



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:48 PM GMT

PDB ID : 1ZZT
Title : Bovine eNOS N368D/V106M double mutant with L-N(omega)-Nitroarginine-(4R)-Amino-L-ProlineAmide Bound
Authors : Li, H.; Flinspach, M.L.; Igarashi, J.; Jamal, J.; Yang, W.; Gomez-Vidal, J.A.; Litzinger, E.A.; Silverman, R.B.; Poulos, T.L.
Deposited on : 2005-06-14
Resolution : 2.14 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>

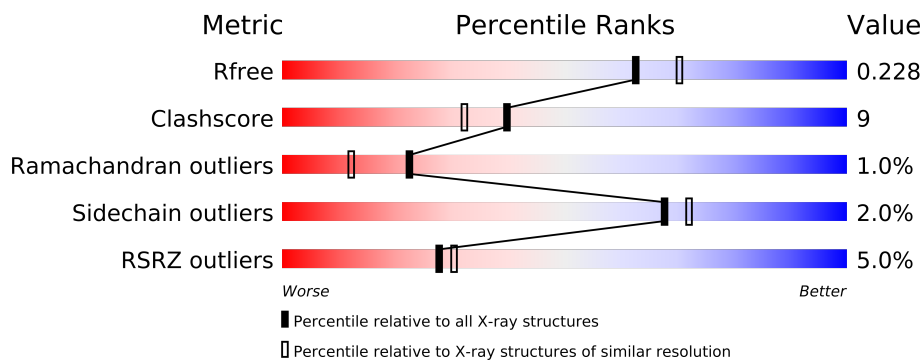
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 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 2.14 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	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
2	ACT	A	860	-	X
2	ACT	B	861	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6994 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.

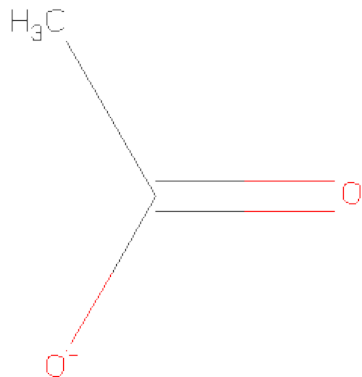
- Molecule 1 is a protein called Nitric-oxide synthase, endothelial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	405	Total	As	C	N	O	S	0	0	0
			3220	1	2048	564	590	17			
1	B	405	Total	As	C	N	O	S	0	0	0
			3227	1	2052	567	590	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	see remark 999	UNP P29473
A	106	MET	VAL	engineered	UNP P29473
A	368	ASP	ASN	engineered	UNP P29473
A	384	CAS	CYS	modified residue	UNP P29473
B	100	ARG	CYS	see remark 999	UNP P29473
B	106	MET	VAL	engineered	UNP P29473
B	368	ASP	ASN	engineered	UNP P29473
B	384	CAS	CYS	modified residue	UNP P29473

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).

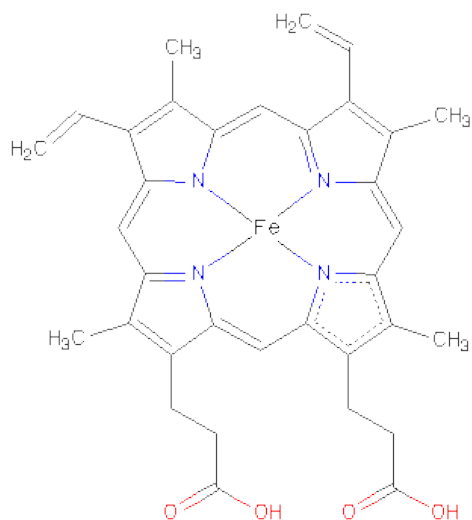


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

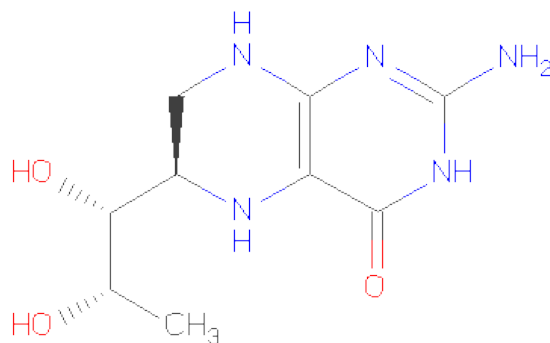
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

