



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 11:09 PM GMT

PDB ID : 3E6L  
Title : Structure of murine INOS oxygenase domain with inhibitor AR-C132283  
Authors : Garcin, E.D.; Arvai, A.S.; Rosenfeld, R.J.; Kroeger, M.D.; Crane, B.R.; Andersson, G.; Andrews, G.; Hamley, P.J.; Mallinder, P.R.; Nicholls, D.J.; St-Gallay, S.A.; Tinker, A.C.; Gensmantel, N.P.; Mete, A.; Cheshire, D.R.; Connolly, S.; Stueh, D.J.; Aberg, A.; Wallace, A.V.; Tainer, J.A.; Getzoff, E.D.  
Deposited on : 2008-08-15  
Resolution : 2.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

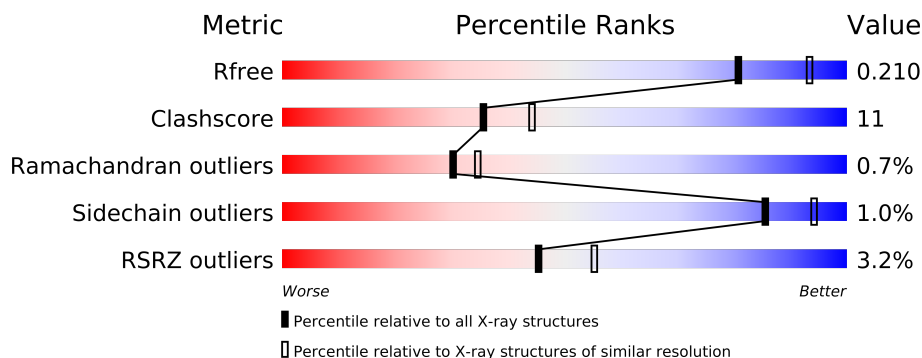
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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  $\geq 3$ , 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	433	
1	B	433	

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	BOG	A	4001	-	X
2	BOG	B	4002	-	X
3	SO4	A	3006	-	X
3	SO4	A	3007	-	X
3	SO4	A	3008	-	X
3	SO4	B	3009	-	X

## 2 Entry composition i

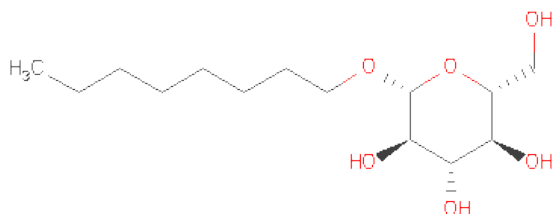
There are 7 unique types of molecules in this entry. The entry contains 7512 atoms, of which 0 are hydrogen and 0 are deuterium.

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, inducible.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3364	2157	580	607	20			
1	B	413	Total	C	N	O	S	0	0	0
			3360	2155	579	606	20			

- Molecule 2 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



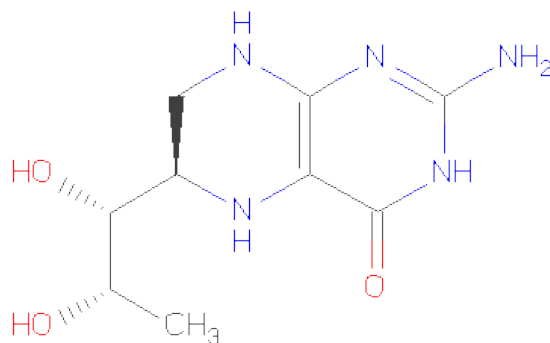
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- 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	0
			43	34	1	4	4		

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



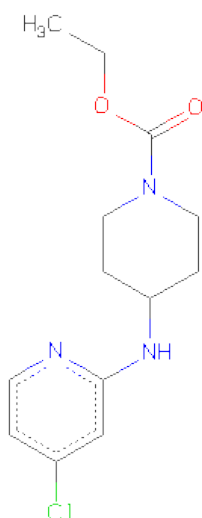
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			17	9	5	3		

*Continued on next page...*

Continued from previous page...

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

- Molecule 6 is ETHYL 4-[(4-CHLOROPYRIDIN-2-YL)AMINO]PIPERIDINE-1-CARBOXYLATE (three-letter code: A11) (formula: C<sub>13</sub>H<sub>18</sub>ClN<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Cl	N	O	0	0
			19	13	1	3	2		
6	B	1	Total	C	Cl	N	O	0	0
			19	13	1	3	2		

- Molecule 7 is water.

