



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:10 PM GMT

PDB ID : 1NSI  
Title : HUMAN INDUCIBLE NITRIC OXIDE SYNTHASE, ZN-BOUND, L-ARG COMPLEX  
Authors : Li, H.; Raman, C.S.; Glaser, C.B.; Blasko, E.; Young, T.A.; Parkinson, J.F.; Whitlow, M.; Poulos, T.L.  
Deposited on : 1999-01-10  
Resolution : 2.55 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

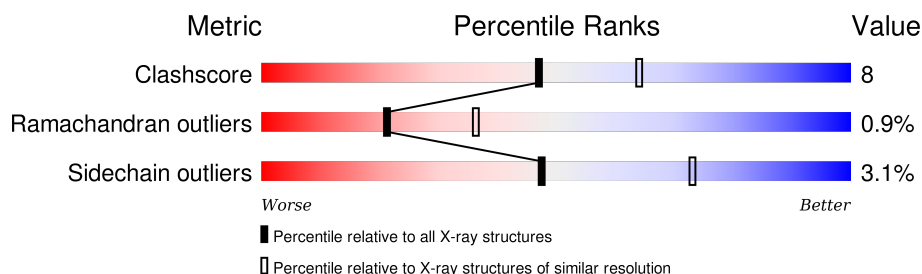
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	431	 82% 14% . .
1	B	431	 78% 16% . .
1	C	431	 80% 16% . .
1	D	431	 73% 22% . .

## 2 Entry composition [i](#)

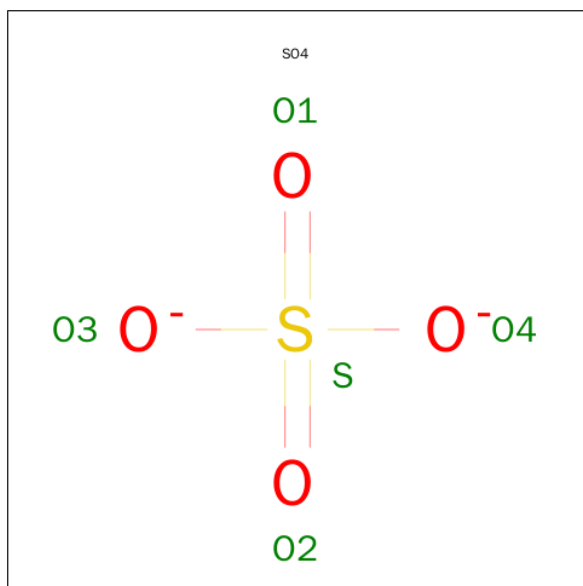
There are 8 unique types of molecules in this entry. The entry contains 14330 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (NITRIC OXIDE SYNTHASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	0	0
			3419	2186	599	612	22			
1	B	420	Total	C	N	O	S	0	0	0
			3419	2186	599	612	22			
1	C	420	Total	C	N	O	S	0	0	0
			3419	2186	599	612	22			
1	D	420	Total	C	N	O	S	0	0	0
			3419	2186	599	612	22			

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (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		

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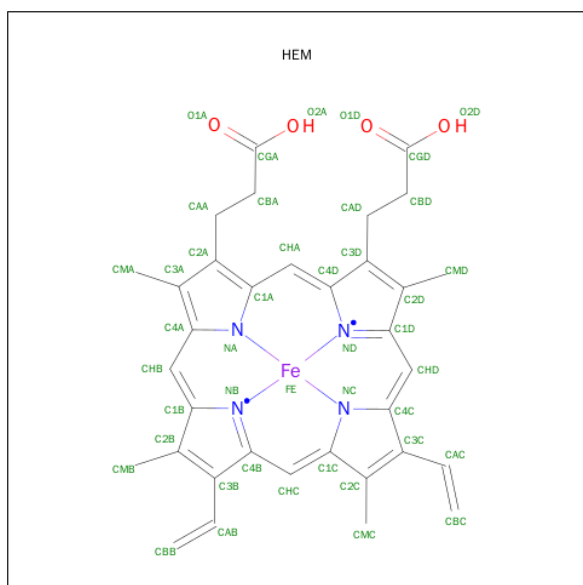
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0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