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



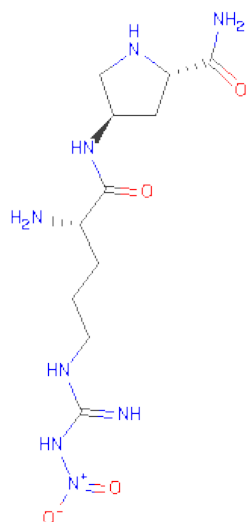
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			17	9	5	3		

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

- Molecule 6 is L-N(OMEGA)-NITROARGININE-(4R)-AMINO-L-PROLINEAMIDE (three-letter code: DP9) (formula: C₁₁H₂₂N₈O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			23	11	8	4		
6	B	1	Total	C	N	O	0	0
			23	11	8	4		

- Molecule 7 is water.

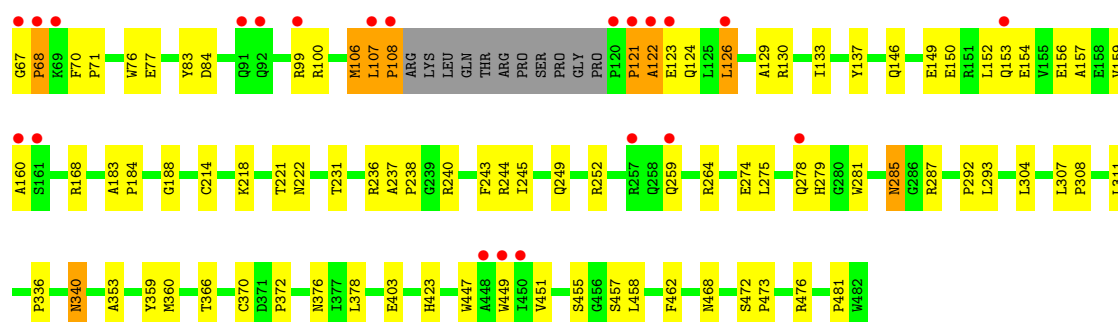
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	189	Total	O	0	0
			189	189		
7	B	183	Total	O	0	0
			183	183		

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.

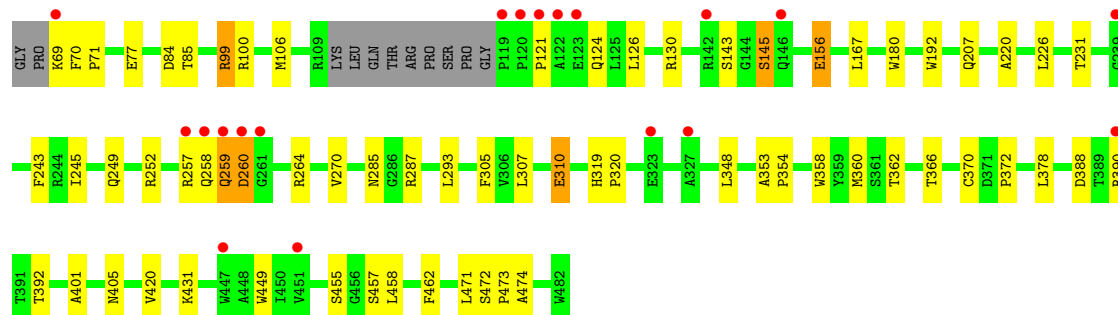
- Molecule 1: Nitric-oxide synthase, endothelial