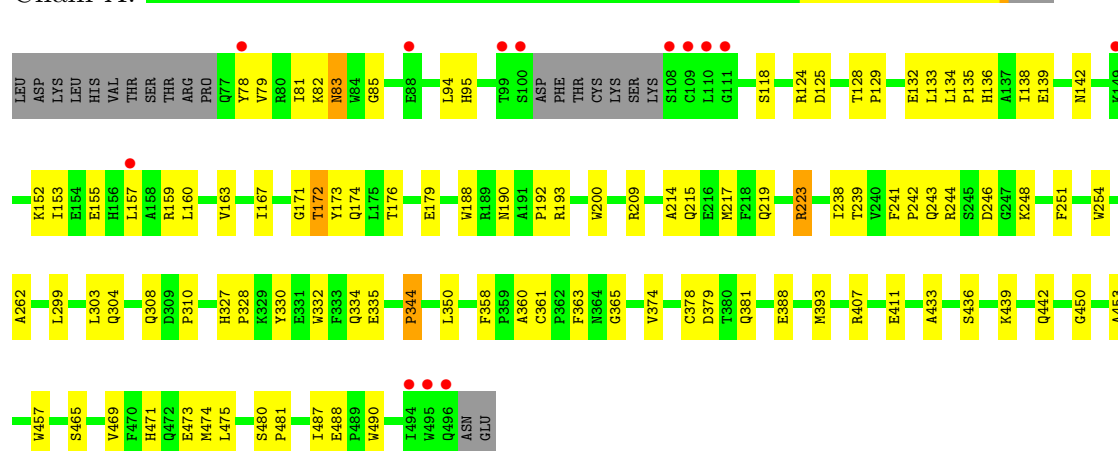
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	274	Total	O	0	0
			274	274		
7	B	271	Total	O	0	0
			271	271		

### 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.

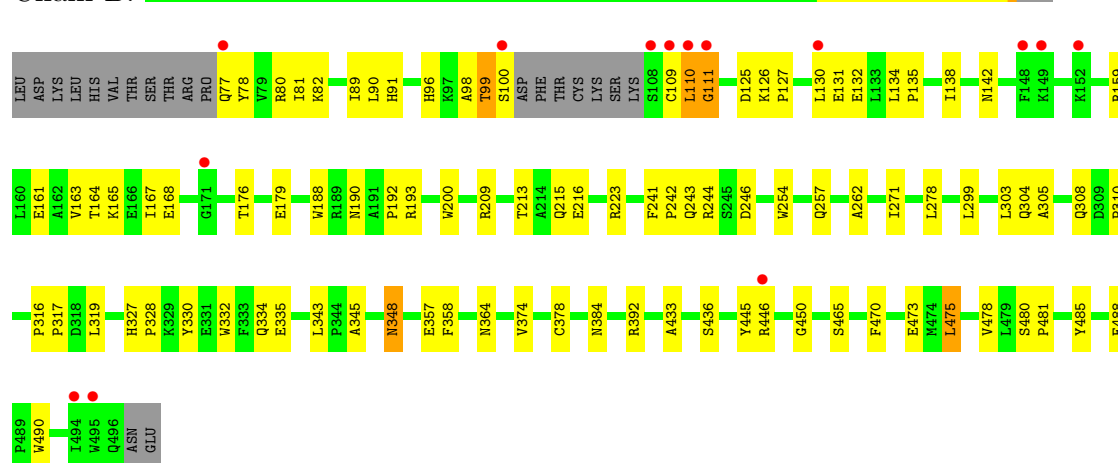
- Molecule 1: Nitric oxide synthase, inducible

Chain A:



- Molecule 1: Nitric oxide synthase, inducible

Chain B:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	213.90Å 213.90Å 116.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.98 – 2.30 29.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.5 (29.98-2.30) 92.5 (29.98-2.30)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.50 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.219 , 0.244 0.207 , 0.210	Depositor DCC
$R_{free}$ test set	3270 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.7	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 68051 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7512	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: HEM, BOG, A11, H4B, SO4

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	0.39	0/3462	0.63	1/4707 (0.0%)
1	B	0.39	0/3458	0.64	0/4702
All	All	0.39	0/6920	0.64	1/9409 (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	A	365	GLY	N-CA-C	-5.05	100.48	113.10

