



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 12:59 AM GMT

PDB ID : 1D0C
Title : BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN
COMPLEXED WITH 3-BROMO-7-NITROINDAZOLE(H4B FREE)
Authors : Raman, C.S.; Li, H.; Martasek, P.; Southan, G.J.; Masters, B.S.S.; Poulos,
T.L.
Deposited on : 1999-09-09
Resolution : 1.65 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>

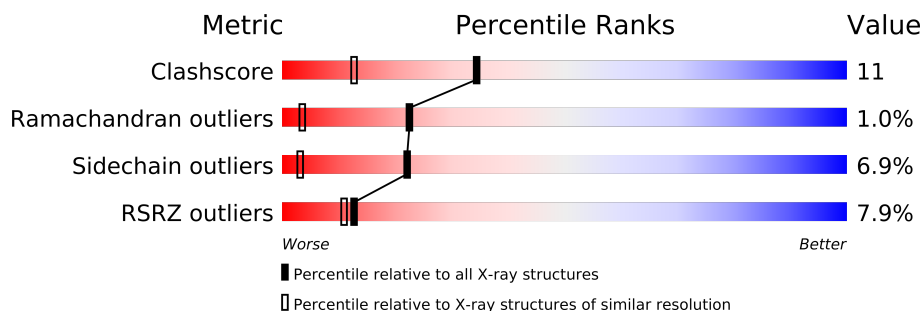
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1001 (1.66-1.66)
Ramachandran outliers	78287	1581 (1.68-1.64)
Sidechain outliers	78261	1580 (1.68-1.64)
RSRZ outliers	66119	1404 (1.68-1.64)

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	444	
1	B	444	

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
6	CAD	A	950	-	X
6	CAD	B	951	-	X
7	GOL	B	881	-	X

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 7428 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.

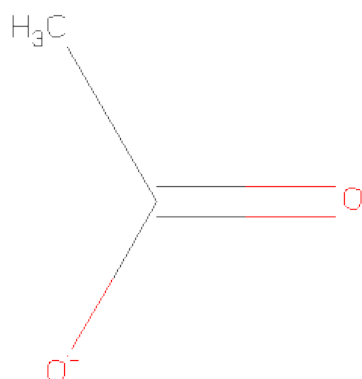
- Molecule 1 is a protein called BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	1	0
			3303	2099	584	604	16			
1	B	414	Total	C	N	O	S	0	1	0
			3292	2092	582	602	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 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		

Continued on next page...

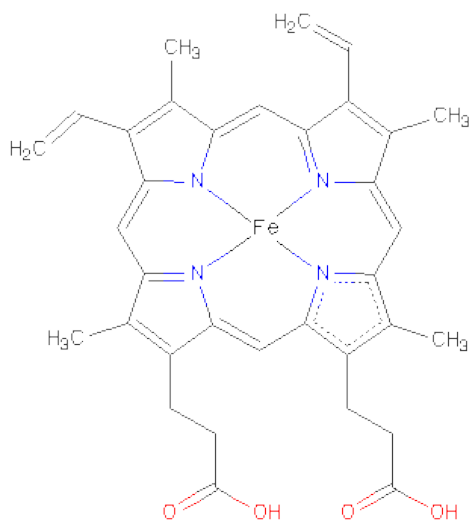
Continued from previous page...

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		
2	B	1	Total	C	O	0	0
			4	2	2		

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

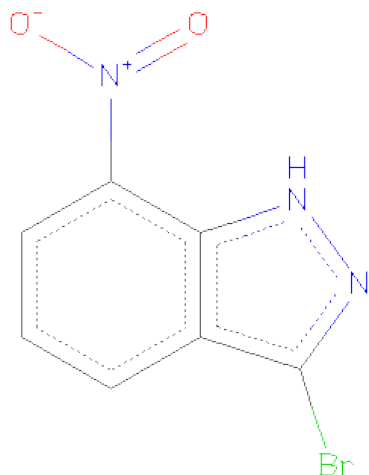
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



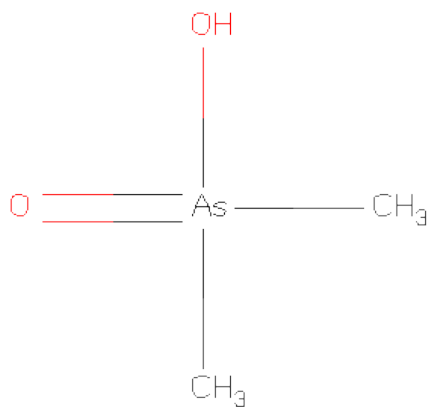
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
4	B	1	Total	C	Fe	N	O	0	1
			48	37	1	4	6		

- Molecule 5 is 3-BROMO-7-NITROINDAZOLE (three-letter code: INE) (formula: $C_7H_4BrN_3O_2$).