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	56.45Å 105.74Å 155.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.43 – 2.14 47.43 – 2.07	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.43-2.14) 95.5 (47.43-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.07Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.189 , 0.233 0.188 , 0.228	Depositor DCC
R_{free} test set	2703 reflections (5.19%)	DCC
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 54769 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6994	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 4.52% 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, DP9, 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	0.49	0/3301	0.72	3/4495 (0.1%)
1	B	0.48	0/3308	0.71	3/4504 (0.1%)
All	All	0.48	0/6609	0.71	6/8999 (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	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	360	MET	N-CA-C	-6.09	94.57	111.00
1	A	360	MET	N-CA-C	-5.71	95.58	111.00
1	B	243	PHE	N-CA-C	-5.29	96.72	111.00
1	B	245	ILE	N-CA-C	-5.29	96.73	111.00
1	A	243	PHE	N-CA-C	-5.20	96.97	111.00
1	A	245	ILE	N-CA-C	-5.05	97.37	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	137	TYR	Sidechain

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	3220	0	3119	73	0
1	B	3227	0	3129	55	0
2	A	4	0	3	1	0
2	B	4	0	3	8	0
3	A	1	0	0	0	0
4	A	43	0	30	0	0
4	B	43	0	30	0	0
5	A	17	0	15	3	0
5	B	17	0	15	3	0
6	A	23	0	21	0	0
6	B	23	0	21	0	0
7	A	189	0	0	6	0
7	B	183	0	0	4	0
All	All	6994	0	6386	123	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 9.