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	3364	0	3259	76	0
1	B	3360	0	3253	67	0
2	A	20	0	28	1	0
2	B	20	0	28	0	0
3	A	30	0	0	0	0
3	B	15	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	43	0	30	1	0
4	B	43	0	30	0	0
5	A	17	0	14	0	0
5	B	17	0	14	0	0
6	A	19	0	18	0	0
6	B	19	0	18	1	0
7	A	274	0	0	7	0
7	B	271	0	0	2	1
All	All	7512	0	6692	144	1

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:81:ILE:HD11	1:B:475:LEU:HD13	1.37	1.05
1:A:83:ASN:ND2	1:A:85:GLY:H	1.82	0.78
1:A:83:ASN:HD22	1:A:85:GLY:H	1.31	0.77
1:A:215:GLN:O	1:A:219:GLN:HG3	1.83	0.77
1:B:125:ASP:O	1:B:126:LYS:HD2	1.84	0.77
1:A:83:ASN:C	1:A:83:ASN:HD22	1.91	0.74
1:A:244:ARG:HA	7:A:2095:HOH:O	1.87	0.74
1:A:129:PRO:HB2	1:A:132:GLU:HG3	1.71	0.71
1:A:132:GLU:O	1:A:135:PRO:HD2	1.90	0.70
1:B:125:ASP:C	1:B:126:LYS:HD2	2.12	0.69
1:A:215:GLN:HE21	1:A:219:GLN:HE21	1.39	0.68
1:A:176:THR:OG1	1:A:179:GLU:HG3	1.95	0.66
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.33	0.64
1:B:81:ILE:HD11	1:B:475:LEU:CD1	2.22	0.63
1:B:130:LEU:HD23	1:B:167:ILE:HG22	1.80	0.62
1:A:223:ARG:HD2	7:A:2156:HOH:O	1.99	0.62
1:A:133:LEU:HD22	1:A:167:ILE:HD13	1.81	0.62
1:A:81:ILE:HD11	1:A:475:LEU:HD13	1.80	0.62
1:A:215:GLN:HE21	1:A:219:GLN:NE2	1.98	0.61
1:B:332:TRP:CE3	1:B:392:ARG:HD2	2.35	0.61
4:A:901:HEM:HBC2	4:A:901:HEM:HMC2	1.82	0.61
1:A:124:ARG:HD2	7:A:2420:HOH:O	2.00	0.61
1:A:388:GLU:HG3	7:A:2359:HOH:O	1.99	0.60
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.32	0.59
1:A:159:ARG:O	1:A:163:VAL:HG23	2.02	0.59
1:B:327:HIS:CG	1:B:328:PRO:HD2	2.38	0.58
1:A:138:ILE:HG22	1:A:142:ASN:HD21	1.67	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:78:TYR:CD1	1:B:78:TYR:C	2.78	0.57
1:B:209:ARG:O	1:B:242:PRO:HG3	2.05	0.56
1:A:241:PHE:HB3	1:A:242:PRO:HD2	1.88	0.56
1:B:98:ALA:O	1:B:99:THR:HG23	2.06	0.56
1:B:110:LEU:N	1:B:110:LEU:HD12	2.22	0.55
1:B:82:LYS:O	1:B:473:GLU:HG3	2.07	0.54
1:B:80:ARG:NH1	7:B:2523:HOH:O	2.40	0.54
1:B:110:LEU:H	1:B:110:LEU:HD12	1.71	0.54
1:B:332:TRP:O	1:B:335:GLU:HB2	2.07	0.54
1:A:304:GLN:HG3	1:A:308:GLN:O	2.08	0.54
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.43	0.53
1:A:83:ASN:ND2	1:A:83:ASN:C	2.62	0.53
1:B:254:TRP:CZ3	1:B:490:TRP:HB3	2.43	0.52
1:A:134:LEU:O	1:A:138:ILE:HG12	2.10	0.52