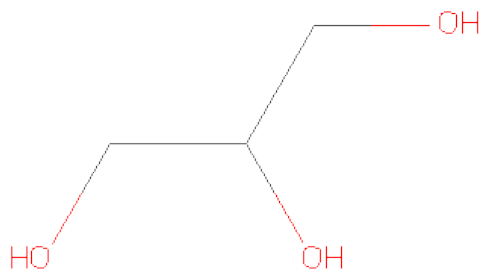
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	Br	C	N	O	0	0
			13	1	7	3	2		
5	B	1	Total	Br	C	N	O	0	0
			13	1	7	3	2		
5	B	1	Total	Br	C	N	O	0	0
			13	1	7	3	2		
5	A	1	Total	Br	C	N	O	0	0
			13	1	7	3	2		

- Molecule 6 is CACODYLIC ACID (three-letter code: CAD) (formula: $C_2H_7AsO_2$).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is water.

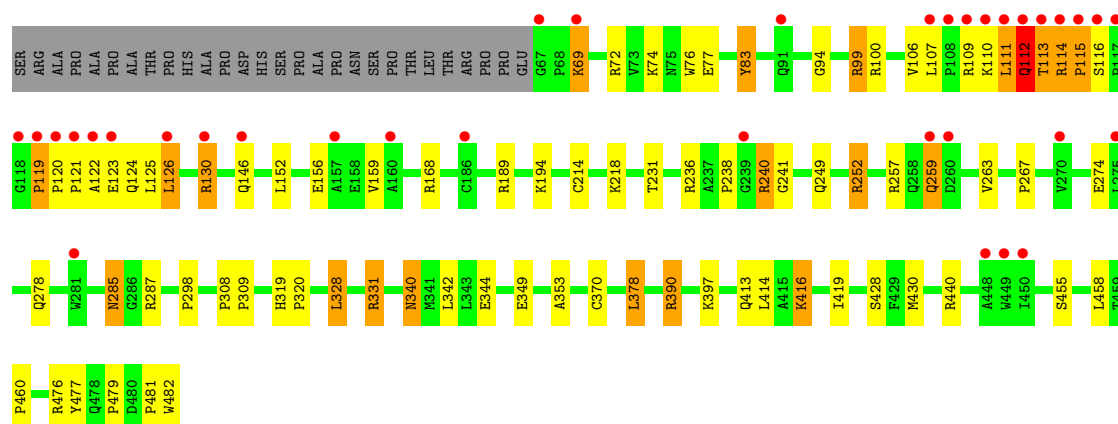
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	348	Total	O	0	0
			348	348		
8	B	307	Total	O	0	0
			307	307		

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.

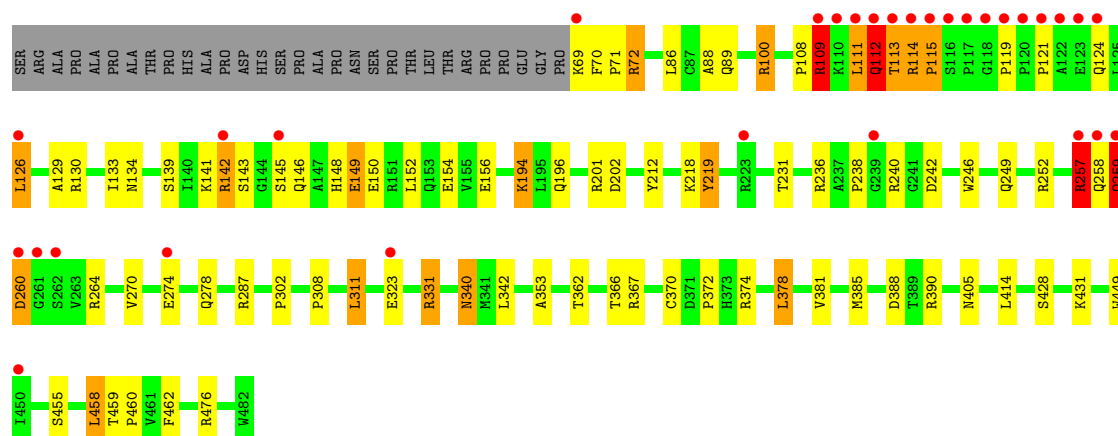
• Molecule 1: BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN

Chain A: 



• Molecule 1: BOVINE ENDOTHELIAL NITRIC OXIDE SYNTHASE HEME DOMAIN

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	57.44Å 105.98Å 155.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 1.65 48.04 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.0 (8.00-1.65) 92.2 (48.04-1.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 1.65Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.213 , 0.259 0.193 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 65.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 113260 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7428	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: GOL, ZN, ACT, HEM, INE, CAD

