



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:43 AM GMT

PDB ID : 2Y37  
Title : THE DISCOVERY OF NOVEL, POTENT AND HIGHLY SELECTIVE INHIBITORS OF INDUCIBLE NITRIC OXIDE SYNTHASE (INOS)  
Authors : Cheshire, D.R.; Andrews, G.; Beaton, H.G.; Birkinshaw, T.N.; Boughton-Smith, N.; Connolly, S.; Cook, T.R.; Cooper, A.; Cooper, S.L.; Cox, D.; Dixon, J.; Gensmantel, N.; Hamley, P.J.; Harrison, R.; Hartopp, P.; Kack, H.; Luker, T.; Mete, A.; Millichip, I.; Nicholls, D.J.; Pimm, A.D.; St-Gallay, S.A.; Wallace, A.V.  
Deposited on : 2010-12-19  
Resolution : 2.60 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

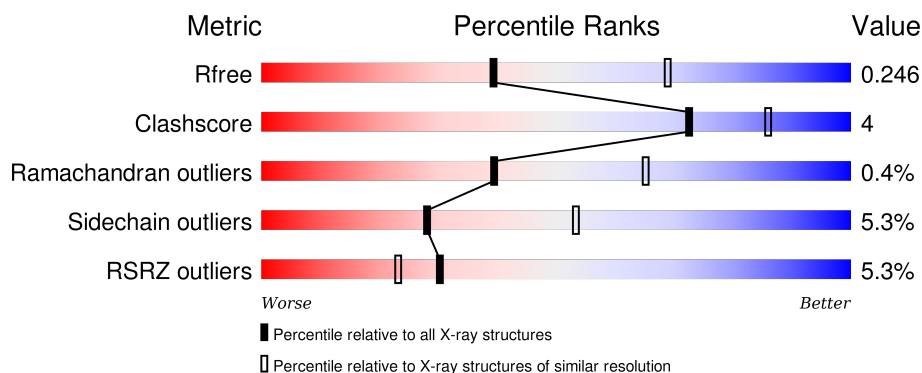
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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. 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	433	<div> <div>5%</div> <div>83%</div> <div>11%</div> <div>5%</div> </div>
1	B	433	<div> <div>5%</div> <div>83%</div> <div>10%</div> <div>5%</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
3	GOL	B	1498	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7222 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, INDUCIBLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3356	2153	579	604	20			
1	B	412	Total	C	N	O	S	0	2	0
			3378	2166	586	606	20			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



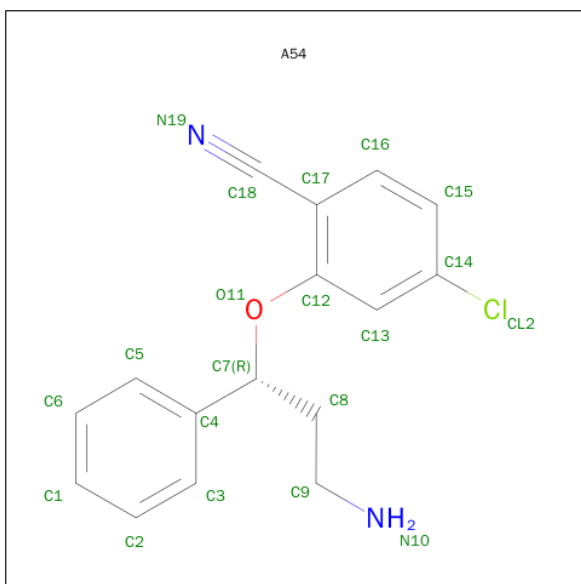
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 4 is 2-[(1R)-3-AMINO-1-PHENYL-PROPOXY]-4-CHLORO-BENZONITRILE (three-letter code: A54) (formula: C<sub>16</sub>H<sub>15</sub>ClN<sub>2</sub>O).