1:A:163:VAL:O	1:A:167:ILE:HG13	2.09	0.52
1:A:465:SER:O	1:A:471:HIS:HE1	1.93	0.52
1:B:304:GLN:HG3	1:B:308:GLN:O	2.10	0.52
1:A:469:VAL:HG13	1:A:474:MET:CE	2.41	0.51
1:B:488:GLU:HB3	1:B:490:TRP:CE2	2.45	0.51
1:B:190:ASN:O	1:B:192:PRO:HD3	2.11	0.51
1:A:330:TYR:HB3	1:A:332:TRP:CE2	2.46	0.51
1:B:130:LEU:CD2	1:B:167:ILE:HG22	2.41	0.50
1:B:213:THR:OG1	1:B:216:GLU:HG3	2.11	0.50
1:B:374:VAL:O	1:B:378:CYS:HB2	2.11	0.50
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.47	0.50
1:A:209:ARG:O	1:A:242:PRO:HG3	2.11	0.50
1:A:94:LEU:HB3	1:A:450:GLY:HA3	1.93	0.50
1:A:303:LEU:O	1:A:310:PRO:HA	2.11	0.49
1:B:176:THR:OG1	1:B:179:GLU:HG3	2.12	0.49
1:A:153:ILE:O	1:A:157:LEU:HD23	2.11	0.49
1:B:445:TYR:CZ	1:B:450:GLY:HA2	2.46	0.49
1:A:344:PRO:O	1:A:344:PRO:HG2	2.12	0.49
1:A:153:ILE:HG22	1:A:157:LEU:HD23	1.94	0.49
1:A:124:ARG:NH2	1:A:128:THR:OG1	2.46	0.48
1:A:138:ILE:O	1:A:142:ASN:ND2	2.46	0.48
1:B:109:CYS:O	1:B:111:GLY:N	2.43	0.48
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.43	0.48
1:A:132:GLU:C	1:A:135:PRO:HD2	2.34	0.48
1:A:138:ILE:HG22	1:A:142:ASN:ND2	2.28	0.48
1:A:334:GLN:HG3	1:A:335:GLU:N	2.29	0.48
1:B:446:ARG:CZ	1:B:446:ARG:HB3	2.44	0.48
1:B:163:VAL:O	1:B:167:ILE:HG13	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:246:ASP:OD2	1:A:248:LYS:HB2	2.14	0.47
1:A:374:VAL:O	1:A:378:CYS:HB2	2.14	0.47
1:B:262:ALA:HB2	1:B:299:LEU:CD2	2.44	0.47
1:B:134:LEU:HB3	1:B:135:PRO:HD3	1.97	0.47
1:A:262:ALA:HB2	1:A:299:LEU:CD2	2.45	0.47
1:B:241:PHE:HB3	1:B:242:PRO:HD2	1.95	0.47
1:B:110:LEU:H	1:B:110:LEU:CD1	2.28	0.47
1:B:445:TYR:HA	1:B:450:GLY:H	1.79	0.47
1:B:77:GLN:O	1:B:96:HIS:HE1	1.98	0.47
1:A:379:ASP:HB3	1:A:381:GLN:NE2	2.29	0.47
1:B:100:SER:HA	1:B:478:VAL:HG11	1.97	0.46
1:A:243:GLN:HB3	1:A:358:PHE:CE2	2.50	0.46
1:A:469:VAL:HG13	1:A:474:MET:HE3	1.97	0.46
1:A:214:ALA:O	1:A:217:MET:HB2	2.16	0.46
1:A:487:ILE:O	1:A:488:GLU:C	2.54	0.46
1:B:127:PRO:HG3	1:B:246:ASP:HA	1.98	0.46
1:B:348:ASN:H	1:B:348:ASN:ND2	2.14	0.46
1:B:244:ARG:NH1	1:B:357:GLU:OE2	2.48	0.46
1:A:133:LEU:HD23	1:A:133:LEU:C	2.36	0.45
1:A:439:LYS:O	1:A:442:GLN:HB3	2.16	0.45
1:A:407:ARG:HD2	7:A:2117:HOH:O	2.15	0.45
1:B:193:ARG:NH1	1:B:485:TYR:OH	2.49	0.45
1:A:193:ARG:HD3	1:A:457:TRP:CD2	2.51	0.45
1:A:453:ALA:HB3	1:A:474:MET:HB3	1.99	0.45