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	0.57	2/3403 (0.1%)	1.07	11/4639 (0.2%)
1	B	0.46	2/3391 (0.1%)	1.05	9/4622 (0.2%)
All	All	0.52	4/6794 (0.1%)	1.06	20/9261 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	428[A]	SER	CB-OG	-15.10	1.22	1.42
1	A	428[B]	SER	CB-OG	-15.10	1.22	1.42
1	B	428[A]	SER	CB-OG	-7.79	1.32	1.42
1	B	428[B]	SER	CB-OG	-7.79	1.32	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	252	ARG	NE-CZ-NH2	-9.45	115.58	120.30
1	B	240	ARG	NE-CZ-NH1	-9.36	115.62	120.30
1	A	252	ARG	NH1-CZ-NH2	7.02	127.12	119.40
1	B	331	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	A	331	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	A	440	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	A	440	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	B	100	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	83	TYR	CB-CG-CD1	-6.22	117.27	121.00
1	A	252	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	B	219	TYR	CB-CG-CD1	5.89	124.53	121.00
1	A	168	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	130	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	374	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	367	ARG	NE-CZ-NH1	5.20	122.90	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	328	LEU	CA-CB-CG	5.14	127.13	115.30
1	B	201	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	462	PHE	CB-CG-CD2	5.02	124.31	120.80
1	B	212	TYR	CB-CG-CD1	-5.01	117.99	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3303	0	3216	71	0
1	B	3292	0	3206	74	0
2	A	8	0	6	0	0
2	B	8	0	6	0	0
3	A	1	0	0	0	0
4	A	43	0	30	0	0
4	B	48	0	8	3	0
5	A	26	0	8	0	0
5	B	26	0	8	1	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
7	A	6	0	8	0	0
7	B	6	0	8	0	0
8	A	348	0	0	12	0
8	B	307	0	0	7	0
All	All	7428	0	6504	143	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 11.

