



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2014 – 03:57 PM EDT

PDB ID : 4CX1
Title : Structure of bovine endothelial nitric oxide synthase L111A 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 : 2.13 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>

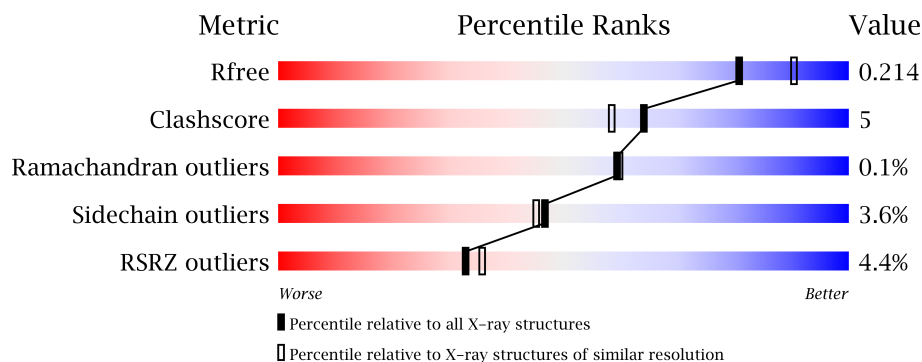
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.13 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	1116 (2.16-2.12)
Clashscore	79885	1302 (2.16-2.12)
Ramachandran outliers	78287	1281 (2.16-2.12)
Sidechain outliers	78261	1281 (2.16-2.12)
RSRZ outliers	66119	1116 (2.16-2.12)

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	B	860	-	X

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 6997 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.

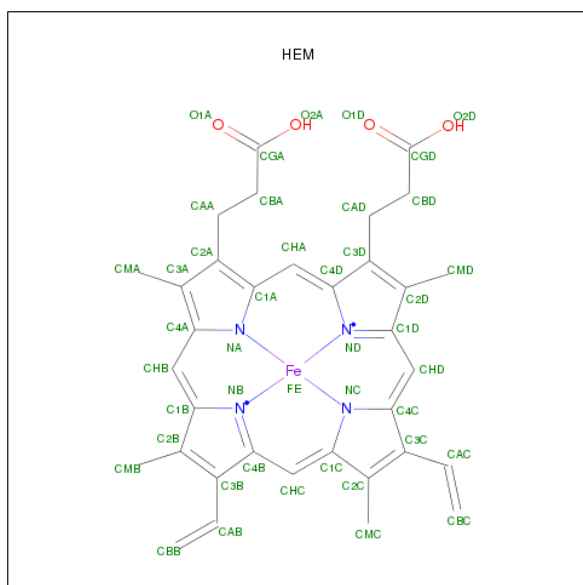
- Molecule 1 is a protein called NITRIC OXIDE SYNTHASE, ENDOTHELIAL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	As	C	N	O	S	0	0	0
			3223	1	2049	568	589	16			
1	B	404	Total	As	C	N	O	S	0	0	0
			3221	1	2048	568	588	16			

There are 4 discrepancies between the modelled and reference sequences:

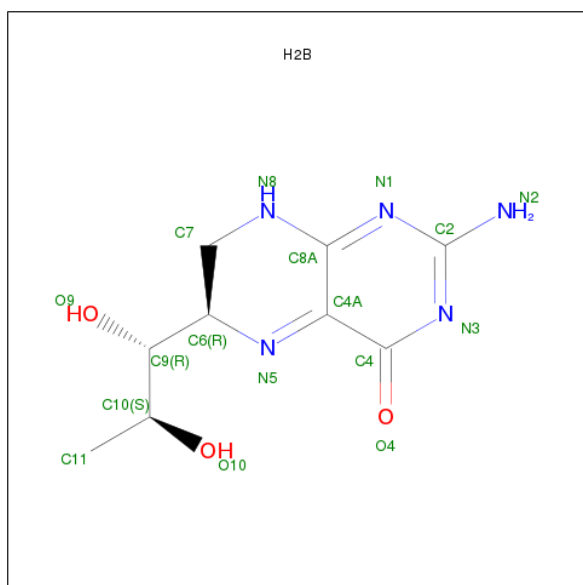
Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	CONFLICT	UNP P29473
A	111	ALA	LEU	ENGINEERED MUTATION	UNP P29473
B	100	ARG	CYS	CONFLICT	UNP P29473
B	111	ALA	LEU	ENGINEERED MUTATION	UNP P29473