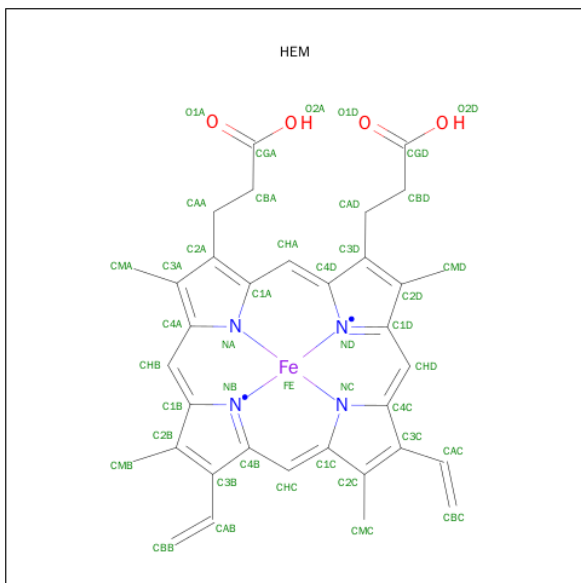
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			20	16	1	2	1		

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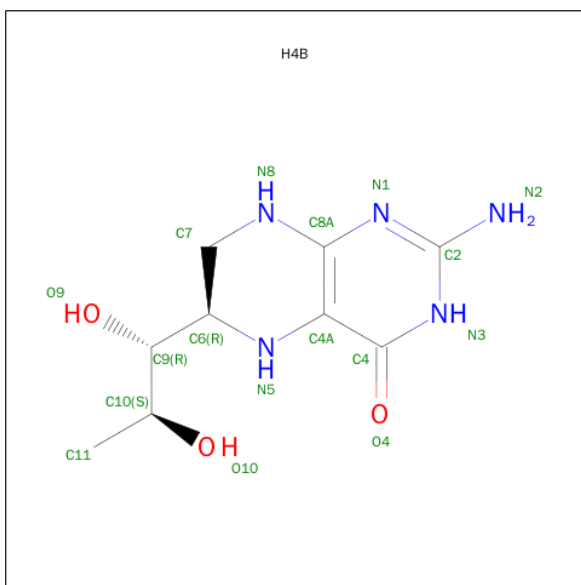
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	Cl	N	O	0	0
			20	16	1	2	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

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



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

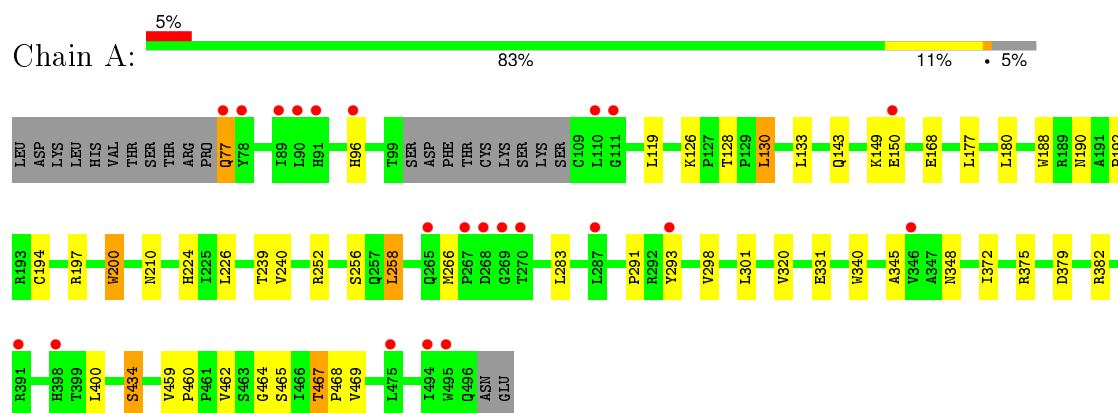
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	152	Total	O	0	0
			152	152		
7	B	149	Total	O	0	0
			149	149		