All (123) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:106:MET:HE2	5:B:761:H4B:H9	1.47	0.97
1:A:126:LEU:HD11	1:A:156:GLU:HG2	1.48	0.92
1:B:126:LEU:O	1:B:130:ARG:HG3	1.74	0.88
1:B:358:TRP:HE1	2:B:861:ACT:H2	1.39	0.86
1:B:358:TRP:HE1	2:B:861:ACT:CH3	1.87	0.86
1:A:249:GLN:HB2	1:A:252:ARG:HG3	1.64	0.80
1:B:388:ASP:OD1	1:B:390:ARG:HB2	1.83	0.78
1:A:126:LEU:O	1:A:130:ARG:HG3	1.86	0.75
1:A:126:LEU:HD12	1:A:130:ARG:HE	1.50	0.75
1:A:68:PRO:HD2	1:A:83:TYR:CE2	2.26	0.71
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.31	0.70
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.33	0.68
1:A:293:LEU:HG	1:A:307:LEU:HD21	1.75	0.67
1:A:126:LEU:HD23	1:A:159:VAL:HG11	1.77	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:77:GLU:HG3	1:B:372:PRO:HG2	1.78	0.66
1:B:257:ARG:HE	1:B:270:VAL:HG11	1.60	0.65
1:B:358:TRP:NE1	2:B:861:ACT:H2	2.09	0.65
1:B:249:GLN:HB2	1:B:252:ARG:HG2	1.78	0.64
1:A:126:LEU:HD12	1:A:130:ARG:NE	2.13	0.63
1:A:293:LEU:HG	1:A:307:LEU:CD2	2.30	0.62
1:A:146:GLN:HG2	1:A:150:GLU:OE2	2.02	0.60
1:A:106:MET:HE1	5:A:760:H4B:HN5	1.66	0.60
1:B:249:GLN:HB2	1:B:252:ARG:CG	2.32	0.60
1:A:279:HIS:HE1	7:A:1069:HOH:O	1.84	0.59
1:A:274:GLU:O	1:A:278:GLN:HG3	2.01	0.59
1:B:293:LEU:HD11	1:B:307:LEU:HD21	1.85	0.59
1:B:167:LEU:HG	1:B:348:LEU:HD12	1.85	0.59
1:A:152:LEU:O	1:A:156:GLU:HG3	2.02	0.58
1:B:420:VAL:HG11	2:B:861:ACT:H3	1.84	0.58
1:A:107:LEU:HB3	1:A:108:PRO:CD	2.33	0.58
1:B:431:LYS:HE3	7:B:936:HOH:O	2.03	0.57
1:A:372:PRO:HG2	1:B:77:GLU:HG3	1.86	0.56
1:B:378:LEU:HB2	7:B:863:HOH:O	2.05	0.56
1:B:449:TRP:HA	5:B:761:H4B:N1	2.20	0.56
1:A:107:LEU:HB3	1:A:108:PRO:HD2	1.87	0.56
1:A:188:GLY:HA2	2:A:860:ACT:H1	1.89	0.55
1:A:68:PRO:CD	1:A:83:TYR:CZ	2.89	0.55
1:B:71:PRO:HG2	1:B:84:ASP:HB3	1.89	0.55
1:A:149:GLU:O	1:A:153:GLN:HG3	2.07	0.55
1:B:310:GLU:HG2	1:B:310:GLU:O	2.07	0.55
1:A:287:ARG:HD2	7:A:962:HOH:O	2.07	0.54
1:A:99:ARG:HH11	1:A:99:ARG:HG3	1.73	0.54
1:A:76:TRP:CD1	1:B:106:MET:HE3	2.43	0.54
1:B:130:ARG:HB3	1:B:130:ARG:HH11	1.71	0.54
1:A:275:LEU:O	1:A:279:HIS:HD2	1.92	0.53
1:A:106:MET:HE1	5:A:760:H4B:N5	2.22	0.53
1:A:423:HIS:HB2	1:B:392:THR:HB	1.92	0.52
1:A:107:LEU:O	1:A:108:PRO:C	2.47	0.52
1:A:237:ALA:HB3	1:A:240:ARG:HB3	1.90	0.52
1:B:106:MET:CE	5:B:761:H4B:H9	2.32	0.52
1:A:146:GLN:O	1:A:150:GLU:HG3	2.11	0.51
1:B:390:ARG:HD2	7:B:972:HOH:O	2.10	0.51
1:A:68:PRO:HG2	1:A:83:TYR:CG	2.44	0.51
1:A:264:ARG:HG3	1:A:264:ARG:HH11	1.73	0.51
1:A:279:HIS:CE1	7:A:1069:HOH:O	2.63	0.51
1:A:70:PHE:HB3	1:A:84:ASP:O	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:264:ARG:NE	1:A:285:ASN:O	2.40	0.50
1:A:244:ARG:NH2	1:A:481:PRO:HD3	2.26	0.50
1:B:287:ARG:HD3	7:B:974:HOH:O	2.11	0.50
1:B:126:LEU:HD11	1:B:156:GLU:HG2	1.93	0.50
1:B:99:ARG:HB2	1:B:99:ARG:HH11	1.76	0.49
1:B:264:ARG:NE	1:B:285:ASN:O	2.44	0.49