1:A:172:THR:HG23	1:A:173:TYR:N	2.31	0.45
1:A:239:THR:O	1:A:361:CYS:HA	2.17	0.45
1:B:445:TYR:CE2	1:B:450:GLY:HA2	2.53	0.44
1:A:136:HIS:O	1:A:139:GLU:HB3	2.17	0.44
1:A:160:LEU:HD13	2:A:4001:BOG:H5'1	2.00	0.44
1:A:82:LYS:O	1:A:473:GLU:HG3	2.18	0.44
1:A:78:TYR:C	1:A:78:TYR:CD1	2.91	0.44
1:A:238:ILE:HG13	1:A:363:PHE:HB3	1.99	0.44
1:B:130:LEU:HD13	1:B:130:LEU:C	2.38	0.43
1:A:327:HIS:CG	1:A:328:PRO:HD2	2.53	0.43
1:B:138:ILE:O	1:B:142:ASN:ND2	2.51	0.43
1:B:348:ASN:H	1:B:348:ASN:HD22	1.65	0.43
1:A:174:GLN:HA	7:A:2052:HOH:O	2.18	0.43
1:A:79:VAL:HG23	1:A:95:HIS:CE1	2.53	0.43
1:B:215:GLN:NE2	7:B:2540:HOH:O	2.51	0.43
1:B:480:SER:HA	1:B:481:PRO:C	2.40	0.43
1:A:125:ASP:O	1:A:248:LYS:HE3	2.19	0.42
1:A:407:ARG:HG2	7:A:2149:HOH:O	2.18	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:215:GLN:NE2	1:A:219:GLN:HE21	2.14	0.42
1:B:348:ASN:N	1:B:348:ASN:HD22	2.18	0.42
1:B:316:PRO:O	1:B:319:LEU:HB2	2.19	0.42
1:B:257:GLN:HG2	6:B:1906:A11:O16	2.19	0.42
1:A:332:TRP:O	1:A:335:GLU:HB2	2.19	0.42
1:B:132:GLU:O	1:B:135:PRO:HD2	2.19	0.42
1:A:350:LEU:C	1:A:350:LEU:HD23	2.40	0.42
1:B:305:ALA:O	1:B:308:GLN:HG2	2.19	0.42
1:B:433:ALA:O	1:B:436:SER:HB3	2.19	0.42
1:B:257:GLN:HA	1:B:345:ALA:O	2.20	0.42
1:B:159:ARG:O	1:B:163:VAL:HG23	2.20	0.42
1:A:433:ALA:O	1:A:436:SER:HB3	2.19	0.42
1:B:271:ILE:HD12	1:B:278:LEU:HD11	2.02	0.42
1:B:188:TRP:CZ3	1:B:200:TRP:HA	2.54	0.41
1:A:171:GLY:O	1:A:172:THR:HB	2.20	0.41
1:B:78:TYR:CE1	1:B:91:HIS:ND1	2.88	0.41
1:A:251:PHE:O	1:A:360:ALA:HB2	2.20	0.41
1:A:480:SER:HA	1:A:481:PRO:C	2.41	0.41
1:A:393:MET:CE	1:A:411:GLU:HG3	2.50	0.41
1:A:81:ILE:HD13	1:A:81:ILE:HA	1.78	0.41
1:B:303:LEU:O	1:B:310:PRO:HA	2.20	0.41
1:B:164:THR:O	1:B:168:GLU:HG3	2.21	0.41
1:A:217:MET:HB3	1:A:303:LEU:HD13	2.03	0.41
1:B:161:GLU:HG2	1:B:165:LYS:HE3	2.03	0.41
1:A:190:ASN:O	1:A:192:PRO:HD3	2.21	0.41
1:B:343:LEU:HD11	1:B:364:ASN:ND2	2.35	0.41
1:B:330:TYR:HB3	1:B:332:TRP:CE2	2.56	0.41
1:B:131:GLU:HG3	1:B:132:GLU:N	2.36	0.41
1:B:316:PRO:HA	1:B:317:PRO:HD3	1.88	0.41
1:B:89:ILE:HG22	1:B:90:LEU:N	2.36	0.41
1:A:152:LYS:HD2	1:A:155:GLU:OE2	2.21	0.40
1:A:254:TRP:CZ3	1:A:490:TRP:HB3	2.56	0.40
1:B:465:SER:HA	1:B:470:PHE:CG	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:B:2227:HOH:O	7:B:2259:HOH:O[9_766]	2.13	0.07