All (143) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:111:LEU:HD23	1:A:476:ARG:HG2	1.35	1.08
1:B:114:ARG:HH11	1:B:114:ARG:HA	1.22	1.04
1:B:115:PRO:HA	1:B:236:ARG:HH12	1.26	0.99
1:B:114:ARG:HD3	1:B:115:PRO:HD2	1.46	0.95
1:A:109:ARG:O	1:A:110:LYS:HD2	1.71	0.90
1:A:99:ARG:HH11	1:A:99:ARG:HB2	1.45	0.81
1:B:121:PRO:HD2	1:B:124:GLN:OE1	1.81	0.81
1:A:111:LEU:CD2	1:A:476:ARG:HG2	2.12	0.80
1:B:152:LEU:O	1:B:156:GLU:HG3	1.83	0.78
1:B:258:GLN:OE1	1:B:264:ARG:HB2	1.83	0.78
1:A:119:PRO:HG3	1:A:238:PRO:HG3	1.66	0.77
1:A:152:LEU:O	1:A:156:GLU:HG3	1.85	0.77
1:A:106:VAL:HG12	1:A:107:LEU:HD23	1.69	0.73
1:B:126:LEU:O	1:B:130:ARG:HG3	1.93	0.69
1:B:86:LEU:O	1:B:89:GLN:HG2	1.94	0.68
1:A:274:GLU:O	1:A:278:GLN:HG3	1.93	0.68
1:B:119:PRO:HG3	1:B:238:PRO:HG3	1.76	0.67
1:B:257:ARG:HH11	1:B:270:VAL:HG11	1.62	0.64
1:B:150:GLU:O	1:B:154:GLU:HG3	1.98	0.63
1:A:126:LEU:HD23	1:A:159:VAL:HG11	1.81	0.62
1:B:113:THR:HG21	1:B:342:LEU:HD22	1.82	0.62
1:B:126:LEU:HD22	1:B:130:ARG:HG3	1.81	0.62
1:B:115:PRO:HA	1:B:236:ARG:NH1	2.07	0.61
1:B:257:ARG:HD3	1:B:270:VAL:HG11	1.84	0.60
1:A:397:LYS:HE3	8:A:1245:HOH:O	2.01	0.59
1:A:413:GLN:O	1:A:416:LYS:HE3	2.01	0.59
1:A:74:LYS:HE2	1:A:76:TRP:CE3	2.37	0.59
1:A:94:GLY:HA3	8:A:1281:HOH:O	2.03	0.59
1:A:113:THR:O	1:A:115:PRO:HD3	2.03	0.59
1:B:126:LEU:HD21	1:B:156:GLU:HG2	1.85	0.58
1:B:370:CYS:SG	1:B:378:LEU:HD13	2.43	0.58
1:A:126:LEU:HD11	1:A:156:GLU:HG2	1.86	0.57
1:A:126:LEU:O	1:A:130:ARG:HG3	2.04	0.57
1:A:340:ASN:H	1:A:340:ASN:HD22	1.51	0.57
1:A:120:PRO:HB2	1:A:125:LEU:HB2	1.87	0.57
1:A:455:SER:HB3	1:A:458:LEU:HD12	1.85	0.57
1:A:481:PRO:HD2	1:A:482:TRP:CZ3	2.40	0.56
1:B:249:GLN:HB2	1:B:252:ARG:HG3	1.87	0.56
1:A:378:LEU:HB2	8:A:1013:HOH:O	2.06	0.56
1:B:114:ARG:NH1	1:B:114:ARG:HA	2.06	0.56
1:A:240:ARG:HD3	1:A:298:PRO:HB3	1.88	0.56
1:B:119:PRO:HG3	1:B:238:PRO:CG	2.36	0.55
1:A:106:VAL:HG12	1:A:107:LEU:CD2	2.35	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:381:VAL:O	1:B:385:MET:HG3	2.07	0.54
1:B:236:ARG:HD2	1:B:242:ASP:OD2	2.07	0.54
1:B:108:PRO:CB	1:B:111:LEU:HB2	2.38	0.54
1:B:108:PRO:HB3	1:B:111:LEU:HB2	1.90	0.54
1:A:285:ASN:HB2	8:A:1190:HOH:O	2.07	0.53
1:A:69:LYS:HG2	1:A:69:LYS:O	2.06	0.53
1:A:99:ARG:HH21	1:B:88:ALA:HA	1.73	0.53
1:A:130:ARG:HD3	8:A:1148:HOH:O	2.08	0.53
1:A:99:ARG:CB	1:A:99:ARG:HH11	2.20	0.53
1:B:111:LEU:O	1:B:112:GLN:O	2.27	0.53
1:B:449:TRP:CZ3	4:B:500[B]:HEM:O1A	2.63	0.52
1:B:449:TRP:CE3	4:B:500[B]:HEM:O1A	2.63	0.52
1:A:390:ARG:N	1:A:390:ARG:HD3	2.24	0.51
1:B:274:GLU:HA	1:B:274:GLU:OE1	2.10	0.51
1:B:114:ARG:O	1:B:115:PRO:O	2.29	0.51
1:B:246:TRP:CZ2	1:B:302:PRO:HG3	2.46	0.51
1:B:388:ASP:OD2	1:B:390:ARG:NH2	2.44	0.51
1:A:72:ARG:HD2	1:A:83:TYR:CE2	2.46	0.51
1:A:115:PRO:CD	1:A:479:PRO:HG2	2.41	0.50
1:A:390:ARG:H	1:A:390:ARG:HD3	1.76	0.50
1:A:112:GLN:NE2	1:A:477:TYR:HB2	2.25	0.50
1:B:149:GLU:OE1	1:B:149:GLU:O	2.30	0.50
1:B:414:LEU:HD23	8:B:1012:HOH:O	2.10	0.50
1:A:109:ARG:C	1:A:110:LYS:HD2	2.32	0.49
1:B:287:ARG:HD3	8:B:1060:HOH:O	2.12	0.49
1:A:236:ARG:NH1	1:A:349:GLU:OE2	2.44	0.49
1:B:126:LEU:HD22	1:B:130:ARG:CG	2.42	0.49
1:A:119:PRO:HG3	1:A:238:PRO:CG	2.39	0.48
1:A:74:LYS:HE2	1:A:76:TRP:CD2	2.48	0.48
1:A:342:LEU:HD11	1:A:349:GLU:HB3	1.94	0.48