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



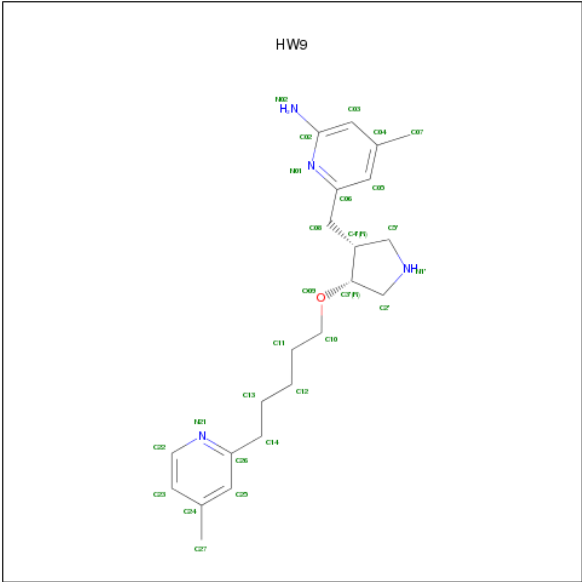
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is 2-AMINO-6-(1,2-DIHYDROXY-PROPYL)-7,8-DIHYDRO-6H-PTERIDIN-4-ONE (three-letter code: H2B) (formula: C₉H₁₃N₅O₃).



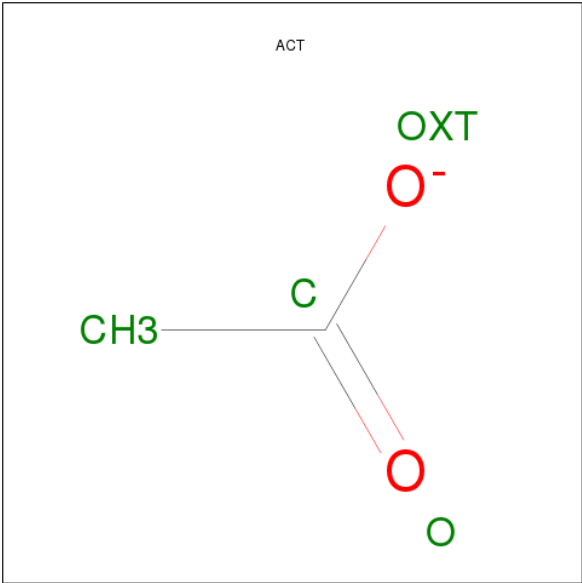
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- 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: C₂₂H₃₂N₄O).



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		

Continued on next page...

Continued from previous page...

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	B	1	Total	Zn	0	0
			1	1		

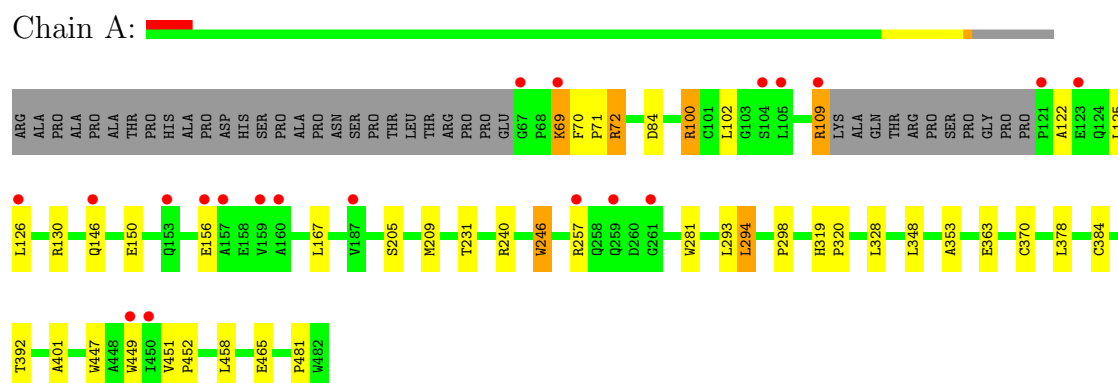
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	209	Total	O	0	0
			209	209		
7	B	153	Total	O	0	0
			153	153		