## 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	409/433 (94%)	379 (93%)	28 (7%)	2 (0%)	38	45
1	B	409/433 (94%)	375 (92%)	30 (7%)	4 (1%)	22	23
All	All	818/866 (94%)	754 (92%)	58 (7%)	6 (1%)	30	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	99	THR
1	B	110	LEU
1	B	111	GLY
1	A	172	THR
1	B	384	ASN
1	A	344	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	360/381 (94%)	357 (99%)	3 (1%)	89	96
1	B	359/381 (94%)	355 (99%)	4 (1%)	84	93
All	All	719/762 (94%)	712 (99%)	7 (1%)	85	94

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	118	SER
1	A	223	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	223	ARG
1	B	334	GLN
1	B	348	ASN
1	B	475	LEU

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

Mol	Chain	Res	Type
1	A	83	ASN
1	A	96	HIS
1	A	142	ASN
1	A	219	GLN
1	A	308	GLN
1	A	421	GLN
1	A	442	GLN
1	A	471	HIS
1	B	96	HIS
1	B	215	GLN
1	B	334	GLN
1	B	348	ASN
1	B	421	GLN

### 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 ⓘ

17 ligands 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$
3	SO4	A	3001	-	4,4,4	0.31	0	6,6,6	0.09	0
3	SO4	A	3002	-	4,4,4	0.41	0	6,6,6	0.09	0
3	SO4	A	3003	-	4,4,4	0.29	0	6,6,6	0.09	0
3	SO4	A	3006	-	4,4,4	0.30	0	6,6,6	0.08	0
3	SO4	A	3007	-	4,4,4	0.42	0	6,6,6	0.07	0
3	SO4	A	3008	-	4,4,4	0.49	0	6,6,6	0.07	0
2	BOG	A	4001	-	20,20,20	1.47	4 (20%)	25,25,25	0.82	1 (4%)
4	HEM	A	901	-	49,50,50	2.80	13 (26%)	46,82,82	1.20	4 (8%)
5	H4B	A	902	-	18,18,18	1.83	3 (16%)	24,26,26	2.31	8 (33%)
6	A11	A	906	-	20,20,20	1.56	3 (15%)	26,26,26	1.67	5 (19%)
4	HEM	B	1901	1	49,50,50	2.22	11 (22%)	46,82,82	1.43	4 (8%)
5	H4B	B	1902	-	18,18,18	2.04	3 (16%)	24,26,26	2.35	8 (33%)
6	A11	B	1906	-	20,20,20	1.59	3 (15%)	26,26,26	1.60	7 (26%)
3	SO4	B	3004	-	4,4,4	0.46	0	6,6,6	0.06	0
3	SO4	B	3005	-	4,4,4	0.31	0	6,6,6	0.11	0
3	SO4	B	3009	-	4,4,4	0.44	0	6,6,6	0.08	0
2	BOG	B	4002	-	20,20,20	1.44	3 (15%)	25,25,25	0.80	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
3	SO4	A	3001	-	-	0/0/0/0	0/0/0/0
3	SO4	A	3002	-	-	0/0/0/0	0/0/0/0
3	SO4	A	3003	-	-	0/0/0/0	0/0/0/0
3	SO4	A	3006	-	-	0/0/0/0	0/0/0/0
3	SO4	A	3007	-	-	0/0/0/0	0/0/0/0
3	SO4	A	3008	-	-	0/0/0/0	0/0/0/0
2	BOG	A	4001	-	-	0/11/31/31	0/1/1/1
4	HEM	A	901	-	-	0/14/114/114	0/0/8/8
5	H4B	A	902	-	1/1/3/5	0/8/17/17	0/0/2/2