1:A:370:CYS:SG	1:A:378:LEU:HD13	2.54	0.48
1:A:109:ARG:HH11	1:A:109:ARG:HG2	1.78	0.48
1:A:214:CYS:O	1:A:218:LYS:HG3	2.14	0.47
1:B:308:PRO:O	1:B:311:LEU:HB2	2.13	0.47
1:B:142:ARG:O	1:B:145:SER:OG	2.30	0.47
1:A:285:ASN:N	1:A:285:ASN:HD22	2.10	0.47
1:B:202:ASP:HB3	8:B:1075:HOH:O	2.15	0.47
1:B:146:GLN:NE2	1:B:150:GLU:OE2	2.48	0.47
1:B:388:ASP:OD1	1:B:390:ARG:HG3	2.15	0.47
1:B:308:PRO:HG2	1:B:311:LEU:HD22	1.96	0.47
1:A:458:LEU:HD22	1:B:378:LEU:HD21	1.96	0.46
1:B:129:ALA:O	1:B:133:ILE:HG12	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:249:GLN:HB2	1:A:252:ARG:HG2	1.97	0.46
1:B:108:PRO:CG	1:B:111:LEU:HB2	2.45	0.46
1:B:459:THR:HB	1:B:460:PRO:HD2	1.96	0.46
1:B:258:GLN:O	1:B:260:ASP:N	2.49	0.46
1:A:331:ARG:HD2	8:A:1242:HOH:O	2.15	0.46
1:B:257:ARG:NH1	1:B:270:VAL:HG11	2.30	0.46
1:A:430:MET:HG3	1:A:460:PRO:HB2	1.97	0.46
1:B:340:ASN:HD22	1:B:340:ASN:H	1.64	0.46
1:B:231:THR:O	1:B:353:ALA:HA	2.15	0.46
1:A:259:GLN:O	1:A:259:GLN:NE2	2.50	0.45
1:B:109:ARG:NH2	8:B:1068:HOH:O	2.48	0.45
1:A:122:ALA:O	1:A:126:LEU:HB2	2.16	0.45
1:A:115:PRO:HD3	1:A:479:PRO:HG2	1.99	0.45
1:B:126:LEU:HD11	1:B:156:GLU:HG2	1.98	0.45
1:A:107:LEU:HD22	1:A:477:TYR:CE2	2.51	0.45
1:B:112:GLN:CG	1:B:113:THR:H	2.29	0.45
1:B:259:GLN:HG3	1:B:260:ASP:OD1	2.16	0.45
1:A:240:ARG:NH2	8:A:1228:HOH:O	2.49	0.45
1:B:431:LYS:NZ	8:B:1108:HOH:O	2.49	0.45
1:B:126:LEU:HD11	1:B:156:GLU:CG	2.46	0.45
1:A:240:ARG:HD3	1:A:241:GLY:O	2.17	0.45
1:A:72:ARG:NH1	8:A:1215:HOH:O	2.49	0.45
1:B:72:ARG:NH1	8:B:1125:HOH:O	2.50	0.45
1:A:231:THR:O	1:A:353:ALA:HA	2.17	0.45
1:A:344:GLU:HG3	8:A:1075:HOH:O	2.17	0.45
1:A:319:HIS:CG	1:A:320:PRO:HD2	2.52	0.45
5:B:765:INE:N1	5:B:765:INE:O12	2.50	0.45
1:A:111:LEU:HD21	8:A:994:HOH:O	2.17	0.44
1:A:477:TYR:HD2	8:A:1211:HOH:O	2.00	0.44
1:B:264:ARG:NH1	1:B:287:ARG:HG3	2.32	0.44
1:A:126:LEU:HA	1:A:126:LEU:HD22	1.64	0.44
1:A:112:GLN:NE2	8:A:1211:HOH:O	2.50	0.44
1:B:257:ARG:HD3	1:B:270:VAL:CG1	2.46	0.44
1:A:340:ASN:HD22	1:A:340:ASN:N	2.17	0.43
1:B:70:PHE:HA	1:B:71:PRO:HD3	1.71	0.43
1:A:106:VAL:C	1:A:107:LEU:HD23	2.39	0.43
1:A:112:GLN:HE21	1:A:112:GLN:HB2	1.57	0.43
1:A:126:LEU:CD2	1:A:159:VAL:HG21	2.49	0.43
1:B:449:TRP:CZ3	4:B:500[A]:HEM:O1A	2.72	0.43
1:A:121:PRO:HB2	1:A:124:GLN:HB2	2.00	0.42
1:A:113:THR:O	1:A:479:PRO:HD3	2.19	0.42
1:B:196:GLN:HG2	1:B:219:TYR:CE1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:134:ASN:OD1	1:B:148:HIS:NE2	2.48	0.42
1:A:263:VAL:HG11	1:A:267:PRO:HA	2.01	0.42
1:B:108:PRO:HB3	1:B:111:LEU:HD22	2.00	0.41
1:B:194:LYS:HD3	8:B:1190:HOH:O	2.20	0.41
1:B:126:LEU:HD23	1:B:126:LEU:HA	1.90	0.41
1:A:114:ARG:HH21	1:A:479:PRO:HB3	1.85	0.41
1:B:246:TRP:CH2	1:B:302:PRO:HG3	2.56	0.41
1:B:218:LYS:HE3	1:B:218:LYS:HB3	1.79	0.41
1:A:194:LYS:O	1:A:194:LYS:HG2	2.20	0.41
1:A:308:PRO:HA	1:A:309:PRO:HD3	1.91	0.41
1:B:455:SER:O	1:B:458:LEU:HB2	2.21	0.41
1:B:264:ARG:NH1	1:B:264:ARG:HG3	2.36	0.41
1:B:86:LEU:HD12	1:B:89:GLN:HG3	2.03	0.41
1:B:366:THR:O	1:B:370:CYS:HB2	2.21	0.41
1:A:77:GLU:HG3	1:B:372:PRO:HG2	2.03	0.40
1:B:362:THR:HA	1:B:405:ASN:HD21	1.86	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	415/444 (94%)	402 (97%)	10 (2%)	3 (1%)	30	8
1	B	413/444 (93%)	396 (96%)	12 (3%)	5 (1%)	19	2
All	All	828/888 (93%)	798 (96%)	22 (3%)	8 (1%)	22	3