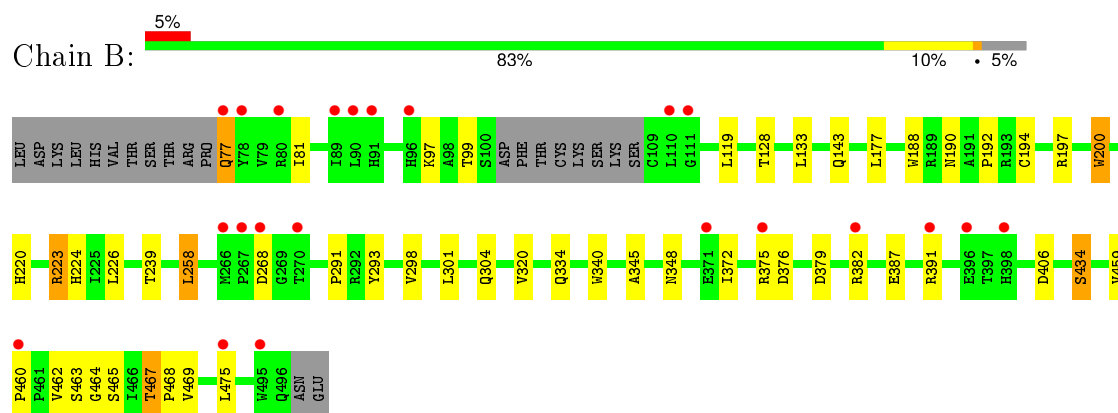
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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



#### • Molecule 1: NITRIC OXIDE SYNTHASE, INDUCIBLE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.49 Å   212.49 Å   115.37 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	26.21 – 2.60 36.80 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (26.21-2.60) 98.8 (36.80-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.61 Å)	Xtriage
Refinement program	BUSTER 2.9.5	Depositor
R, $R_{free}$	0.208   ,   0.242 0.209   ,   0.246	Depositor DCC
$R_{free}$ test set	2389 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	51.8	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 64.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 47053 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7222	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A54, GOL, H4B, HEM, 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	0.49	0/3454	0.71	0/4696
1	B	0.49	0/3482	0.72	0/4732
All	All	0.49	0/6936	0.71	0/9428

There are no bond length outliers.

There are no bond angle outliers.

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	3356	0	3255	23	0
1	B	3378	0	3286	26	1
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	6	0	8	2	0
3	B	6	0	8	1	0
4	A	20	0	15	1	0
4	B	20	0	15	1	0
5	A	43	0	30	5	0
5	B	43	0	30	6	0
6	A	17	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	17	0	15	1	0
7	A	152	0	0	1	0
7	B	149	0	0	2	1
All	All	7222	0	6677	57	2

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 4.