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

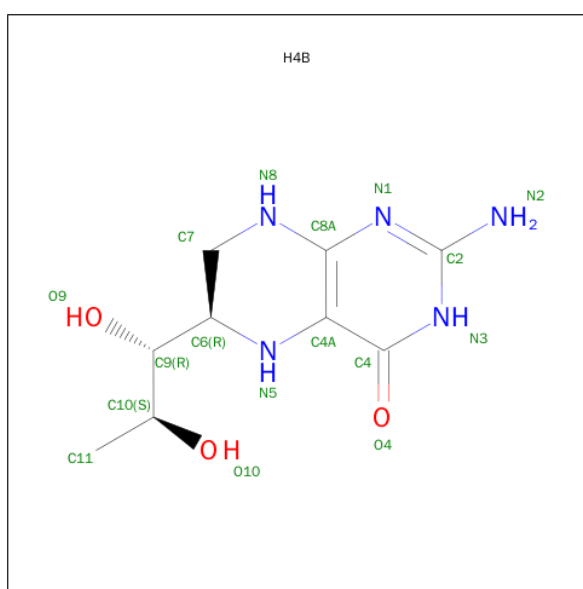
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

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



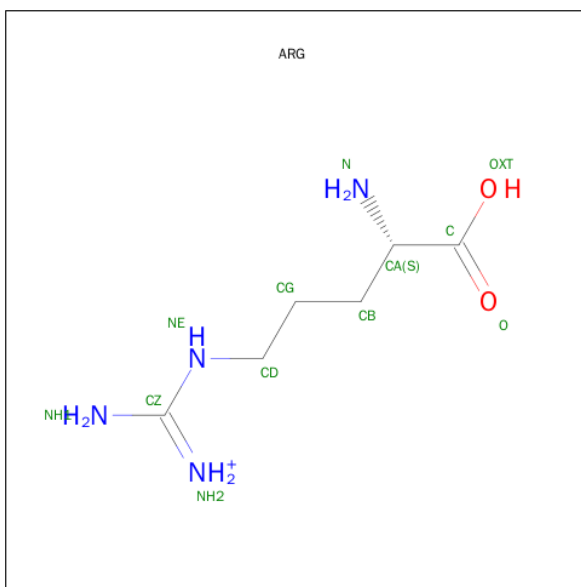
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
4	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- 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		
			17	9	5	3		
5	B	1	Total	C	N	O		
			17	9	5	3		
5	C	1	Total	C	N	O		
			17	9	5	3		
5	D	1	Total	C	N	O		
			17	9	5	3		

- Molecule 6 is ARGinine (three-letter code: ARG) (formula:  $C_6H_{15}N_4O_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			12	6	4	2		
6	B	1	Total	C	N	O	0	0
			12	6	4	2		
6	C	1	Total	C	N	O	0	0
			12	6	4	2		
6	D	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 7 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
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

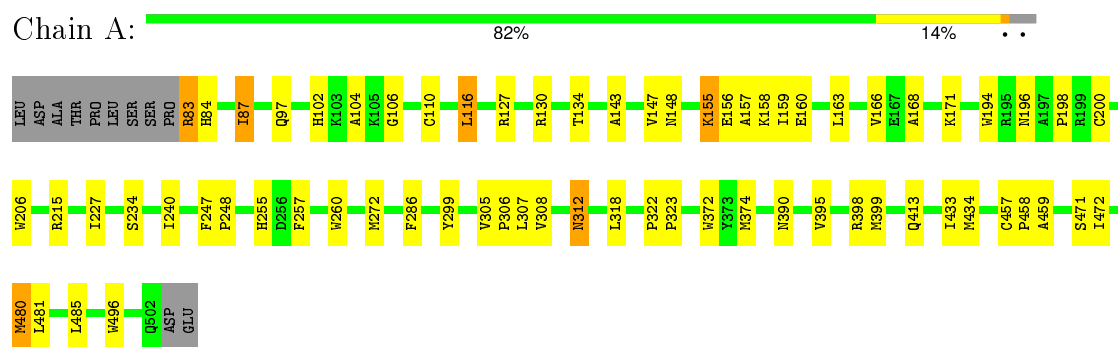
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	92	Total	O	0	0
			92	92		
8	B	77	Total	O	0	0
			77	77		
8	C	88	Total	O	0	0
			88	88		
8	D	38	Total	O	0	0
			38	38		