1:A:154:GLU:OE1	1:A:168:ARG:NH2	2.46	0.49
1:B:455:SER:HB3	1:B:458:LEU:HD12	1.94	0.49
1:B:420:VAL:CB	2:B:861:ACT:H3	2.43	0.48
1:A:68:PRO:HD3	1:A:83:TYR:CZ	2.48	0.48
1:A:472:SER:HA	1:A:473:PRO:C	2.34	0.48
1:A:281:TRP:HB2	1:A:304:LEU:HD21	1.94	0.48
1:A:99:ARG:NH1	1:A:99:ARG:HG3	2.29	0.48
1:B:264:ARG:HG3	1:B:264:ARG:HH11	1.78	0.48
1:A:293:LEU:CG	1:A:307:LEU:HD21	2.43	0.47
1:B:69:LYS:HD2	1:B:70:PHE:CE1	2.49	0.47
1:A:236:ARG:NH1	7:A:1073:HOH:O	2.44	0.47
1:B:130:ARG:HB3	1:B:130:ARG:NH1	2.30	0.47
1:A:336:PRO:HB3	1:A:359:TYR:CZ	2.49	0.47
1:A:378:LEU:HB2	7:A:909:HOH:O	2.14	0.47
1:B:180:TRP:CE3	1:B:192:TRP:HA	2.50	0.47
1:B:319:HIS:CG	1:B:320:PRO:HD2	2.51	0.46
1:A:366:THR:O	1:A:370:CYS:HB2	2.15	0.46
1:B:362:THR:HA	1:B:405:ASN:HD21	1.80	0.46
1:B:362:THR:HA	1:B:405:ASN:ND2	2.29	0.46
1:A:292:PRO:HA	7:A:970:HOH:O	2.15	0.46
1:B:207:GLN:NE2	1:B:305:PHE:HE2	2.13	0.46
1:A:68:PRO:CD	1:A:83:TYR:CE2	2.98	0.45
1:A:121:PRO:O	1:A:124:GLN:N	2.50	0.45
1:A:457:SER:HA	1:A:462:PHE:CG	2.51	0.45
1:A:157:ALA:O	1:A:160:ALA:HB3	2.17	0.45
1:A:449:TRP:HA	5:A:760:H4B:N1	2.32	0.45
1:A:121:PRO:O	1:A:123:GLU:N	2.51	0.44
1:A:403:GLU:HA	1:A:403:GLU:OE1	2.16	0.44
1:B:457:SER:HA	1:B:462:PHE:CG	2.52	0.44
1:B:472:SER:HA	1:B:473:PRO:C	2.38	0.44
1:B:70:PHE:HD2	1:B:85:THR:HA	1.83	0.44
1:B:121:PRO:HG2	1:B:124:GLN:HE21	1.83	0.44
1:A:308:PRO:HD2	1:A:311:LEU:HD12	2.00	0.43
1:A:455:SER:HB3	1:A:458:LEU:HD12	2.00	0.43
1:A:476:ARG:HH11	1:A:476:ARG:HG2	1.82	0.43
1:A:214:CYS:O	1:A:218:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:126:LEU:CD2	1:A:159:VAL:HG11	2.48	0.43
1:B:420:VAL:CG1	2:B:861:ACT:H3	2.46	0.43
1:A:447:TRP:CZ2	1:A:451:VAL:HG21	2.53	0.43
1:B:358:TRP:HE1	2:B:861:ACT:H1	1.77	0.43
1:A:129:ALA:O	1:A:133:ILE:HG12	2.19	0.43
1:B:231:THR:O	1:B:353:ALA:HA	2.18	0.43
1:A:121:PRO:C	1:A:123:GLU:N	2.72	0.43
1:A:476:ARG:NH1	1:A:476:ARG:HG2	2.33	0.42
1:A:231:THR:O	1:A:353:ALA:HA	2.19	0.42
1:A:458:LEU:HD11	1:B:401:ALA:CB	2.50	0.42
1:B:143:SER:C	1:B:145:SER:H	2.23	0.42
1:B:126:LEU:HG	1:B:130:ARG:HD2	2.01	0.42
1:A:67:GLY:HA3	1:A:68:PRO:HD3	1.54	0.42
1:B:471:LEU:O	1:B:474:ALA:HB2	2.19	0.42
1:A:122:ALA:O	1:A:126:LEU:HB2	2.19	0.41
1:A:285:ASN:HD22	1:A:285:ASN:C	2.24	0.41
1:A:71:PRO:HD2	1:A:84:ASP:O	2.20	0.41
1:B:420:VAL:HG21	2:B:861:ACT:H3	2.02	0.41
1:A:183:ALA:HA	1:A:184:PRO:HD3	1.93	0.41
1:A:340:ASN:HD22	1:A:340:ASN:H	1.68	0.41
1:B:366:THR:O	1:B:370:CYS:HB2	2.21	0.41
1:B:258:GLN:O	1:B:259:GLN:C	2.59	0.40
1:A:221:THR:O	1:A:222:ASN:C	2.60	0.40
1:B:231:THR:O	1:B:354:PRO:HD2	2.21	0.40
1:B:220:ALA:O	1:B:226:LEU:HA	2.22	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	400/416 (96%)	380 (95%)	15 (4%)	5 (1%)	18	9
1	B	400/416 (96%)	384 (96%)	13 (3%)	3 (1%)	27	16
All	All	800/832 (96%)	764 (96%)	28 (4%)	8 (1%)	22	12

