



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2017 – 12:22 AM EST

PDB ID : 4KCS
Title : Structure of bovine endothelial nitric oxide synthase heme domain in complex with N-(3-((ethyl(3-fluorophenethyl)amino)methyl)phenyl)thiophene-2-carboximidamide
Authors : Chreifi, G.; Li, H.; Poulos, T.L.
Deposited on : unknown
Resolution : 2.05 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

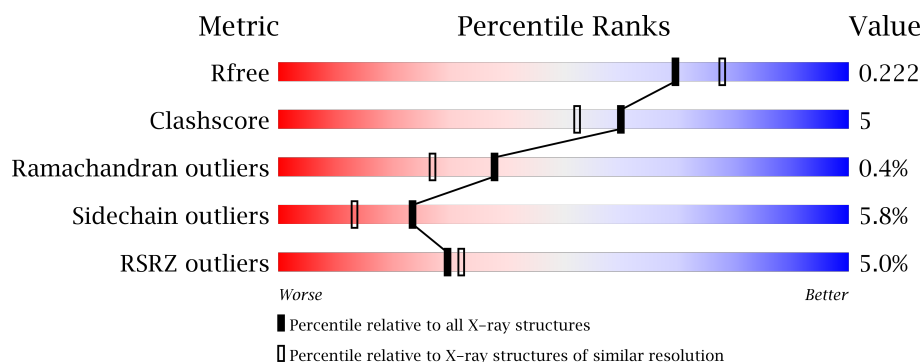
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	100719	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	443	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	443	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>9%</div> <div>••</div> <div>9%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	B	505	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6993 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nitric oxide synthase, 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	405	Total	As	C	N	O	S	0	0	0
			3229	1	2054	569	589	16			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	CYS	CONFLICT	UNP P29473
B	100	ARG	CYS	CONFLICT	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	C	Fe	N	O	0	0
			43	34	1	4	4		

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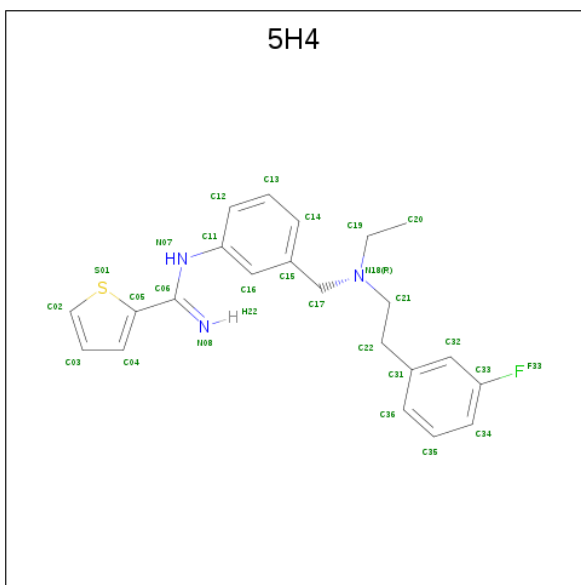
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



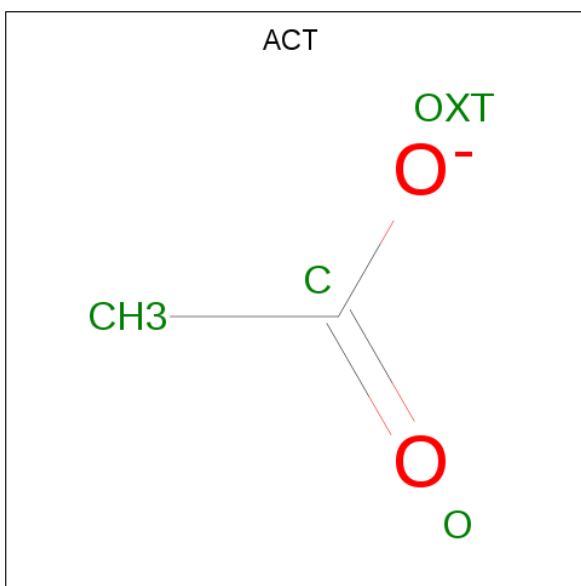
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			17	9	5	3		
3	B	1	Total	C	N	O	0	0
			17	9	5	3		