All (57) 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:B:304:GLN:HE22	3:B:1498:GOL:H12	1.64	0.61
1:B:376:ASP:HA	1:B:382[B]:ARG:HD3	1.83	0.61
5:A:1501:HEM:HBB2	5:A:1501:HEM:HHC	1.84	0.59
1:B:298:VAL:HG21	1:B:320:VAL:HG11	1.87	0.57
1:A:252:ARG:NH1	3:A:1499:GOL:H11	2.21	0.56
1:A:298:VAL:HG21	1:A:320:VAL:HG11	1.89	0.54
1:B:81:ILE:HD11	1:B:475:LEU:HG	1.89	0.54
1:B:220:HIS:HD2	1:B:223[B]:ARG:HH21	1.56	0.53
1:B:194:CYS:HB3	1:B:197:ARG:HD2	1.91	0.53
4:B:1499:A54:H92C	5:B:1500:HEM:O1A	2.10	0.52
1:B:220:HIS:HD2	1:B:223[B]:ARG:NH2	2.08	0.52
1:A:258:LEU:HB2	1:A:345:ALA:HB3	1.93	0.51
1:B:258:LEU:HB2	1:B:345:ALA:HB3	1.92	0.51
1:A:143:GLN:NE2	7:A:2019:HOH:O	2.44	0.51
1:A:190:ASN:O	1:A:192:PRO:HD3	2.10	0.51
1:A:194:CYS:HB3	1:A:197:ARG:HD2	1.91	0.51
1:B:190:ASN:O	1:B:192:PRO:HD3	2.10	0.51
4:A:1500:A54:H92C	5:A:1501:HEM:O1A	2.12	0.50
1:A:252:ARG:HH11	3:A:1499:GOL:H11	1.78	0.48
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.49	0.47
5:B:1500:HEM:HBA2	5:B:1500:HEM:HHA	1.96	0.47
1:A:460:PRO:HD2	1:A:467:THR:HG21	1.96	0.47
1:B:460:PRO:HD2	1:B:467:THR:HG21	1.97	0.47
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.49	0.46
1:B:465:SER:C	1:B:467:THR:H	2.19	0.46
1:B:375:ARG:NH1	1:B:379:ASP:OD2	2.48	0.46
1:A:375:ARG:NH1	1:A:379:ASP:OD2	2.47	0.46
5:A:1501:HEM:HBC2	5:A:1501:HEM:HMC1	1.98	0.45
1:B:224:HIS:HD2	1:B:239:THR:OG1	2.00	0.45
1:A:130:LEU:HD11	1:A:168:GLU:HA	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ARG:HH21	6:A:1502:H4B:C4	2.29	0.45
1:A:465:SER:C	1:A:467:THR:H	2.19	0.45
1:B:77:GLN:HA	7:B:2002:HOH:O	2.16	0.45
1:A:77:GLN:O	1:A:96:HIS:HE1	2.00	0.45
1:A:224:HIS:HD2	1:A:239:THR:OG1	1.99	0.44
1:B:258:LEU:HA	1:B:258:LEU:HD12	1.86	0.44
1:B:143:GLN:NE2	7:B:2017:HOH:O	2.50	0.44
1:B:464:GLY:O	1:B:467:THR:HG22	2.18	0.43
1:B:340:TRP:CD1	1:B:372:ILE:HG12	2.53	0.43
1:A:459:VAL:HG22	1:A:469:VAL:HG23	1.99	0.43
1:A:464:GLY:O	1:A:467:THR:HG22	2.18	0.43
1:B:459:VAL:HG22	1:B:469:VAL:HG23	2.00	0.43
1:A:434:SER:HB3	1:A:468:PRO:HD2	2.00	0.42
1:B:434:SER:HB3	1:B:468:PRO:HD2	2.01	0.41
1:A:291:PRO:HG2	1:A:293:TYR:CE2	2.55	0.41
1:A:379:ASP:HB2	1:A:382:ARG:HG2	2.03	0.41
1:B:224:HIS:CD2	1:B:239:THR:OG1	2.74	0.41
1:A:188:TRP:CH2	5:A:1501:HEM:HMC3	2.56	0.41
1:B:188:TRP:CH2	5:B:1500:HEM:HMC3	2.56	0.41
1:B:291:PRO:HG2	1:B:293:TYR:CE2	2.56	0.41
5:B:1500:HEM:HHC	5:B:1500:HEM:HBB2	2.03	0.41
5:B:1500:HEM:O2A	6:B:1501:H4B:N2	2.51	0.40
1:B:188:TRP:CZ3	5:B:1500:HEM:HMC3	2.56	0.40
1:A:180:LEU:HD11	1:A:240:VAL:HG11	2.02	0.40
1:A:340:TRP:CD1	1:A:372:ILE:HG12	2.56	0.40
1:B:387:GLU:HG2	1:B:391:ARG:HE	1.86	0.40
5:A:1501:HEM:HBC2	5:A:1501:HEM:CMC	2.51	0.40

All (2) 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	Interatomic distance (Å)	Clash overlap (Å)
7:B:2138:HOH:O	7:B:2138:HOH:O[11_554]	1.94	0.26
1:B:406:ASP:OD1	1:B:463:SER:OG[11_554]	2.17	0.03

## 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	407/433 (94%)	391 (96%)	15 (4%)	1 (0%)	52	77
1	B	410/433 (95%)	384 (94%)	24 (6%)	2 (0%)	34	60
All	All	817/866 (94%)	775 (95%)	39 (5%)	3 (0%)	39	65