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	PRO
1	B	259	GLN
1	B	145	SER
1	B	260	ASP
1	A	121	PRO
1	A	122	ALA
1	A	238	PRO
1	A	107	LEU

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	343/353 (97%)	334 (97%)	9 (3%)	59	60
1	B	344/353 (98%)	339 (98%)	5 (2%)	76	82
All	All	687/706 (97%)	673 (98%)	14 (2%)	68	72

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	ARG
1	A	106	MET
1	A	108	PRO
1	A	126	LEU
1	A	259	GLN
1	A	285	ASN
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN
1	B	99	ARG
1	B	100	ARG
1	B	156	GLU
1	B	260	ASP
1	B	310	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	191	GLN
1	A	207	GLN
1	A	279	HIS
1	A	285	ASN
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN
1	B	124	GLN
1	B	146	GLN
1	B	191	GLN
1	B	207	GLN
1	B	215	ASN
1	B	222	ASN
1	B	279	HIS
1	B	405	ASN
1	B	413	GLN

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	7.82	6 (75%)	7,9,11	2.72	2 (28%)
1	CAS	B	384	1	8,8,9	6.86	5 (62%)	7,9,11	2.79	3 (42%)

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 (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	384	CAS	O-C	17.71	1.23	1.11
1	B	384	CAS	O-C	16.89	1.23	1.11
1	A	384	CAS	AS-SG	11.32	2.33	2.26
1	B	384	CAS	AS-SG	6.74	2.30	2.26
1	B	384	CAS	AS-CE1	-4.46	1.83	1.96
1	B	384	CAS	AS-CE2	-4.42	1.84	1.96
1	A	384	CAS	AS-CE2	-4.31	1.84	1.96
1	A	384	CAS	AS-CE1	-4.27	1.84	1.96
1	A	384	CAS	CA-C	2.30	1.52	1.48
1	A	384	CAS	CB-SG	-2.28	1.76	1.84
1	B	384	CAS	CA-C	2.21	1.52	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	CAS	AS-SG-CB	-6.01	92.22	102.24
1	B	384	CAS	AS-SG-CB	-5.18	93.61	102.24
1	B	384	CAS	C-CA-N	-4.28	109.55	113.83
1	A	384	CAS	C-CA-N	-3.19	110.64	113.83
1	B	384	CAS	CA-CB-SG	2.57	121.51	111.64

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 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\# Z > 2$
4	HEM	A	700	1	49,50,50	2.25	13 (26%)	46,82,82	1.81	10 (21%)
5	H4B	A	760	-	18,18,18	1.52	4 (22%)	24,26,26	2.55	7 (29%)
6	DP9	A	799	-	22,23,23	2.05	3 (13%)	26,30,30	1.60	4 (15%)
2	ACT	A	860	-	1,3,3	0.36	0	0,3,3	0.00	-
4	HEM	B	700	1	49,50,50	1.88	9 (18%)	46,82,82	1.51	7 (15%)
5	H4B	B	761	-	18,18,18	1.51	4 (22%)	24,26,26	2.53	8 (33%)
6	DP9	B	800	-	22,23,23	1.54	2 (9%)	26,30,30	1.70	5 (19%)
2	ACT	B	861	-	1,3,3	0.71	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
4	HEM	A	700	1	-	0/14/114/114	0/0/8/8
5	H4B	A	760	-	-	0/8/17/17	0/0/2/2
6	DP9	A	799	-	-	0/20/32/32	0/1/1/1
2	ACT	A	860	-	-	0/0/0/0	0/0/0/0
4	HEM	B	700	1	-	0/14/114/114	0/0/8/8
5	H4B	B	761	-	-	0/8/17/17	0/0/2/2
6	DP9	B	800	-	-	0/20/32/32	0/1/1/1
2	ACT	B	861	-	-	0/0/0/0	0/0/0/0