- Molecule 4 is N-[3-({ethyl[2-(3-fluorophenyl)ethyl]amino}methyl)phenyl]thiophene-2-carboximidamide (three-letter code: 5H4) (formula: $C_{22}H_{24}FN_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	S	0	0
			27	22	1	3	1		
4	B	1	Total	C	F	N	S	0	0
			27	22	1	3	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

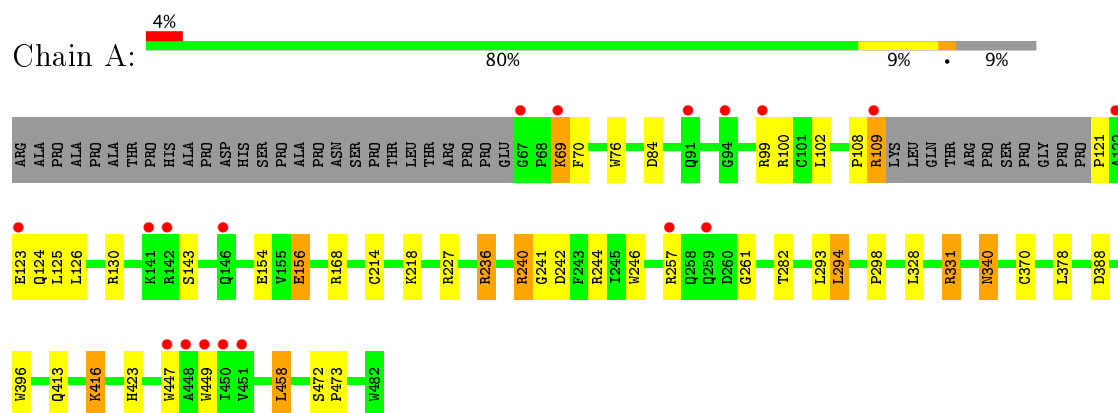
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	169	Total	O	0	0
			169	169		
8	B	177	Total	O	0	0
			177	177		

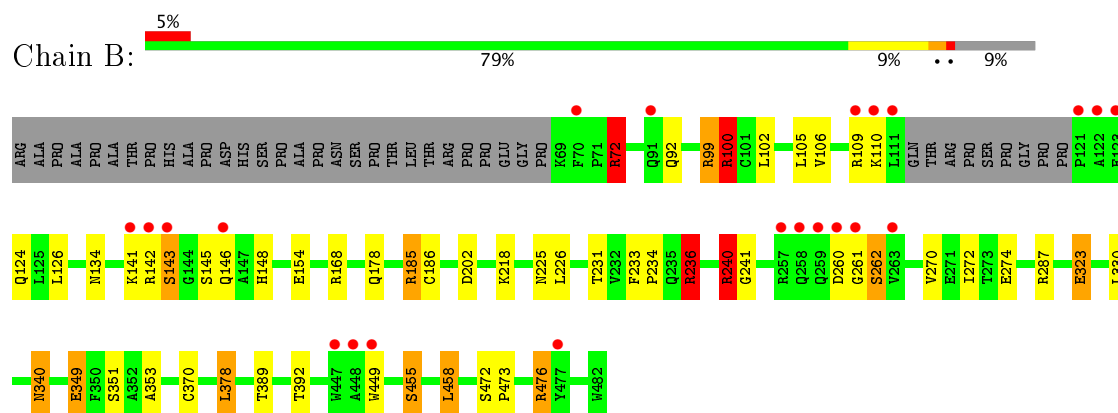
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nitric oxide synthase, 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 106.41Å 157.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.02 – 2.05 46.98 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.02-2.05) 99.0 (46.98-2.05)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.05Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.168 , 0.213 0.177 , 0.222	Depositor DCC
R_{free} test set	3031 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6993	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, H4B, CAS, 5H4, 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	1.00	2/3303 (0.1%)	0.99	8/4497 (0.2%)
1	B	1.01	2/3308 (0.1%)	1.02	7/4502 (0.2%)
All	All	1.00	4/6611 (0.1%)	1.00	15/8999 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	455	SER	CB-OG	6.03	1.50	1.42
1	B	349	GLU	CD-OE2	-5.19	1.20	1.25
1	A	396	TRP	CE3-CZ3	5.05	1.47	1.38
1	A	447	TRP	CZ3-CH2	5.02	1.48	1.40