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	112	GLN
1	B	115	PRO
1	B	259	GLN
1	A	119	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	257	ARG
1	B	109	ARG
1	A	112	GLN
1	A	115	PRO

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	355/377 (94%)	332 (94%)	23 (6%)	24	4
1	B	354/377 (94%)	328 (93%)	26 (7%)	20	3
All	All	709/754 (94%)	660 (93%)	49 (7%)	22	3

All (49) 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	111	LEU
1	A	112	GLN
1	A	113	THR
1	A	114	ARG
1	A	116	SER
1	A	123	GLU
1	A	126	LEU
1	A	146	GLN
1	A	240	ARG
1	A	257	ARG
1	A	259	GLN
1	A	285	ASN
1	A	287	ARG
1	A	328	LEU
1	A	340	ASN
1	A	378	LEU
1	A	390	ARG
1	A	414	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	416	LYS
1	A	419	ILE
1	B	69	LYS
1	B	72	ARG
1	B	100	ARG
1	B	109	ARG
1	B	111	LEU
1	B	112	GLN
1	B	113	THR
1	B	114	ARG
1	B	126	LEU
1	B	139	SER
1	B	141	LYS
1	B	142	ARG
1	B	143	SER
1	B	149	GLU
1	B	194	LYS
1	B	257	ARG
1	B	259	GLN
1	B	260	ASP
1	B	278	GLN
1	B	311	LEU
1	B	323	GLU
1	B	331	ARG
1	B	340	ASN
1	B	378	LEU
1	B	458	LEU
1	B	476	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	124	GLN
1	A	153	GLN
1	A	191	GLN
1	A	258	GLN
1	A	259	GLN
1	A	278	GLN
1	A	285	ASN
1	A	340	ASN
1	A	376	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	413	GLN
1	A	468	ASN
1	B	146	GLN
1	B	191	GLN
1	B	222	ASN
1	B	225	ASN
1	B	278	GLN
1	B	340	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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	500	1	49,50,50	1.82	9 (18%)	46,82,82	1.72	12 (26%)
5	INE	A	760	-	14,14,14	3.80	7 (50%)	15,20,20	2.44	6 (40%)
5	INE	A	766	-	14,14,14	3.73	7 (50%)	15,20,20	1.78	3 (20%)
2	ACT	A	850	-	1,3,3	2.30	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	A	860	-	1,3,3	2.44	1 (100%)	0,3,3	0.00	-
7	GOL	A	880	-	5,5,5	0.19	0	5,5,5	0.31	0
6	CAD	A	950	1	2,2,4	0.47	0	0,1,6	0.00	-
4	HEM	B	500[A]	-	4,4,50	8.83	1 (25%)	3,4,82	1.03	0
4	HEM	B	500[B]	-	4,4,50	6.07	1 (25%)	3,4,82	1.73	1 (33%)
5	INE	B	761	-	14,14,14	3.54	6 (42%)	15,20,20	1.89	4 (26%)
5	INE	B	765	-	14,14,14	3.74	6 (42%)	15,20,20	1.95	3 (20%)
2	ACT	B	851	-	1,3,3	2.43	1 (100%)	0,3,3	0.00	-
2	ACT	B	861	-	1,3,3	2.71	1 (100%)	0,3,3	0.00	-
7	GOL	B	881	-	5,5,5	0.61	0	5,5,5	0.80	0
6	CAD	B	951	1	2,2,4	0.49	0	0,1,6	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	500	1	-	0/14/114/114	0/0/8/8
5	INE	A	760	-	-	0/4/4/4	0/0/2/2
5	INE	A	766	-	-	0/4/4/4	0/0/2/2
2	ACT	A	850	-	-	0/0/0/0	0/0/0/0
2	ACT	A	860	-	-	0/0/0/0	0/0/0/0
7	GOL	A	880	-	-	0/4/4/4	0/0/0/0
6	CAD	A	950	1	-	0/0/0/0	0/0/0/0
4	HEM	B	500[A]	-	-	0/2/2/114	0/0/0/8
4	HEM	B	500[B]	-	-	0/2/2/114	0/0/0/8
5	INE	B	761	-	-	0/4/4/4	0/0/2/2
5	INE	B	765	-	-	0/4/4/4	0/0/2/2
2	ACT	B	851	-	-	0/0/0/0	0/0/0/0
2	ACT	B	861	-	-	0/0/0/0	0/0/0/0
7	GOL	B	881	-	-	0/4/4/4	0/0/0/0
6	CAD	B	951	1	-	0/0/0/0	0/0/0/0