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	200	TRP
1	B	268	ASP
1	B	200	TRP

### 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	359/381 (94%)	337 (94%)	22 (6%)	23	46
1	B	362/381 (95%)	345 (95%)	17 (5%)	32	59
All	All	721/762 (95%)	682 (95%)	39 (5%)	28	52

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	119	LEU
1	A	126	LYS

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Mol	Chain	Res	Type
1	A	128	THR
1	A	130	LEU
1	A	133	LEU
1	A	149	LYS
1	A	150	GLU
1	A	177	LEU
1	A	210	ASN
1	A	226	LEU
1	A	256	SER
1	A	258	LEU
1	A	266	MET
1	A	283	LEU
1	A	301	LEU
1	A	331	GLU
1	A	348	ASN
1	A	400	LEU
1	A	434	SER
1	A	462	VAL
1	A	467	THR
1	B	77	GLN
1	B	97	LYS
1	B	99	THR
1	B	119	LEU
1	B	128	THR
1	B	133	LEU
1	B	177	LEU
1	B	223[A]	ARG
1	B	223[B]	ARG
1	B	226	LEU
1	B	258	LEU
1	B	301	LEU
1	B	334	GLN
1	B	348	ASN
1	B	434	SER
1	B	462	VAL
1	B	467	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	210	ASN

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Mol	Chain	Res	Type
1	A	220	HIS
1	A	224	HIS
1	A	231	ASN
1	A	233	ASN
1	A	257	GLN
1	A	348	ASN
1	B	77	GLN
1	B	143	GLN
1	B	220	HIS
1	B	224	HIS
1	B	231	ASN
1	B	233	ASN
1	B	257	GLN
1	B	348	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

11 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
2	SO4	A	1497	-	4,4,4	0.47	0	6,6,6	0.33	0
2	SO4	A	1498	-	4,4,4	0.49	0	6,6,6	0.08	0
3	GOL	A	1499	-	5,5,5	0.82	0	5,5,5	1.79	2 (40%)
4	A54	A	1500	-	20,21,21	0.79	0	25,27,27	0.84	1 (4%)
5	HEM	A	1501	1	30,50,50	2.44	7 (23%)	24,82,82	2.74	12 (50%)
6	H4B	A	1502	-	13,18,18	2.13	7 (53%)	11,26,26	2.69	5 (45%)
2	SO4	B	1497	-	4,4,4	0.19	0	6,6,6	0.27	0
3	GOL	B	1498	-	5,5,5	0.35	0	5,5,5	0.52	0
4	A54	B	1499	-	20,21,21	0.73	1 (5%)	25,27,27	0.96	1 (4%)
5	HEM	B	1500	1	30,50,50	2.34	8 (26%)	24,82,82	2.67	10 (41%)
6	H4B	B	1501	-	13,18,18	2.18	6 (46%)	11,26,26	2.28	4 (36%)