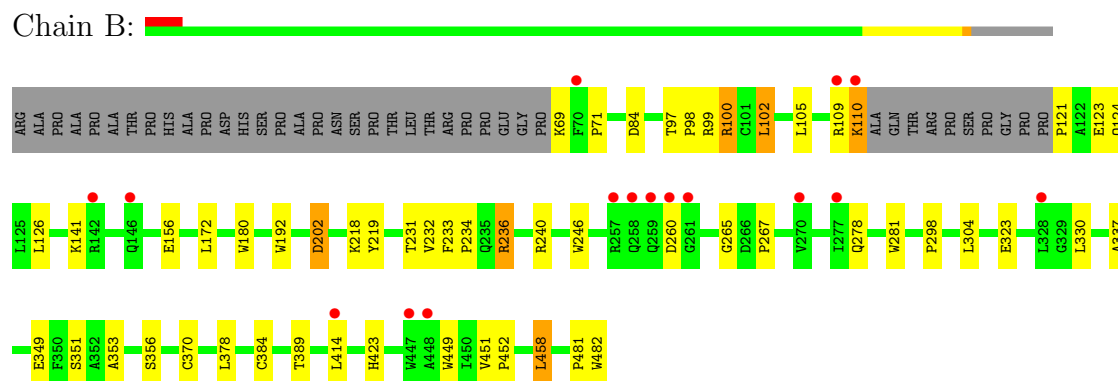
3 Residue-property plots

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



• Molecule 1: NITRIC OXIDE SYNTHASE, ENDOTHELIAL



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	57.73Å 106.20Å 156.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.19 – 2.13 48.23 – 2.12	Depositor EDS
% Data completeness (in resolution range)	98.9 (92.19-2.13) 97.8 (48.23-2.12)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.172 , 0.214 0.172 , 0.214	Depositor DCC
R_{free} test set	2712 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.9	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 54290 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6997	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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, CAS, HW9, ACT, HEM, H2B

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	0.69	3/3303 (0.1%)	0.72	0/4497
1	B	0.68	1/3300 (0.0%)	0.70	0/4491
All	All	0.69	4/6603 (0.1%)	0.71	0/8988

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	447	TRP	CD2-CE2	5.66	1.48	1.41
1	A	281	TRP	CD2-CE2	5.62	1.48	1.41
1	B	482	TRP	CD2-CE2	5.54	1.48	1.41
1	A	246	TRP	CD2-CE2	5.02	1.47	1.41

There are no bond angle outliers.

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	3223	0	3127	34	0
1	B	3221	0	3130	35	0
2	A	43	0	30	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	4	0
3	A	17	0	13	1	0
3	B	17	0	13	1	0
4	A	27	0	32	2	0
4	B	27	0	32	1	0
5	A	8	0	6	0	0
5	B	8	0	6	0	0
6	B	1	0	0	0	0
7	A	209	0	0	3	0
7	B	153	0	0	1	0
All	All	6997	0	6419	70	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 5.