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	799	DP9	O2-NO	8.67	1.28	1.22
4	A	700	HEM	C2D-C1D	7.64	1.46	1.44
6	B	800	DP9	O2-NO	6.00	1.26	1.22
4	A	700	HEM	C3D-C4D	-5.42	1.43	1.44
4	B	700	HEM	C3B-C2B	-5.19	1.34	1.43
4	A	700	HEM	C3B-C2B	-5.11	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	700	HEM	C2B-C1B	-4.98	1.43	1.44
4	B	700	HEM	C3C-C2C	-4.58	1.35	1.43
4	A	700	HEM	C4A-C3A	4.53	1.45	1.40
4	B	700	HEM	C3D-C2D	-4.08	1.36	1.43
4	A	700	HEM	C3D-C2D	-4.06	1.36	1.43
4	A	700	HEM	C2B-C1B	4.01	1.45	1.44
5	A	760	H4B	C6-N5	3.85	1.54	1.46
4	B	700	HEM	C3D-C4D	-3.53	1.43	1.44
4	B	700	HEM	C4A-C3A	3.36	1.44	1.40
5	B	761	H4B	C6-N5	3.20	1.52	1.46
5	B	761	H4B	C4-N3	3.00	1.42	1.37
4	A	700	HEM	C4A-NA	2.99	1.42	1.36
4	B	700	HEM	CHB-C1B	2.98	1.40	1.35
4	A	700	HEM	CMD-C2D	2.74	1.55	1.47
4	A	700	HEM	C4C-NC	2.69	1.41	1.38
5	A	760	H4B	C4-N3	2.68	1.41	1.37
5	B	761	H4B	C4A-N5	2.60	1.47	1.38
6	B	800	DP9	CG'-N2'	2.55	1.51	1.46
4	A	700	HEM	C3C-C2C	-2.53	1.39	1.43
5	A	760	H4B	C4A-N5	2.47	1.46	1.38
4	A	700	HEM	CHA-C4D	2.42	1.39	1.35
4	B	700	HEM	CMB-C2B	2.40	1.54	1.47
6	A	799	DP9	CG'-N2'	2.35	1.51	1.46
6	A	799	DP9	CD'-CG'	2.25	1.56	1.53
5	B	761	H4B	C8A-N1	2.20	1.39	1.34
4	A	700	HEM	CMC-C2C	2.16	1.54	1.47
4	A	700	HEM	CHB-C1B	2.15	1.38	1.35
5	A	760	H4B	C7-C6	2.10	1.54	1.52
4	B	700	HEM	C2D-C1D	-2.03	1.44	1.44

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	761	H4B	C4-C4A-C8A	8.50	122.44	114.56
5	A	760	H4B	C4-C4A-C8A	8.50	122.43	114.56
4	A	700	HEM	CBA-CAA-C2A	-5.46	103.07	112.69
4	B	700	HEM	CBA-CAA-C2A	-5.03	103.83	112.69
4	A	700	HEM	C3A-C4A-NA	4.44	112.76	109.41
4	B	700	HEM	C3B-C4B-NB	-3.98	111.15	114.00
6	B	800	DP9	C'-CA'-N'	-3.78	104.63	111.72
6	A	799	DP9	CD-NE-CZ	3.64	130.41	124.03
5	A	760	H4B	C2-N1-C8A	3.61	122.74	117.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	700	HEM	C4A-C3A-C2A	-3.59	104.50	107.00
6	B	800	DP9	CD-NE-CZ	3.55	130.26	124.03
6	B	800	DP9	O'-C'-N1'	-3.54	117.03	123.03
5	B	761	H4B	C2-N1-C8A	3.47	122.53	117.61
6	A	799	DP9	C'-CA'-N'	-3.28	105.58	111.72
5	A	760	H4B	C4A-N5-C6	-3.26	112.29	121.16
4	A	700	HEM	CBD-CAD-C3D	-3.21	107.36	114.37
5	A	760	H4B	C4-N3-C2	3.20	125.10	119.51
4	B	700	HEM	CBD-CAD-C3D	-3.17	107.45	114.37
5	B	761	H4B	C4-N3-C2	3.06	124.86	119.51
4	A	700	HEM	C1A-CHA-C4D	-3.05	123.46	127.47
4	A	700	HEM	C4A-NA-C1A	-2.99	102.82	106.76
5	A	760	H4B	N3-C2-N1	-2.97	117.61	121.78
4	A	700	HEM	C4A-CHB-C1B	-2.97	123.56	127.47
5	B	761	H4B	N3-C2-N1	-2.94	117.65	121.78
5	B	761	H4B	C4A-N5-C6	-2.94	113.16	121.16
6	A	799	DP9	O'-C'-N1'	-2.87	118.17	123.03
5	A	760	H4B	C4A-C8A-N8	2.78	123.05	119.23
4	A	700	HEM	C4C-NC-C1C	-2.68	102.75	105.53
4	B	700	HEM	C1A-CHA-C4D	-2.64	124.00	127.47
4	A	700	HEM	C3B-C4B-NB	-2.64	112.11	114.00
5	B	761	H4B	C4A-C8A-N8	2.48	122.63	119.23
4	B	700	HEM	C4A-CHB-C1B	-2.46	124.24	127.47
6	B	800	DP9	CA'-C'-N1'	2.36	121.34	116.78
6	A	799	DP9	CG'-N2'-C	2.32	126.91	123.18
5	A	760	H4B	O9-C9-C6	2.29	114.63	109.07
5	B	761	H4B	O9-C9-C6	2.29	114.62	109.07
4	A	700	HEM	C1B-NB-C4B	-2.26	102.85	105.16
4	B	700	HEM	C4A-NA-C1A	-2.20	103.87	106.76
6	B	800	DP9	CG'-N2'-C	2.16	126.65	123.18
5	B	761	H4B	N8-C8A-N1	2.15	118.97	115.82
4	B	700	HEM	C4D-ND-C1D	-2.11	103.00	105.16