### 3 Residue-property plots

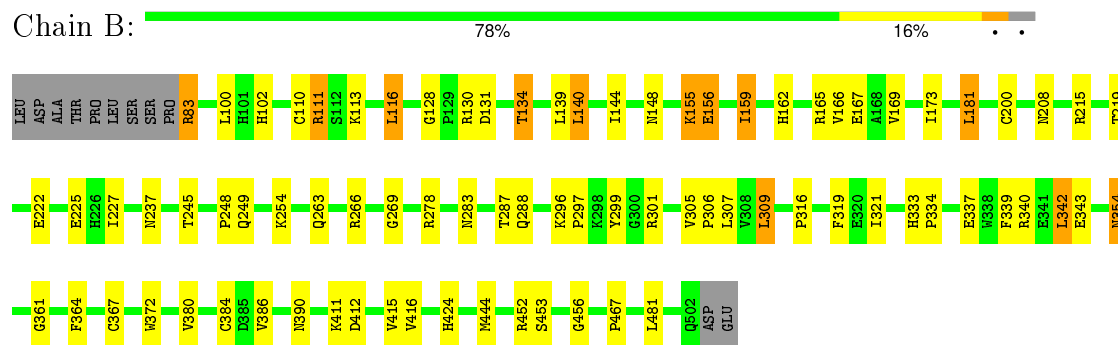
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

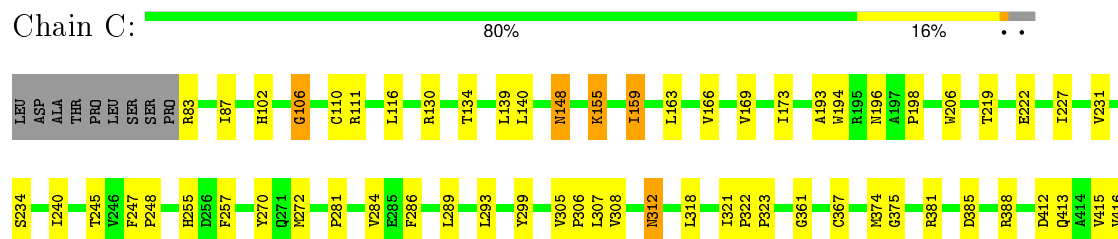
#### • Molecule 1: PROTEIN (NITRIC OXIDE SYNTHASE)



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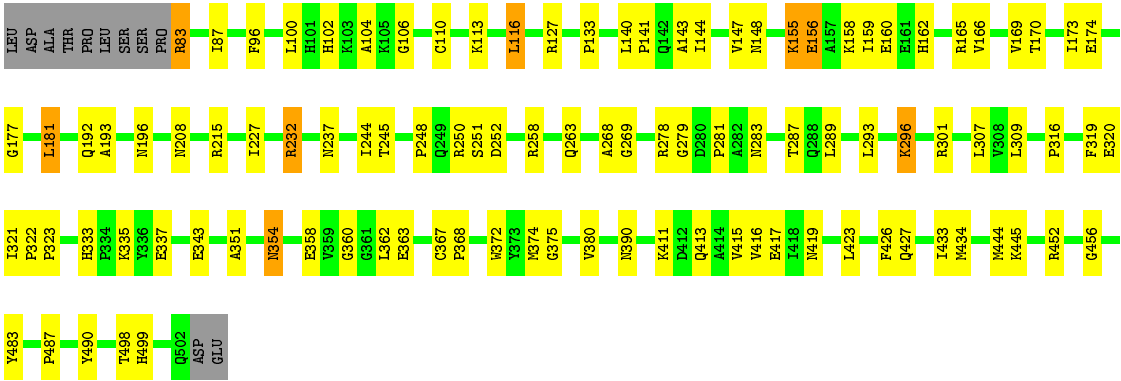






● Molecule 1: PROTEIN (NITRIC OXIDE SYNTHASE)

Chain D: 73% 22% . .



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	187.35Å 187.35Å 227.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.55	Depositor
% Data completeness (in resolution range)	80.5 (30.00-2.55)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.209 , 0.243	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14330	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

## 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, 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	0.37	0/3518	0.63	1/4774 (0.0%)
1	B	0.38	0/3518	0.63	0/4774
1	C	0.36	0/3518	0.61	0/4774
1	D	0.38	0/3518	0.62	1/4774 (0.0%)
All	All	0.37	0/14072	0.62	2/19096 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	CYS	CA-CB-SG	-8.77	98.22	114.00
1	D	110	CYS	CA-CB-SG	6.20	125.16	114.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3419	0	3326	46	0
1	B	3419	0	3326	59	0
1	C	3419	0	3326	52	0
1	D	3419	0	3326	63	0
2	A	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	43	0	30	1	0
4	B	43	0	30	2	0
4	C	43	0	30	0	0
4	D	43	0	30	2	0
5	A	17	0	15	0	0
5	B	17	0	15	0	0
5	C	17	0	15	1	0
5	D	17	0	15	0	0
6	A	12	0	12	0	0
6	B	12	0	12	0	0
6	C	12	0	12	0	0
6	D	12	0	12	0	0
7	A	6	0	8	0	0
7	B	6	0	8	0	0
7	C	6	0	8	0	0
7	D	6	0	8	3	0
8	A	92	0	0	1	0
8	B	77	0	0	0	0
8	C	88	0	0	0	0
8	D	38	0	0	0	0
All	All	14330	0	13564	208	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 8.