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	240	ARG	NE-CZ-NH1	11.43	126.02	120.30
1	B	240	ARG	NE-CZ-NH2	-9.74	115.43	120.30
1	B	185	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	A	240	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	A	331	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	244	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	A	240	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	236	ARG	NE-CZ-NH1	-6.41	117.09	120.30
1	A	458	LEU	CB-CG-CD1	6.13	121.42	111.00
1	B	100	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	331	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	72	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	476	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	388	ASP	CB-CG-OD1	5.24	123.01	118.30
1	A	227	ARG	NE-CZ-NH1	5.14	122.87	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3223	0	3127	30	0
1	B	3229	0	3141	32	0
2	A	43	0	30	2	0
2	B	43	0	30	6	0
3	A	17	0	15	1	0
3	B	17	0	15	1	0
4	A	27	0	23	2	0
4	B	27	0	23	2	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
7	A	1	0	0	0	0
8	A	169	0	0	3	0
8	B	177	0	0	3	0
All	All	6993	0	6426	69	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (69) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PRO:HD3	8:A:735:HOH:O	1.67	0.94
1:A:126:LEU:HD23	1:A:130:ARG:NH2	1.95	0.82
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.65	0.76
1:B:236:ARG:HD3	1:B:351:SER:HB3	1.72	0.72
1:A:240:ARG:HD3	1:A:298:PRO:CB	2.23	0.68
1:B:287:ARG:HD3	8:B:683:HOH:O	1.95	0.67
2:B:501:HEM:HBC2	2:B:501:HEM:HMC1	1.79	0.64
1:B:233:PHE:HB3	1:B:234:PRO:CD	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD21	1:A:156:GLU:HB3	1.82	0.61
2:B:501:HEM:HBC2	2:B:501:HEM:CMC	2.31	0.59
1:B:186:CYS:HB2	2:B:501:HEM:ND	2.18	0.58
1:B:240:ARG:HD2	1:B:241:GLY:O	2.04	0.58
1:A:121:PRO:O	1:A:124:GLN:HB3	2.05	0.57
1:A:449:TRP:HA	3:A:502:H4B:N1	2.19	0.57
1:A:340:ASN:HD22	1:A:340:ASN:H	1.53	0.57
1:B:141:LYS:HB2	1:B:142:ARG:NH1	2.19	0.56
1:B:236:ARG:HG3	1:B:349:GLU:HB2	1.88	0.55
1:A:240:ARG:HD2	1:A:241:GLY:O	2.06	0.55
1:B:146:GLN:HA	1:B:146:GLN:OE1	2.07	0.55
1:B:186:CYS:HB2	2:B:501:HEM:C4D	2.41	0.55
1:A:214:CYS:O	1:A:218:LYS:HG3	2.07	0.53
1:A:109:ARG:CZ	1:B:72:ARG:HD3	2.39	0.53
