
2	B	500	HEM	C3D-C2D	-3.60	1.34	1.43
2	A	500	HEM	FE-NB	3.35	2.07	1.95
2	B	500	HEM	C3C-C4C	-2.91	1.43	1.45
2	B	500	HEM	C3B-CAB	2.81	1.49	1.40
2	B	500	HEM	FE-NC	2.68	2.06	1.95
2	A	500	HEM	C4A-NA	2.52	1.40	1.36
2	B	500	HEM	C1B-C2B	-2.44	1.43	1.45
2	B	500	HEM	C3C-CAC	2.36	1.48	1.40
2	A	500	HEM	FE-NC	2.25	2.04	1.95
2	A	500	HEM	C3B-CAB	2.23	1.47	1.40
2	A	500	HEM	C1B-C2B	-2.21	1.43	1.45
3	B	600	H4B	C4-C4A	-2.18	1.38	1.41
3	B	600	H4B	C2-N2	2.07	1.35	1.32

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	H4B	C4-C4A-C8A	5.22	119.29	114.56
3	B	600	H4B	C4-C4A-C8A	4.61	118.74	114.56
2	B	500	HEM	CBA-CAA-C2A	-3.87	106.18	112.63
4	B	800	HW9	C02-N01-C06	3.43	120.65	118.24
3	B	600	H4B	N2-C2-N3	3.31	121.37	117.82
4	B	800	HW9	C22-N21-C26	3.16	121.80	117.37
4	B	800	HW9	C25-C26-N21	-3.09	119.31	122.88
2	B	500	HEM	CAD-C3D-C4D	3.06	129.91	125.60
4	A	800	HW9	C14-C26-C25	-3.03	116.94	121.15
2	A	500	HEM	CAD-C3D-C4D	2.99	129.82	125.60
3	A	600	H4B	N2-C2-N3	2.97	121.00	117.82
3	A	600	H4B	C4A-C8A-N8	2.95	121.90	118.43
4	A	800	HW9	C23-C22-N21	-2.91	120.66	123.88
3	A	600	H4B	C4-N3-C2	2.87	121.82	120.20
4	A	800	HW9	C5'-N1'-C2'	2.84	113.08	105.92
2	A	500	HEM	CBA-CAA-C2A	-2.78	108.00	112.63
3	B	600	H4B	N2-C2-N1	-2.75	116.73	120.29
4	B	800	HW9	C08-C4'-C3'	2.74	117.72	113.62
4	B	800	HW9	C3'-C2'-N1'	-2.68	100.54	105.46
4	B	800	HW9	C5'-N1'-C2'	2.66	112.62	105.92
4	B	800	HW9	C23-C22-N21	-2.61	120.99	123.88
3	A	600	H4B	C4-C4A-N5	2.61	122.80	119.07
2	A	500	HEM	C4A-NA-C1A	-2.58	104.72	107.93
4	B	800	HW9	C2'-C3'-C4'	-2.54	101.50	103.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	HW9	N02-C02-N01	2.53	121.33	116.61
2	B	500	HEM	C4A-C3A-C2A	2.44	108.70	107.00
4	B	800	HW9	N02-C02-N01	2.44	121.16	116.61
4	A	800	HW9	C02-N01-C06	2.37	119.91	118.24
3	B	600	H4B	N8-C8A-N1	2.36	119.27	115.82
4	A	800	HW9	C14-C26-N21	2.32	122.12	116.92
2	A	500	HEM	O2A-CGA-O1A	-2.32	117.45	123.31
4	A	800	HW9	C06-C08-C4'	-2.31	106.80	115.31
4	B	800	HW9	C05-C06-N01	-2.27	120.43	122.96
3	B	600	H4B	C4-N3-C2	-2.26	118.93	120.20
3	A	600	H4B	C6-C7-N8	-2.25	108.62	111.56
4	A	800	HW9	C3'-C2'-N1'	-2.19	101.44	105.46
4	B	800	HW9	C06-C08-C4'	-2.06	107.72	115.31
2	B	500	HEM	O2D-CGD-CBD	2.05	121.29	114.19

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(Å ²)	Q<0.9
1	A	405/443 (91%)	0.08	22 (5%) 25 27	24, 35, 61, 99	0
1	B	404/443 (91%)	0.02	13 (3%) 45 50	24, 37, 64, 101	0
All	All	809/886 (91%)	0.05	35 (4%) 34 37	24, 35, 63, 101	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	GLN	5.7
1	A	259	GLN	5.3
1	B	110	LYS	4.6
1	A	67	GLY	4.6
1	A	123	GLU	3.9
1	A	160	ALA	3.9
1	A	122	ALA	3.8
1	A	69	LYS	3.5
1	A	239	GLY	3.4
1	B	142	ARG	3.3
1	A	121	PRO	3.3
1	A	238	PRO	3.3
1	B	261	GLY	3.2
1	B	123	GLU	3.2
1	A	126	LEU	3.0
1	A	124	GLN	3.0
1	A	261	GLY	2.8
1	B	239	GLY	2.8
1	B	121	PRO	2.8
1	A	109	ARG	2.8
1	B	260	ASP	2.7
1	A	99	ARG	2.5
1	B	109	ARG	2.5
1	B	122	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	260	ASP	2.4
1	A	338	VAL	2.4
1	A	156	GLU	2.4
1	A	153	GLN	2.4
1	B	414	LEU	2.3
1	A	414	LEU	2.2
1	B	223	ARG	2.1
1	B	146	GLN	2.1
1	A	230	ILE	2.1
1	A	146	GLN	2.0
1	A	91	GLN	2.0

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

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.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CAS	A	384	9/10	0.08	-0.47	33,34,54,57	0
1	CAS	B	384	9/10	0.07	-1.08	44,45,51,52	0

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.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	ACT	B	860	4/4	0.26	15.22	43,44,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	ACT	A	860	4/4	0.13	2.20	38,41,43,46	0
5	ACT	A	861	4/4	0.17	1.61	30,33,33,34	0
4	HW9	B	800	27/27	0.21	1.46	26,39,57,60	0
4	HW9	A	800	27/27	0.21	1.19	26,41,55,61	0
3	H4B	A	600	17/17	0.16	0.91	26,28,32,33	0
2	HEM	A	500	43/43	0.17	0.78	25,27,34,36	0
2	HEM	B	500	43/43	0.14	0.54	26,28,36,39	0
3	H4B	B	600	17/17	0.14	0.52	25,27,30,30	0
5	ACT	B	861	4/4	0.13	-0.13	34,37,38,38	0
6	ZN	A	900	1/1	0.06	-1.97	29,29,29,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.