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	405/416 (97%)	0.41	22 (5%) 25 27	27, 37, 63, 85	0
1	B	405/416 (97%)	0.41	19 (4%) 30 33	29, 40, 65, 92	0
All	All	810/832 (97%)	0.41	41 (5%) 28 29	27, 39, 64, 92	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	67	GLY	11.2
1	B	120	PRO	8.9
1	B	259	GLN	6.5
1	A	120	PRO	6.4
1	B	119	PRO	5.9
1	A	121	PRO	4.3
1	A	126	LEU	4.3
1	B	122	ALA	4.2
1	A	122	ALA	4.1
1	B	121	PRO	3.9
1	B	257	ARG	3.8
1	A	259	GLN	3.6
1	B	258	GLN	3.5
1	A	123	GLU	3.4
1	A	91	GLN	3.4
1	B	261	GLY	3.4
1	B	123	GLU	3.3
1	A	108	PRO	3.2
1	A	99	ARG	3.1
1	A	69	LYS	3.1
1	B	323	GLU	3.1
1	B	146	GLN	3.1
1	B	69	LYS	3.0
1	A	160	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	68	PRO	2.7
1	A	161	SER	2.7
1	A	153	GLN	2.6
1	A	448	ALA	2.5
1	B	451	VAL	2.4
1	B	260	ASP	2.4
1	A	92	GLN	2.4
1	A	257	ARG	2.4
1	A	107	LEU	2.3
1	A	278	GLN	2.3
1	B	142	ARG	2.2
1	A	450	ILE	2.2
1	B	390	ARG	2.2
1	A	449	TRP	2.2
1	B	447	TRP	2.2
1	B	327	ALA	2.0
1	B	239	GLY	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	-1.17	36,37,52,56	0
1	CAS	B	384	9/10	0.10	-1.49	49,51,66,67	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(\AA^2)	Q<0.9
2	ACT	B	861	4/4	0.25	5.85	46,48,51,53	0
2	ACT	A	860	4/4	0.34	5.62	41,42,42,43	0
5	H4B	B	761	17/17	0.21	1.18	30,32,36,36	0
4	HEM	A	700	43/43	0.19	0.94	23,28,34,42	0
6	DP9	B	800	23/23	0.18	0.76	31,38,51,53	0
4	HEM	B	700	43/43	0.17	0.64	25,29,37,39	0
5	H4B	A	760	17/17	0.19	0.45	30,35,38,39	0
6	DP9	A	799	23/23	0.15	-0.15	33,38,49,52	0
3	ZN	A	900	1/1	0.07	-2.14	40,40,40,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.