1:A:126:LEU:HD11	1:A:156:GLU:HA	1.91	0.53
1:B:323:GLU:CD	1:B:323:GLU:H	2.13	0.53
1:A:378:LEU:HB2	8:A:648:HOH:O	2.07	0.53
1:B:472:SER:HA	1:B:473:PRO:C	2.30	0.52
2:B:501:HEM:HBB2	2:B:501:HEM:HHC	1.92	0.52
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.50	0.51
1:A:70:PHE:HB3	1:A:84:ASP:O	2.11	0.50
2:A:501:HEM:HBB2	2:A:501:HEM:HHC	1.94	0.50
1:A:108:PRO:CD	8:A:735:HOH:O	2.42	0.50
1:B:340:ASN:HD22	1:B:340:ASN:H	1.60	0.49
1:A:246:TRP:HB2	1:A:294:LEU:HB3	1.94	0.49
1:A:282:THR:HG22	1:A:282:THR:O	2.13	0.49
1:A:472:SER:HA	1:A:473:PRO:C	2.34	0.48
1:B:455:SER:HB3	1:B:458:LEU:HD22	1.94	0.47
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.53	0.47
1:B:260:ASP:OD2	1:B:260:ASP:O	2.31	0.47
1:A:236:ARG:HG2	1:A:242:ASP:OD1	2.15	0.47
1:A:69:LYS:HE2	1:A:69:LYS:HA	1.97	0.47
4:A:503:5H4:C05	4:A:503:5H4:C12	2.92	0.47
1:B:455:SER:O	1:B:458:LEU:HB2	2.15	0.47
1:B:99:ARG:HG2	1:B:100:ARG:HD2	1.96	0.46
2:B:501:HEM:CBC	2:B:501:HEM:HMC1	2.44	0.46
1:B:134:ASN:OD1	1:B:148:HIS:NE2	2.49	0.46
1:B:449:TRP:HA	3:B:502:H4B:N1	2.31	0.45
1:A:121:PRO:O	1:A:124:GLN:N	2.49	0.45
1:B:185:ARG:HG2	1:B:449:TRP:CG	2.51	0.45
1:B:260:ASP:O	1:B:262:SER:N	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ASN:H	1:A:340:ASN:ND2	2.15	0.44
4:A:503:5H4:H5	4:A:503:5H4:H11	1.68	0.43
1:B:231:THR:O	1:B:353:ALA:HA	2.18	0.43
1:A:340:ASN:HD22	1:A:340:ASN:N	2.13	0.43
1:A:76:TRP:CZ2	1:B:106:VAL:HB	2.53	0.43
1:B:145:SER:O	1:B:146:GLN:C	2.57	0.43
1:B:476:ARG:NH1	8:B:673:HOH:O	2.52	0.43
1:A:126:LEU:O	1:A:130:ARG:HG3	2.19	0.42
1:A:154:GLU:OE1	1:A:168:ARG:NH2	2.51	0.42
4:B:503:5H4:C05	4:B:503:5H4:C12	2.98	0.42
1:A:257:ARG:NH1	1:A:261:GLY:O	2.45	0.42
1:B:233:PHE:HB3	1:B:234:PRO:HD2	2.01	0.41
4:B:503:5H4:H5	4:B:503:5H4:H11	1.81	0.41
1:A:413:GLN:O	1:A:416:LYS:HE3	2.20	0.41
1:B:270:VAL:O	1:B:274:GLU:HG3	2.19	0.41
1:A:423:HIS:HB2	1:B:392:THR:HB	2.02	0.41
1:B:154:GLU:OE1	1:B:168:ARG:NH2	2.53	0.41
1:B:126:LEU:HD12	1:B:126:LEU:HA	1.85	0.41
2:A:501:HEM:HBC2	2:A:501:HEM:CMC	2.51	0.41
1:B:272:ILE:HG22	8:B:666:HOH:O	2.21	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%)	391 (98%)	9 (2%)	0	100	100
1	B	400/443 (90%)	376 (94%)	21 (5%)	3 (1%)	22	12
All	All	800/886 (90%)	767 (96%)	30 (4%)	3 (0%)	38	27