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	500[A]	HEM	CAA-CBA	-17.56	1.48	1.55
4	B	500[B]	HEM	CAA-CBA	12.04	1.60	1.55
5	A	760	INE	C7-N10	-9.04	1.32	1.46
5	A	760	INE	BR-C3	-8.55	1.76	1.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	761	INE	C7-N10	-8.52	1.33	1.46
5	A	766	INE	BR-C3	-8.19	1.77	1.90
5	B	765	INE	C7-N10	-8.08	1.34	1.46
5	A	766	INE	C7-N10	-7.93	1.34	1.46
5	B	765	INE	BR-C3	-7.88	1.77	1.90
5	B	761	INE	BR-C3	-6.90	1.79	1.90
5	B	765	INE	C3-N2	5.60	1.45	1.34
5	A	766	INE	C3-N2	5.50	1.45	1.34
4	A	500	HEM	C3C-C2C	-4.75	1.35	1.43
4	A	500	HEM	C4A-C3A	4.45	1.45	1.40
5	A	760	INE	C3-N2	4.41	1.43	1.34
4	A	500	HEM	CHB-C1B	4.38	1.42	1.35
5	B	761	INE	C3-N2	4.24	1.42	1.34
4	A	500	HEM	C3D-C2D	-4.23	1.36	1.43
4	A	500	HEM	C3B-C2B	-4.04	1.36	1.43
5	B	761	INE	O11-N10	-3.85	1.18	1.25
5	B	765	INE	O11-N10	-3.62	1.19	1.25
4	A	500	HEM	CHA-C4D	3.21	1.40	1.35
5	A	766	INE	O11-N10	-3.20	1.19	1.25
5	B	761	INE	C8-N1	-3.10	1.31	1.38
5	B	765	INE	C8-N1	-3.08	1.31	1.38
4	A	500	HEM	C3D-C4D	-3.08	1.43	1.44
5	A	766	INE	C8-N1	-2.96	1.31	1.38
5	A	760	INE	C8-N1	-2.95	1.31	1.38
2	B	861	ACT	CH3-C	2.71	1.52	1.48
2	A	860	ACT	CH3-C	2.44	1.52	1.48
2	B	851	ACT	CH3-C	2.43	1.52	1.48
2	A	850	ACT	CH3-C	2.30	1.52	1.48
5	A	760	INE	C9-C8	-2.28	1.37	1.41
5	A	766	INE	C3-C9	-2.22	1.38	1.45
5	A	760	INE	C5-C4	2.18	1.41	1.36
5	B	765	INE	C9-C8	-2.16	1.37	1.41
5	A	760	INE	O11-N10	-2.12	1.21	1.25
4	A	500	HEM	CHD-C4C	2.10	1.40	1.36
5	A	766	INE	C9-C8	-2.10	1.37	1.41
4	A	500	HEM	CMC-C2C	2.06	1.53	1.47
5	B	761	INE	C9-C8	-2.05	1.37	1.41

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	765	INE	C6-C7-N10	4.84	123.59	116.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	760	INE	C6-C7-N10	4.46	123.04	116.61
5	A	760	INE	BR-C3-C9	4.40	128.68	122.87
5	A	760	INE	C7-C8-C9	4.09	121.60	117.31
4	A	500	HEM	C4A-CHB-C1B	-3.93	122.30	127.47
5	A	766	INE	C6-C7-N10	3.85	122.16	116.61
4	A	500	HEM	C1B-NB-C4B	-3.78	101.30	105.16
5	B	761	INE	C6-C7-N10	3.73	121.98	116.61
5	A	766	INE	BR-C3-C9	3.64	127.67	122.87
5	B	765	INE	BR-C3-C9	3.36	127.30	122.87
5	B	761	INE	BR-C3-C9	3.31	127.24	122.87
4	A	500	HEM	C4D-ND-C1D	-3.30	101.78	105.16
5	B	761	INE	C7-C8-C9	3.22	120.69	117.31
5	A	760	INE	O12-N10-C7	3.04	127.56	119.33
5	A	760	INE	O11-N10-O12	-3.02	115.24	121.35
4	A	500	HEM	CMA-C3A-C2A	2.92	130.44	124.94
4	A	500	HEM	CHD-C1D-ND	-2.91	122.17	124.58
4	A	500	HEM	CMA-C3A-C4A	-2.89	124.17	128.62
4	A	500	HEM	C4A-C3A-C2A	-2.69	105.12	107.00
4	A	500	HEM	C3A-C4A-CHB	-2.67	120.93	126.00
4	A	500	HEM	CAD-C3D-C4D	2.67	129.33	124.53
5	B	765	INE	C7-C8-C9	2.65	120.09	117.31
4	A	500	HEM	C3A-C4A-NA	2.61	111.38	109.41
5	B	761	INE	O11-N10-O12	-2.51	116.28	121.35
5	A	766	INE	C7-C8-C9	2.40	119.83	117.31
4	B	500[B]	HEM	O2A-CGA-CBA	2.35	121.04	113.70
4	A	500	HEM	C3B-C4B-NB	-2.34	112.32	114.00
5	A	760	INE	C5-C4-C9	-2.18	117.70	120.88
4	A	500	HEM	C1A-CHA-C4D	-2.11	124.69	127.47