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	A11	A	906	-	-	0/11/21/21	0/2/2/2
4	HEM	B	1901	1	-	0/14/114/114	0/0/8/8
5	H4B	B	1902	-	1/1/3/5	0/8/17/17	0/0/2/2
6	A11	B	1906	-	-	0/11/21/21	0/2/2/2
3	SO4	B	3004	-	-	0/0/0/0	0/0/0/0
3	SO4	B	3005	-	-	0/0/0/0	0/0/0/0
3	SO4	B	3009	-	-	0/0/0/0	0/0/0/0
2	BOG	B	4002	-	-	0/11/31/31	0/1/1/1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	HEM	C2D-C1D	12.39	1.47	1.44
4	B	1901	HEM	C2D-C1D	8.42	1.46	1.44
4	A	901	HEM	C3D-C4D	7.17	1.46	1.44
4	A	901	HEM	C4A-C3A	7.07	1.49	1.40
4	B	1901	HEM	C3D-C4D	5.76	1.46	1.44
5	B	1902	H4B	C7-C6	-5.74	1.45	1.52
5	B	1902	H4B	C7-N8	-5.18	1.38	1.46
5	A	902	H4B	C7-N8	-4.87	1.38	1.46
5	A	902	H4B	C7-C6	-4.86	1.46	1.52
4	A	901	HEM	C3D-C2D	-4.65	1.35	1.43
4	B	1901	HEM	C3D-C2D	-4.62	1.35	1.43
4	B	1901	HEM	C3B-C4B	4.58	1.49	1.44
2	B	4002	BOG	C3-C2	-4.20	1.41	1.52
4	A	901	HEM	CHB-C1B	3.99	1.41	1.35
6	A	906	A11	O16-C15	3.94	1.27	1.21
2	A	4001	BOG	C3-C2	-3.89	1.42	1.52
6	B	1906	A11	O16-C15	3.84	1.27	1.21
6	A	906	A11	C6-N5	3.60	1.41	1.34
6	B	1906	A11	C6-N5	3.59	1.41	1.34
2	B	4002	BOG	C4-C3	-3.45	1.43	1.52
4	A	901	HEM	C1A-C2A	3.35	1.49	1.43
4	B	1901	HEM	C4A-C3A	3.20	1.44	1.40
4	A	901	HEM	C3B-C2B	-3.06	1.38	1.43
2	A	4001	BOG	C4-C3	-3.05	1.44	1.52
4	B	1901	HEM	CHA-C4D	3.00	1.40	1.35
6	B	1906	A11	C4-N5	2.82	1.41	1.34
2	A	4001	BOG	O1-C1	2.66	1.45	1.40
6	A	906	A11	C4-N5	2.64	1.40	1.34
4	B	1901	HEM	C3C-C2C	-2.63	1.39	1.43
4	A	901	HEM	C3B-C4B	2.58	1.47	1.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1901	HEM	FE-ND	2.49	2.06	1.97
4	A	901	HEM	FE-NC	2.47	2.07	1.97
4	B	1901	HEM	CHB-C1B	2.47	1.39	1.35
2	A	4001	BOG	O5-C1	2.46	1.48	1.41
4	A	901	HEM	FE-NA	2.38	2.02	1.92
4	A	901	HEM	CMC-C2C	2.27	1.54	1.47
4	A	901	HEM	C3C-C2C	-2.27	1.39	1.43
4	B	1901	HEM	FE-NC	2.27	2.06	1.97
5	A	902	H4B	C4-N3	-2.21	1.33	1.37
4	B	1901	HEM	CMC-C2C	2.19	1.54	1.47
5	B	1902	H4B	C4-N3	-2.15	1.33	1.37
2	B	4002	BOG	O1-C1	2.06	1.43	1.40
4	A	901	HEM	CBC-CAC	2.04	1.40	1.28

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1902	H4B	C7-C6-C9	7.41	125.09	113.66
5	A	902	H4B	C7-C6-C9	6.91	124.31	113.66
4	B	1901	HEM	C3B-C4B-NB	-5.80	109.85	114.00
5	A	902	H4B	C6-C7-N8	5.69	119.01	111.66
5	B	1902	H4B	C6-C7-N8	5.05	118.18	111.66
4	A	901	HEM	C3B-C4B-NB	-3.94	111.18	114.00
6	A	906	A11	O17-C15-N12	3.71	114.71	111.60
6	A	906	A11	C3-C4-N5	-3.60	119.89	123.88
6	B	1906	A11	O17-C15-N12	3.51	114.53	111.60
6	B	1906	A11	C3-C4-N5	-3.36	120.14	123.88
5	A	902	H4B	C4-C4A-C8A	3.11	117.44	114.56
5	A	902	H4B	N8-C8A-N1	2.98	120.19	115.82
5	B	1902	H4B	C4-C4A-C8A	2.97	117.31	114.56
4	B	1901	HEM	CBD-CAD-C3D	-2.96	107.92	114.37
5	B	1902	H4B	N8-C8A-N1	2.90	120.08	115.82
5	B	1902	H4B	C7-C6-N5	2.80	116.64	109.85
6	A	906	A11	C4-C3-C2	2.75	119.32	117.76
4	B	1901	HEM	CHC-C4B-NB	-2.70	122.34	124.58
5	A	902	H4B	C7-C6-N5	2.66	116.30	109.85
4	A	901	HEM	C2D-C1D-ND	-2.64	109.81	112.93
5	B	1902	H4B	C2-N1-C8A	2.45	121.09	117.61
6	B	1906	A11	C2-C7-C6	2.42	120.03	117.97
4	A	901	HEM	CBD-CAD-C3D	-2.40	109.14	114.37
5	B	1902	H4B	C4A-C4-N3	2.31	119.99	114.06
6	A	906	A11	O16-C15-N12	-2.31	119.82	124.36