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	262	SER
1	B	143	SER
1	B	261	GLY

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	343/375 (92%)	326 (95%)	17 (5%)	28	19
1	B	344/375 (92%)	321 (93%)	23 (7%)	19	10
All	All	687/750 (92%)	647 (94%)	40 (6%)	23	13

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
1	A	99	ARG
1	A	100	ARG
1	A	102	LEU
1	A	109	ARG
1	A	123	GLU
1	A	125	LEU
1	A	143	SER
1	A	156	GLU
1	A	236	ARG
1	A	293	LEU
1	A	294	LEU
1	A	328	LEU
1	A	331	ARG
1	A	340	ASN
1	A	416	LYS
1	A	458	LEU
1	B	72	ARG
1	B	92	GLN
1	B	99	ARG
1	B	100	ARG

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Mol	Chain	Res	Type
1	B	102	LEU
1	B	105	LEU
1	B	109	ARG
1	B	110	LYS
1	B	124	GLN
1	B	143	SER
1	B	178	GLN
1	B	202	ASP
1	B	218	LYS
1	B	225	ASN
1	B	226	LEU
1	B	236	ARG
1	B	240	ARG
1	B	323	GLU
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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	166	HIS
1	A	191	GLN
1	A	340	ASN
1	A	376	ASN
1	A	468	ASN
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 molecules 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	6,8,9	1.16	0	2,9,11	1.06	0
1	CAS	B	384	1	6,8,9	1.00	0	2,9,11	1.59	1 (50%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	CAS	O-C-CA	-2.24	118.84	125.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	501	1	28,50,50	1.75	4 (14%)	17,82,82	1.56	2 (11%)
3	H4B	A	502	-	14,18,18	1.21	1 (7%)	12,26,26	2.11	4 (33%)
4	5H4	A	503	-	29,29,29	1.19	2 (6%)	31,38,38	1.49	4 (12%)
5	ACT	A	504	-	1,3,3	3.75	1 (100%)	0,3,3	0.00	-
6	GOL	A	505	-	5,5,5	0.53	0	5,5,5	1.14	0
2	HEM	B	501	1	28,50,50	1.38	3 (10%)	17,82,82	1.80	4 (23%)
3	H4B	B	502	-	14,18,18	1.18	2 (14%)	12,26,26	2.26	5 (41%)
4	5H4	B	503	-	29,29,29	1.35	4 (13%)	31,38,38	1.19	1 (3%)
5	ACT	B	504	-	1,3,3	2.81	1 (100%)	0,3,3	0.00	-
6	GOL	B	505	-	5,5,5	0.33	0	5,5,5	1.04	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
2	HEM	A	501	1	-	0/6/54/54	0/0/8/8
3	H4B	A	502	-	-	0/8/17/17	0/2/2/2
4	5H4	A	503	-	-	0/15/19/19	0/3/3/3
5	ACT	A	504	-	-	0/0/0/0	0/0/0/0
6	GOL	A	505	-	-	0/4/4/4	0/0/0/0
2	HEM	B	501	1	-	0/6/54/54	0/0/8/8
3	H4B	B	502	-	-	0/8/17/17	0/2/2/2
4	5H4	B	503	-	-	0/15/19/19	0/3/3/3
5	ACT	B	504	-	-	0/0/0/0	0/0/0/0
6	GOL	B	505	-	-	0/4/4/4	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C1B-NB	-5.36	1.30	1.36
5	A	504	ACT	CH3-C	-3.75	1.43	1.48
2	B	501	HEM	C3B-C2B	-3.68	1.35	1.40
2	B	501	HEM	C3C-C2C	-3.51	1.35	1.40
4	B	503	5H4	C06-N07	-3.33	1.32	1.39
4	B	503	5H4	C11-N07	-3.27	1.35	1.41
3	A	502	H4B	C4-C4A	-3.13	1.37	1.41
2	A	501	HEM	C3B-C2B	-2.94	1.36	1.40
5	B	504	ACT	CH3-C	-2.81	1.45	1.48
4	A	503	5H4	C06-N07	-2.76	1.33	1.39
3	B	502	H4B	C4-C4A	-2.41	1.38	1.41
4	B	503	5H4	C32-C33	2.09	1.41	1.37
3	B	502	H4B	C2-N3	2.11	1.39	1.35
2	A	501	HEM	C1A-NA	2.16	1.40	1.36
2	B	501	HEM	CAD-C3D	2.20	1.56	1.52
4	B	503	5H4	C05-S01	3.00	1.76	1.72
4	A	503	5H4	C05-C06	3.32	1.50	1.45
2	A	501	HEM	C4C-NC	5.20	1.42	1.36