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	416/444 (93%)	0.53	35 (8%) 11 9	17, 27, 63, 123	0
1	B	414/444 (93%)	0.47	31 (7%) 14 12	19, 29, 65, 137	0
All	All	830/888 (93%)	0.50	66 (7%) 13 10	17, 28, 65, 137	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	111	LEU	17.6
1	B	117	PRO	16.6
1	A	113	THR	16.6
1	B	113	THR	15.4
1	A	119	PRO	14.6
1	B	115	PRO	11.9
1	B	114	ARG	11.7
1	A	111	LEU	11.1
1	A	117	PRO	10.7
1	B	110	LYS	10.4
1	B	118	GLY	10.2
1	B	259	GLN	9.9
1	B	119	PRO	9.8
1	B	261	GLY	9.1
1	B	116	SER	9.1
1	A	110	LYS	9.0
1	A	120	PRO	8.5
1	B	112	GLN	7.3
1	A	121	PRO	6.6
1	A	115	PRO	6.6
1	B	120	PRO	6.2
1	A	259	GLN	5.7
1	A	118	GLY	5.7
1	A	116	SER	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	112	GLN	4.8
1	A	160	ALA	4.7
1	A	239	GLY	4.4
1	A	109	ARG	4.4
1	A	123	GLU	4.3
1	B	260	ASP	4.2
1	A	114	ARG	4.0
1	A	122	ALA	3.9
1	A	260	ASP	3.9
1	A	67	GLY	3.2
1	A	146	GLN	3.1
1	A	69	LYS	3.1
1	A	449	TRP	3.1
1	B	257	ARG	3.1
1	B	69	LYS	3.0
1	B	239	GLY	2.8
1	A	450	ILE	2.8
1	B	258	GLN	2.8
1	A	108	PRO	2.8
1	B	142	ARG	2.7
1	A	126	LEU	2.7
1	A	281	TRP	2.6
1	B	323	GLU	2.6
1	B	109	ARG	2.5
1	A	270	VAL	2.5
1	A	91	GLN	2.5
1	B	223	ARG	2.4
1	A	107	LEU	2.4
1	B	126	LEU	2.4
1	A	130	ARG	2.4
1	B	262	SER	2.3
1	B	274	GLU	2.2
1	B	450	ILE	2.2
1	A	157	ALA	2.2
1	A	186	CYS	2.2
1	A	448	ALA	2.2
1	A	275	LEU	2.1
1	B	145	SER	2.1
1	B	123	GLU	2.1
1	B	122	ALA	2.0
1	B	121	PRO	2.0
1	B	124	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	CAD	A	950	3/5	0.47	20.77	24,24,47,53	0
7	GOL	B	881	6/6	0.26	8.99	44,54,59,62	0
6	CAD	B	951	3/5	0.40	8.13	19,19,38,50	0
2	ACT	A	860	4/4	0.18	2.89	28,34,36,39	0
2	ACT	B	851	4/4	0.10	1.73	25,32,34,35	0
7	GOL	A	880	6/6	0.16	1.52	34,45,53,61	0
4	HEM	B	500[A]	5/43	0.12	0.79	20,22,31,49	5
4	HEM	B	500[B]	5/43	0.12	0.79	22,23,30,32	5
4	HEM	A	500	43/43	0.15	0.73	15,19,42,53	0
2	ACT	B	861	4/4	0.08	0.64	24,26,31,32	0
5	INE	A	760	13/13	0.11	0.02	17,21,25,32	0
5	INE	A	766	13/13	0.12	-0.06	36,42,59,59	0
5	INE	B	765	13/13	0.12	-0.25	36,44,56,57	0
2	ACT	A	850	4/4	0.07	-0.55	22,27,31,34	0
5	INE	B	761	13/13	0.06	-0.71	19,24,29,36	0
3	ZN	A	900	1/1	0.02	-4.02	26,26,26,26	0

6.5 Other polymers ⓘ

There are no such residues in this entry.