All (70) 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	2.49	1.31
1:B:384:CAS:AS	1:B:384:CAS:SG	2.57	1.22
1:A:72:ARG:HD3	7:A:2002:HOH:O	1.77	0.84
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.62	0.81
1:A:72:ARG:H	1:B:109:ARG:HE	1.37	0.70
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.74	0.70
1:A:384:CAS:CB	1:A:384:CAS:AS	3.02	0.67
2:B:500:HEM:HBC2	2:B:500:HEM:HMC1	1.78	0.66
1:A:109:ARG:H	1:A:109:ARG:HH11	1.44	0.64
2:B:500:HEM:HBC2	2:B:500:HEM:CMC	2.29	0.63
1:B:240:ARG:HD3	1:B:298:PRO:HB3	1.82	0.62
1:B:281:TRP:HB2	1:B:304:LEU:HD21	1.82	0.61
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.68	0.58
1:A:146:GLN:O	1:A:150:GLU:CG	2.53	0.56
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.35	0.56
1:A:126:LEU:HD11	1:A:156:GLU:HA	1.87	0.56
1:A:449:TRP:HA	3:A:600:H2B:N1	2.21	0.55
1:B:110:LYS:C	1:B:110:LYS:HD2	2.28	0.54
1:A:72:ARG:H	1:B:109:ARG:NE	2.05	0.53
1:B:236:ARG:HG3	1:B:349:GLU:HB2	1.90	0.53
1:B:231:THR:O	1:B:353:ALA:HA	2.08	0.53
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.47	0.53
1:A:146:GLN:O	1:A:150:GLU:HG2	2.09	0.53
1:A:384:CAS:HB2	1:A:384:CAS:AS	2.70	0.51
1:A:384:CAS:SG	1:A:384:CAS:CE1	2.99	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.93	0.49
1:A:257:ARG:NH1	1:A:257:ARG:HG3	2.27	0.48
1:B:97:THR:HB	1:B:98:PRO:HD2	1.94	0.48
1:B:172:LEU:HD11	1:B:232:VAL:HG11	1.95	0.47
1:B:337:ALA:HB2	1:B:356:SER:HB3	1.96	0.47
1:A:146:GLN:O	1:A:150:GLU:HG3	2.12	0.47
1:A:205:SER:O	1:A:209:MET:HG3	2.15	0.47
1:A:69:LYS:HG3	1:A:69:LYS:O	2.14	0.47
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.55	0.46
1:B:378:LEU:HB2	7:B:2118:HOH:O	2.16	0.46
2:A:500:HEM:CMC	2:A:500:HEM:HBC2	2.46	0.45
1:B:219:TYR:CD1	1:B:219:TYR:C	2.90	0.45
1:B:99:ARG:HG2	1:B:100:ARG:HD2	1.97	0.45
1:B:449:TRP:HA	3:B:600:H2B:N1	2.32	0.45
1:A:167:LEU:HG	1:A:348:LEU:HD12	1.99	0.45
1:B:246:TRP:CD1	1:B:481:PRO:HG2	2.52	0.44
1:B:121:PRO:HB2	1:B:123:GLU:OE1	2.17	0.44
1:B:84:ASP:C	1:B:84:ASP:OD1	2.56	0.44
1:B:109:ARG:HD2	1:B:109:ARG:HA	1.72	0.44
1:A:392:THR:HB	1:B:423:HIS:HB2	2.00	0.43
2:B:500:HEM:C1C	4:B:800:HW9:H33	2.53	0.43
1:B:71:PRO:HG2	1:B:84:ASP:HB3	2.00	0.43
1:A:100:ARG:NE	7:A:2027:HOH:O	2.37	0.43
1:A:126:LEU:HD23	1:A:130:ARG:NH2	2.34	0.43
1:A:451:VAL:HA	1:A:452:PRO:HD3	1.81	0.43
2:A:500:HEM:C1C	4:A:800:HW9:H33	2.54	0.43
1:B:141:LYS:HA	1:B:141:LYS:HD3	1.86	0.43
1:A:401:ALA:CB	1:B:458:LEU:HD21	2.49	0.42
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.55	0.42
1:A:71:PRO:HB3	1:B:102:LEU:HD21	2.01	0.42
1:A:465:GLU:HB3	1:B:105:LEU:HD22	2.02	0.42
1:B:451:VAL:HA	1:B:452:PRO:HD3	1.92	0.41
1:A:231:THR:O	1:A:353:ALA:HA	2.19	0.41
2:B:500:HEM:HMC1	2:B:500:HEM:CBC	2.47	0.41
1:A:378:LEU:HB2	7:A:2153:HOH:O	2.19	0.41
1:A:70:PHE:HB3	1:A:84:ASP:O	2.21	0.41
1:B:202:ASP:CG	1:B:202:ASP:O	2.58	0.41
2:A:500:HEM:CBB	2:A:500:HEM:HHC	2.51	0.41
1:A:246:TRP:CD1	1:A:481:PRO:HG2	2.56	0.41
1:B:110:LYS:CD	1:B:110:LYS:C	2.89	0.41
1:B:97:THR:HB	1:B:98:PRO:CD	2.50	0.40
1:A:363:GLU:OE1	4:A:800:HW9:N21	2.55	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:126:LEU:HD11	1:B:156:GLU:HA	2.03	0.40
1:B:265:GLY:O	1:B:267:PRO:HD3	2.21	0.40
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.56	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	400/443 (90%)	387 (97%)	12 (3%)	1 (0%)	50	46
1	B	399/443 (90%)	387 (97%)	12 (3%)	0	100	100
All	All	799/886 (90%)	774 (97%)	24 (3%)	1 (0%)	59	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ALA