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	SO4	A	1497	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1498	-	-	0/0/0/0	0/0/0/0
3	GOL	A	1499	-	-	0/4/4/4	0/0/0/0
4	A54	A	1500	-	-	0/13/13/13	0/2/2/2
5	HEM	A	1501	1	-	0/10/54/54	0/0/8/8
6	H4B	A	1502	-	-	0/8/17/17	0/2/2/2
2	SO4	B	1497	-	-	0/0/0/0	0/0/0/0
3	GOL	B	1498	-	-	0/4/4/4	0/0/0/0
4	A54	B	1499	-	-	0/13/13/13	0/2/2/2
5	HEM	B	1500	1	-	0/10/54/54	0/0/8/8
6	H4B	B	1501	-	-	0/8/17/17	0/2/2/2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1501	HEM	C2D-C3D	-8.08	1.30	1.54
5	B	1500	HEM	C2D-C3D	-7.43	1.32	1.54
5	A	1501	HEM	C3D-C4D	-5.41	1.44	1.51
5	B	1500	HEM	C3D-C4D	-4.74	1.45	1.51
5	A	1501	HEM	C2C-C1C	-4.69	1.43	1.52
5	B	1500	HEM	C2C-C1C	-4.25	1.44	1.52
5	B	1500	HEM	CAD-C3D	-3.77	1.46	1.54
5	B	1500	HEM	C3B-C4B	-3.50	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1500	HEM	C3B-CAB	-3.28	1.45	1.51
5	A	1501	HEM	CAD-C3D	-3.03	1.48	1.54
5	B	1500	HEM	C3C-CAC	-2.70	1.46	1.51
5	A	1501	HEM	C3B-CAB	-2.68	1.46	1.51
5	A	1501	HEM	CMA-C3A	-2.51	1.46	1.51
4	B	1499	A54	O11-C12	2.01	1.41	1.37
6	A	1502	H4B	C7-N8	2.08	1.48	1.46
6	B	1501	H4B	C4A-C8A	2.10	1.45	1.41
6	B	1501	H4B	C2-N3	2.18	1.39	1.35
6	A	1502	H4B	C8A-N1	2.22	1.38	1.34
6	B	1501	H4B	C8A-N1	2.40	1.38	1.34
6	A	1502	H4B	C4A-N5	2.54	1.43	1.38
6	A	1502	H4B	C4A-C8A	2.59	1.46	1.41
5	B	1500	HEM	C1C-NC	2.79	1.39	1.36
6	A	1502	H4B	C2-N1	2.93	1.40	1.35
6	A	1502	H4B	C2-N3	3.28	1.41	1.35
6	B	1501	H4B	C4-N3	3.38	1.39	1.33
6	A	1502	H4B	C2-N2	3.50	1.41	1.34
6	B	1501	H4B	C7-N8	3.56	1.50	1.46
6	B	1501	H4B	C6-N5	3.58	1.52	1.45
5	A	1501	HEM	C4C-NC	3.95	1.40	1.36

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1501	HEM	CBA-CAA-C2A	-6.38	101.10	112.53
5	B	1500	HEM	CBD-CAD-C3D	-4.28	101.08	113.55
5	A	1501	HEM	CBD-CAD-C3D	-3.19	104.27	113.55
5	B	1500	HEM	CBA-CAA-C2A	-3.14	106.90	112.53
3	A	1499	GOL	O3-C3-C2	-2.88	96.20	110.18
5	B	1500	HEM	C1D-CHD-C4C	-2.85	121.06	125.82
6	A	1502	H4B	N3-C2-N1	-2.81	120.93	125.53
4	A	1500	A54	C8-C7-C4	-2.11	109.14	112.98
5	A	1501	HEM	C3C-CAC-CBC	-2.09	121.24	124.46
5	A	1501	HEM	C1D-CHD-C4C	-2.02	122.44	125.82
6	A	1502	H4B	C2-N1-C8A	2.04	119.13	114.54
3	A	1499	GOL	O2-C2-C1	2.08	118.18	108.65
6	B	1501	H4B	N2-C2-N1	2.09	120.66	117.20
5	A	1501	HEM	CAA-C2A-C1A	2.19	129.38	127.01
5	A	1501	HEM	CAA-CBA-CGA	2.30	116.97	112.75
6	B	1501	H4B	C2-N1-C8A	2.49	120.14	114.54
5	B	1500	HEM	CMD-C2D-C3D	2.71	126.32	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1502	H4B	N2-C2-N1	2.72	121.70	117.20
6	B	1501	H4B	C4-N3-C2	2.92	119.99	115.94
4	B	1499	A54	O11-C7-C4	2.94	115.47	110.26
5	A	1501	HEM	CMD-C2D-C3D	3.25	128.72	114.35
5	A	1501	HEM	CAD-C3D-C4D	3.44	124.59	112.47
5	A	1501	HEM	C2D-C3D-C4D	3.64	107.68	101.50
5	B	1500	HEM	CAD-C3D-C4D	3.73	125.61	112.47
5	B	1500	HEM	C2D-C3D-C4D	3.83	107.99	101.50
5	B	1500	HEM	C3B-CAB-CBB	3.90	130.44	124.46
5	A	1501	HEM	CMB-C2B-C3B	3.98	126.48	116.53
5	B	1500	HEM	CMB-C2B-C3B	4.15	126.89	116.53
6	A	1502	H4B	C4-N3-C2	4.27	121.86	115.94
5	B	1500	HEM	CAD-C3D-C2D	4.57	126.37	113.22
5	A	1501	HEM	CMC-C2C-C3C	4.85	128.64	116.53
5	A	1501	HEM	CAD-C3D-C2D	5.03	127.68	113.22
5	B	1500	HEM	CMC-C2C-C3C	5.44	130.11	116.53
6	B	1501	H4B	C4-C4A-C8A	5.66	119.69	114.56
6	A	1502	H4B	C4-C4A-C8A	6.13	120.11	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1499	GOL	2	0
4	A	1500	A54	1	0
5	A	1501	HEM	5	0
6	A	1502	H4B	1	0
3	B	1498	GOL	1	0
4	B	1499	A54	1	0
5	B	1500	HEM	6	0
6	B	1501	H4B	1	0