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	503	5H4	C03-C02-S01	-4.50	108.33	113.18
2	B	501	HEM	CBA-CAA-C2A	-3.84	105.13	112.48
2	B	501	HEM	CMA-C3A-C4A	-2.98	123.89	128.46
4	A	503	5H4	C34-C33-C32	-2.87	119.52	123.29
3	B	502	H4B	N3-C2-N1	-2.30	121.72	125.45
2	A	501	HEM	C4C-C3C-C2C	-2.29	105.30	106.90
4	A	503	5H4	C12-C11-C16	-2.27	117.00	119.66
3	A	502	H4B	N3-C2-N1	-2.04	122.14	125.45
3	B	502	H4B	O9-C9-C6	2.55	115.08	108.98
3	B	502	H4B	C2-N1-C8A	2.58	120.33	114.51
3	A	502	H4B	C4-N3-C2	2.86	120.17	116.06
2	B	501	HEM	C4A-C3A-C2A	2.91	109.02	107.00
3	A	502	H4B	N2-C2-N3	3.27	122.47	117.24
2	B	501	HEM	CBD-CAD-C3D	3.27	118.71	112.47
4	A	503	5H4	C15-C17-N18	3.67	120.23	113.17
3	B	502	H4B	N2-C2-N3	3.92	123.50	117.24
2	A	501	HEM	CAA-CBA-CGA	4.00	119.50	112.66
4	B	503	5H4	C15-C17-N18	4.12	121.10	113.17
3	B	502	H4B	C4-C4A-C8A	4.20	118.36	114.56
3	A	502	H4B	C4-C4A-C8A	4.29	118.45	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	2	0
3	A	502	H4B	1	0
4	A	503	5H4	2	0
2	B	501	HEM	6	0
3	B	502	H4B	1	0
4	B	503	5H4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	404/443 (91%)	-0.05	18 (4%) 34 37	30, 42, 69, 98	0
1	B	404/443 (91%)	-0.02	22 (5%) 26 29	29, 43, 72, 105	0
All	All	808/886 (91%)	-0.04	40 (4%) 30 32	29, 43, 71, 105	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	GLN	5.5
1	B	110	LYS	5.0
1	A	67	GLY	4.0
1	A	123	GLU	3.8
1	B	121	PRO	3.8
1	A	91	GLN	3.6
1	B	142	ARG	3.5
1	A	99	ARG	3.4
1	A	122	ALA	3.4
1	B	146	GLN	3.1
1	A	259	GLN	3.1
1	B	448	ALA	3.1
1	A	450	ILE	3.1
1	B	122	ALA	3.1
1	B	261	GLY	3.1
1	B	263	VAL	3.0
1	B	449	TRP	2.8
1	B	123	GLU	2.7
1	A	448	ALA	2.7
1	B	447	TRP	2.7
1	A	109	ARG	2.7
1	B	141	LYS	2.7
1	A	451	VAL	2.6
1	A	449	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	146	GLN	2.5
1	A	141	LYS	2.5
1	A	447	TRP	2.4
1	B	109	ARG	2.4
1	B	260	ASP	2.4
1	A	69	LYS	2.4
1	B	477	TYR	2.3
1	B	70	PHE	2.3
1	B	143	SER	2.3
1	B	91	GLN	2.2
1	B	258	GLN	2.2
1	A	142	ARG	2.2
1	A	94	GLY	2.2
1	B	111	LEU	2.1
1	A	257	ARG	2.1
1	B	257	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CAS	A	384	9/10	0.97	0.08	-	40,42,63,69	0
1	CAS	B	384	9/10	0.97	0.08	-	43,48,62,66	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	GOL	B	505	6/6	0.93	0.25	2.20	58,66,76,86	0
5	ACT	B	504	4/4	0.91	0.17	1.80	47,48,55,60	0
6	GOL	A	505	6/6	0.91	0.21	1.67	60,66,73,73	0
5	ACT	A	504	4/4	0.90	0.17	1.23	41,42,46,59	0
4	5H4	B	503	27/27	0.96	0.17	1.02	27,40,95,99	0
2	HEM	A	501	43/43	0.98	0.17	0.74	30,36,40,42	0
4	5H4	A	503	27/27	0.95	0.16	0.74	28,43,96,105	0
2	HEM	B	501	43/43	0.98	0.16	0.38	29,34,45,48	0
3	H4B	A	502	17/17	0.98	0.18	0.20	34,38,43,45	0
3	H4B	B	502	17/17	0.98	0.18	0.12	33,36,48,54	0
7	ZN	A	506	1/1	0.99	0.04	-2.29	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.