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	343/374 (92%)	333 (97%)	10 (3%)	55	55
1	B	343/374 (92%)	328 (96%)	15 (4%)	39	34
All	All	686/748 (92%)	661 (96%)	25 (4%)	47	45

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	72	ARG
1	A	100	ARG
1	A	102	LEU
1	A	109	ARG
1	A	125	LEU
1	A	293	LEU
1	A	294	LEU
1	A	328	LEU
1	A	458	LEU
1	B	69	LYS
1	B	100	ARG
1	B	102	LEU
1	B	110	LYS
1	B	124	GLN
1	B	202	ASP
1	B	218	LYS
1	B	236	ARG
1	B	260	ASP
1	B	278	GLN
1	B	323	GLU
1	B	330	LEU
1	B	389	THR
1	B	414	LEU
1	B	458	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	191	GLN
1	A	376	ASN
1	A	413	GLN
1	A	468	ASN
1	B	178	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	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	13.76	2 (25%)	7,9,11	5.93	4 (57%)
1	CAS	B	384	1	8,8,9	18.27	4 (50%)	7,9,11	5.95	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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	384	CAS	AS-SG	48.94	2.57	2.26
1	A	384	CAS	AS-SG	35.44	2.49	2.26
1	B	384	CAS	O-C	16.15	1.22	1.11
1	A	384	CAS	O-C	15.82	1.22	1.11
1	B	384	CAS	CA-C	2.10	1.53	1.49
1	B	384	CAS	AS-CE2	2.01	2.01	1.96

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	CAS	CE2-AS-CE1	14.75	119.78	96.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	CAS	CE2-AS-CE1	12.22	115.82	96.77
1	A	384	CAS	AS-SG-CB	-8.72	87.70	102.24
1	A	384	CAS	CE1-AS-SG	-3.54	83.23	96.44
1	B	384	CAS	C-CA-N	-3.32	110.51	113.83
1	B	384	CAS	CE2-AS-SG	3.26	108.60	96.44
1	B	384	CAS	AS-SG-CB	-2.77	97.61	102.24
1	A	384	CAS	C-CA-N	-2.63	111.20	113.83