## 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	411/433 (94%)	0.08	22 (5%)	29 22	34, 54, 86, 104	0
1	B	412/433 (95%)	0.10	22 (5%)	30 23	33, 53, 88, 115	0
All	All	823/866 (95%)	0.09	44 (5%)	30 23	33, 54, 88, 115	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	78	TYR	4.7
1	A	78	TYR	4.2
1	A	494	ILE	4.1
1	B	382[A]	ARG	3.8
1	B	111	GLY	3.8
1	B	268	ASP	3.7
1	A	91	HIS	3.4
1	B	91	HIS	3.4
1	B	77	GLN	3.4
1	B	90	LEU	3.2
1	A	268	ASP	3.2
1	A	111	GLY	3.2
1	B	270	THR	3.2
1	B	96	HIS	3.1
1	B	391	ARG	3.0
1	A	77	GLN	3.0
1	B	398	HIS	2.9
1	B	267	PRO	2.9
1	B	495	TRP	2.8
1	A	89	ILE	2.8
1	A	269	GLY	2.7
1	A	270	THR	2.7
1	A	265	GLN	2.6
1	A	391	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	267	PRO	2.5
1	B	460	PRO	2.5
1	B	266	MET	2.4
1	A	293	TYR	2.4
1	A	495	TRP	2.4
1	B	110	LEU	2.4
1	B	396	GLU	2.4
1	B	80	ARG	2.3
1	A	287	LEU	2.3
1	B	89	ILE	2.3
1	B	475	LEU	2.2
1	A	398	HIS	2.2
1	B	371	GLU	2.1
1	A	96	HIS	2.1
1	A	110	LEU	2.1
1	A	90	LEU	2.1
1	A	346	VAL	2.1
1	A	475	LEU	2.0
1	A	150	GLU	2.0
1	B	375	ARG	2.0

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

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

## 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, 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	B	1498	6/6	0.95	0.20	2.09	56,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	A	1499	6/6	0.89	0.28	0.96	71,71,72,72	0
5	HEM	A	1501	43/43	0.98	0.22	0.41	35,36,43,47	0
4	A54	A	1500	20/20	0.99	0.23	0.22	28,39,54,58	0
5	HEM	B	1500	43/43	0.98	0.19	-0.04	33,34,41,45	0
6	H4B	A	1502	17/17	0.93	0.20	-0.04	53,56,58,60	0
6	H4B	B	1501	17/17	0.94	0.20	-0.11	53,58,60,61	0
4	A54	B	1499	20/20	0.98	0.20	-0.52	27,39,52,58	0
2	SO4	B	1497	5/5	0.87	0.28	-	112,116,118,118	0
2	SO4	A	1498	5/5	0.95	0.88	-	198,202,203,204	5
2	SO4	A	1497	5/5	0.81	0.30	-	119,123,123,125	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.