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1906	A11	C18-O17-C15	2.24	119.22	115.65
5	A	902	H4B	C4A-C4-N3	2.24	119.79	114.06
6	B	1906	A11	O16-C15-N12	-2.22	119.98	124.36
6	B	1906	A11	C4-C3-C2	2.19	119.00	117.76
5	A	902	H4B	C8A-C4A-N5	2.12	121.40	118.50
4	A	901	HEM	CHC-C4B-NB	-2.11	122.83	124.58
6	A	906	A11	C18-O17-C15	2.11	119.01	115.65
5	A	902	H4B	C2-N1-C8A	2.08	120.56	117.61
5	B	1902	H4B	C8A-C4A-N5	2.07	121.33	118.50
4	B	1901	HEM	C4A-C3A-C2A	2.06	108.43	107.00
6	B	1906	A11	C7-C6-N5	-2.05	119.75	122.69
2	A	4001	BOG	C4-C3-C2	2.01	114.52	110.82

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	1902	H4B	C6
5	A	902	H4B	C6

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	413/433 (95%)	0.00	13 (3%) 47 56	28, 44, 70, 95	0
1	B	413/433 (95%)	-0.02	14 (3%) 43 53	26, 42, 67, 98	0
All	All	826/866 (95%)	-0.01	27 (3%) 45 54	26, 43, 69, 98	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	108	SER	5.7
1	A	110	LEU	5.6
1	A	494	ILE	4.7
1	B	100	SER	4.5
1	A	108	SER	4.2
1	B	495	TRP	4.1
1	A	100	SER	3.9
1	A	149	LYS	3.5
1	B	109	CYS	3.4
1	A	495	TRP	3.2
1	A	109	CYS	3.1
1	B	110	LEU	3.0
1	B	494	ILE	2.9
1	A	157	LEU	2.7
1	B	446	ARG	2.7
1	A	496	GLN	2.6
1	A	111	GLY	2.5
1	B	111	GLY	2.5
1	B	149	LYS	2.2
1	B	148	PHE	2.2
1	B	130	LEU	2.2
1	B	152	LYS	2.2
1	A	99	THR	2.1
1	B	77	GLN	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	88	GLU	2.0
1	B	171	GLY	2.0
1	A	78	TYR	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	SO4	A	3006	5/5	0.33	8.37	104,104,105,106	0
2	BOG	A	4001	20/20	0.43	4.21	84,95,97,98	0
3	SO4	B	3009	5/5	0.25	3.23	118,119,119,120	0
3	SO4	A	3008	5/5	0.25	3.01	123,123,124,124	0
2	BOG	B	4002	20/20	0.31	2.30	83,87,88,89	0
3	SO4	A	3007	5/5	0.19	2.07	115,115,116,116	0
3	SO4	B	3004	5/5	0.25	1.81	117,118,118,118	0
3	SO4	A	3002	5/5	0.27	1.47	112,112,113,113	0
3	SO4	A	3003	5/5	0.12	0.67	99,99,99,100	0
5	H4B	B	1902	17/17	0.15	0.64	30,32,38,40	0
4	HEM	B	1901	43/43	0.14	0.22	22,27,29,29	0
4	HEM	A	901	43/43	0.14	0.15	24,27,30,34	0
6	A11	B	1906	19/19	0.14	0.14	27,29,31,37	0
6	A11	A	906	19/19	0.14	0.11	26,28,34,35	0
5	H4B	A	902	17/17	0.10	-0.63	31,32,37,37	0
3	SO4	B	3005	5/5	0.19	-1.78	97,97,98,99	0
3	SO4	A	3001	5/5	0.17	-4.62	102,103,103,103	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.