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	2.62	20 (47%)	27,82,82	2.75	7 (25%)
3	H2B	A	600	-	18,18,18	1.39	3 (16%)	26,26,26	1.92	6 (23%)
4	HW9	A	800	-	29,29,29	0.70	0	38,38,38	1.77	7 (18%)
5	ACT	A	860	-	1,3,3	1.19	0	0,3,3	0.00	-
5	ACT	A	861	-	1,3,3	1.96	0	0,3,3	0.00	-
2	HEM	B	500	1	42,50,50	2.68	19 (45%)	27,82,82	2.47	7 (25%)
3	H2B	B	600	-	18,18,18	1.41	3 (16%)	26,26,26	1.66	5 (19%)
4	HW9	B	800	-	29,29,29	0.66	0	38,38,38	2.08	12 (31%)
5	ACT	B	860	-	1,3,3	1.48	0	0,3,3	0.00	-
5	ACT	B	861	-	1,3,3	1.71	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	H2B	A	600	-	-	0/8/33/33	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	H2B	B	600	-	-	0/8/33/33	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 (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C4A-NA	6.06	1.46	1.36
2	B	500	HEM	CHC-C4B	5.89	1.47	1.39
2	A	500	HEM	C1B-C2B	5.51	1.49	1.45
2	B	500	HEM	C4A-NA	5.32	1.45	1.36
2	B	500	HEM	C3C-C4C	5.15	1.49	1.45
2	B	500	HEM	C1A-NA	4.76	1.44	1.36
2	A	500	HEM	C4C-NC	4.65	1.45	1.33
2	B	500	HEM	C1C-NC	4.41	1.44	1.33
2	B	500	HEM	C4C-NC	4.35	1.44	1.33
2	A	500	HEM	C1A-NA	4.23	1.43	1.36
2	A	500	HEM	FE-NB	4.10	2.10	1.95
2	B	500	HEM	FE-NB	4.02	2.10	1.95
2	A	500	HEM	C3C-C2C	3.97	1.48	1.45
2	A	500	HEM	C1C-NC	3.80	1.43	1.33
2	B	500	HEM	FE-ND	3.78	2.10	1.95
2	A	500	HEM	CHC-C4B	3.64	1.44	1.39
2	B	500	HEM	C1B-C2B	3.62	1.48	1.45
2	A	500	HEM	CMC-C2C	3.61	1.51	1.45
2	B	500	HEM	C2A-C3A	3.44	1.47	1.37
2	B	500	HEM	C3C-C2C	3.43	1.48	1.45
2	A	500	HEM	C3C-C4C	3.39	1.47	1.45
2	B	500	HEM	CMC-C2C	3.36	1.51	1.45
2	B	500	HEM	C4A-C3A	3.32	1.48	1.43
2	A	500	HEM	CMD-C2D	3.24	1.50	1.45
3	B	600	H2B	C4A-N5	3.21	1.37	1.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C2A-C3A	3.12	1.46	1.37
2	A	500	HEM	C1A-C2A	3.09	1.48	1.43
2	A	500	HEM	C4A-C3A	3.05	1.48	1.43
2	B	500	HEM	C3B-CAB	3.02	1.50	1.40
3	A	600	H2B	C4A-N5	2.99	1.37	1.28
2	B	500	HEM	CMD-C2D	2.98	1.50	1.45
3	B	600	H2B	C4-C4A	-2.87	1.39	1.47
2	A	500	HEM	CMB-C2B	2.84	1.50	1.45
2	B	500	HEM	C1C-C2C	2.81	1.50	1.43
2	A	500	HEM	FE-ND	2.75	2.06	1.95
2	A	500	HEM	C4D-C3D	2.74	1.50	1.43
3	A	600	H2B	C4-C4A	-2.72	1.39	1.47
2	A	500	HEM	C3B-CAB	2.63	1.49	1.40
2	B	500	HEM	C1A-C2A	2.58	1.47	1.43
2	A	500	HEM	C3C-CAC	2.53	1.48	1.40
3	A	600	H2B	C9-C6	2.44	1.55	1.52
2	B	500	HEM	C3C-CAC	2.42	1.48	1.40
2	B	500	HEM	CMB-C2B	2.15	1.49	1.45
2	A	500	HEM	C1D-C2D	2.07	1.48	1.43
3	B	600	H2B	C8A-N1	2.03	1.37	1.32

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	500	HEM	C3A-C4A-NA	8.68	115.30	109.50
4	B	800	HW9	C02-N01-C06	7.78	123.70	118.24
2	B	500	HEM	CBA-CAA-C2A	-6.98	101.01	112.63
4	A	800	HW9	C02-N01-C06	6.60	122.87	118.24
2	A	500	HEM	C4A-NA-C1A	-6.05	100.40	107.93
2	A	500	HEM	C4A-C3A-C2A	-5.55	103.13	107.00
2	B	500	HEM	C3A-C4A-NA	5.54	113.20	109.50
3	A	600	H2B	C4-C4A-N5	5.53	123.25	117.83
2	B	500	HEM	C4A-NA-C1A	-4.77	101.99	107.93
3	B	600	H2B	C4-C4A-N5	4.77	122.51	117.83
3	A	600	H2B	C6-C7-N8	-4.33	107.48	111.33
2	B	500	HEM	CBD-CAD-C3D	-3.82	106.23	114.51
3	A	600	H2B	N1-C2-N3	-3.56	120.80	126.37
4	B	800	HW9	C23-C22-N21	-3.48	120.03	123.88
4	A	800	HW9	C05-C06-N01	-3.48	119.07	122.96
2	A	500	HEM	CBD-CAD-C3D	-3.38	107.17	114.51
3	B	600	H2B	N1-C2-N3	-3.38	121.08	126.37
2	A	500	HEM	CBA-CAA-C2A	-3.36	107.04	112.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	HW9	C08-C4'-C3'	3.31	118.57	113.62
4	B	800	HW9	C05-C06-N01	-3.26	119.32	122.96
2	B	500	HEM	C2A-C1A-NA	3.24	114.24	109.73
4	B	800	HW9	C22-N21-C26	3.23	121.90	117.37
3	A	600	H2B	N2-C2-N1	3.22	120.64	116.53
3	B	600	H2B	N2-C2-N1	3.13	120.53	116.53
2	A	500	HEM	C2A-C1A-NA	3.10	114.04	109.73
4	A	800	HW9	C25-C26-N21	-3.05	119.36	122.88
4	A	800	HW9	C3'-C2'-N1'	-2.94	100.05	105.46
4	B	800	HW9	C5'-N1'-C2'	2.92	113.27	105.92
4	A	800	HW9	C5'-N1'-C2'	2.91	113.24	105.92
4	B	800	HW9	C24-C25-C26	-2.87	118.39	120.28
4	A	800	HW9	C22-N21-C26	2.72	121.18	117.37
3	A	600	H2B	C7-N8-C8A	2.61	124.34	119.95
2	B	500	HEM	C4A-C3A-C2A	-2.55	105.22	107.00
3	B	600	H2B	C4A-C4-N3	2.53	121.45	117.08
4	B	800	HW9	C06-C08-C4'	-2.49	106.14	115.31
4	B	800	HW9	C3'-C2'-N1'	-2.46	100.94	105.46
4	A	800	HW9	C08-C4'-C3'	2.45	117.29	113.62
3	A	600	H2B	C8A-C4A-N5	-2.35	118.41	124.46
4	B	800	HW9	C25-C26-N21	-2.33	120.19	122.88
4	B	800	HW9	C04-C05-C06	-2.30	118.77	120.28
4	B	800	HW9	C10-O09-C3'	2.20	119.23	113.94
2	B	500	HEM	CAD-C3D-C4D	2.19	128.69	125.60
2	A	500	HEM	CMB-C2B-C3B	2.10	131.04	126.21
3	B	600	H2B	C6-C7-N8	-2.09	109.47	111.33

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%)	0.40	20 (4%) 28 31	26, 38, 67, 95	0
1	B	404/443 (91%)	0.24	16 (3%) 36 39	25, 41, 69, 99	0
All	All	809/886 (91%)	0.32	36 (4%) 33 36	25, 40, 68, 99	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	GLN	6.1
1	A	67	GLY	4.4
1	B	270	VAL	4.3
1	A	126	LEU	4.2
1	A	121	PRO	3.8
1	A	261	GLY	3.6
1	A	146	GLN	3.5
1	A	259	GLN	3.4
1	A	160	ALA	3.3
1	A	157	ALA	3.2
1	B	261	GLY	3.1
1	A	450	ILE	3.0
1	B	142	ARG	2.8
1	B	328	LEU	2.7
1	A	257	ARG	2.7
1	A	449	TRP	2.6
1	A	156	GLU	2.6
1	B	146	GLN	2.6
1	B	448	ALA	2.5
1	A	123	GLU	2.5
1	A	109	ARG	2.5
1	A	153	GLN	2.5
1	B	110	LYS	2.5
1	B	414	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	109	ARG	2.3
1	B	70	PHE	2.3
1	A	159	VAL	2.3
1	B	277	ILE	2.2
1	A	69	LYS	2.2
1	A	187	VAL	2.1
1	B	258	GLN	2.1
1	B	447	TRP	2.1
1	A	105	LEU	2.1
1	B	260	ASP	2.1
1	A	104	SER	2.0
1	B	257	ARG	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	0.09	-0.59	39,41,56,65	0
1	CAS	B	384	9/10	0.10	-1.35	51,57,86,91	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	0.31	14.82	49,53,55,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	HEM	A	500	43/43	0.19	0.86	24,26,32,34	0
2	HEM	B	500	43/43	0.14	0.77	28,30,34,34	0
4	HW9	B	800	27/27	0.13	0.38	29,32,35,36	0
5	ACT	B	861	4/4	0.11	0.38	34,35,38,38	0
4	HW9	A	800	27/27	0.16	0.23	26,30,34,35	0
3	H2B	A	600	17/17	0.18	-0.07	25,28,30,30	0
3	H2B	B	600	17/17	0.16	-0.43	23,27,28,28	0
5	ACT	A	860	4/4	0.14	-0.55	47,48,49,52	0
5	ACT	A	861	4/4	0.10	-0.60	29,30,32,32	0
6	ZN	B	900	1/1	0.12	-2.95	33,33,33,33	0

6.5 Other polymers ⓘ

There are no such residues in this entry.