All (208) 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:481:LEU:HD22	1:B:116:LEU:HD22	1.54	0.90
1:C:481:LEU:HD22	1:D:116:LEU:HD22	1.56	0.86
1:A:83:ARG:HH11	1:A:83:ARG:HB2	1.42	0.84
1:D:411:LYS:O	1:D:415:VAL:HG23	1.81	0.80
1:A:116:LEU:HD22	1:B:481:LEU:HG	1.68	0.76
1:D:83:ARG:HH11	1:D:83:ARG:HB2	1.49	0.75
1:C:227:ILE:HG21	1:C:307:LEU:HD21	1.74	0.69
1:C:257:PHE:CE1	1:C:312:ASN:HB3	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:GLY:H	1:B:287:THR:HG21	1.59	0.68
1:A:372:TRP:H	4:A:550:HEM:HAB	1.58	0.66
1:B:305:VAL:HG22	1:B:306:PRO:HD2	1.77	0.66
1:D:227:ILE:HG21	1:D:307:LEU:HD21	1.77	0.66
1:D:100:LEU:HB3	1:D:456:GLY:HA3	1.78	0.66
1:B:227:ILE:HG21	1:B:307:LEU:HD21	1.76	0.65
1:D:258:ARG:HH21	7:D:883:GOL:H2	1.60	0.65
1:B:411:LYS:O	1:B:415:VAL:HG23	1.97	0.64
1:D:140:LEU:O	1:D:144:ILE:HG12	1.98	0.64
1:A:83:ARG:NH1	1:A:83:ARG:HB2	2.13	0.64
1:B:144:ILE:HG22	1:B:148:ASN:HD21	1.63	0.63
1:D:143:ALA:O	1:D:147:VAL:HG23	1.99	0.63
1:D:354:ASN:H	1:D:354:ASN:HD22	1.46	0.62
1:A:84:HIS:HB3	1:A:97:GLN:NE2	2.15	0.62
1:C:255:HIS:HB3	1:C:312:ASN:HB2	1.82	0.62
1:B:283:ASN:O	1:B:287:THR:HG23	2.00	0.61
1:C:130:ARG:NH1	1:C:134:THR:HG22	2.17	0.60
1:B:354:ASN:HD22	1:B:354:ASN:N	2.00	0.60
1:A:83:ARG:HB3	1:A:102:HIS:NE2	2.18	0.59
1:D:170:THR:O	1:D:174:GLU:HB2	2.02	0.59
1:D:301:ARG:HH22	1:D:343:GLU:HB2	1.67	0.59
1:B:83:ARG:HB2	1:B:83:ARG:HH11	1.67	0.59
1:D:269:GLY:H	1:D:287:THR:HG21	1.67	0.59
1:B:111:ARG:HD2	1:B:111:ARG:N	2.17	0.59
1:A:257:PHE:CE1	1:A:312:ASN:HB3	2.38	0.58
1:A:227:ILE:HG21	1:A:307:LEU:HD21	1.84	0.58
1:B:215:ARG:O	1:B:248:PRO:HG3	2.03	0.57
1:C:412:ASP:O	1:C:416:VAL:HG23	2.03	0.57
1:B:140:LEU:HD22	1:B:173:ILE:HD12	1.87	0.56
1:B:83:ARG:HB3	1:B:102:HIS:NE2	2.20	0.56
1:C:305:VAL:HG13	1:C:306:PRO:HD2	1.86	0.56
1:A:168:ALA:O	1:A:171:LYS:HE2	2.05	0.56
1:D:309:LEU:HD23	1:D:319:PHE:CD2	2.40	0.56
1:B:372:TRP:H	4:B:550:HEM:HAB	1.71	0.56
1:D:162:HIS:O	1:D:166:VAL:HG23	2.07	0.55
1:A:472:ILE:HG13	1:B:415:VAL:HG21	1.88	0.55
1:B:130:ARG:CZ	1:B:134:THR:HG23	2.36	0.55
1:D:333:HIS:CE1	1:D:335:LYS:HG3	2.42	0.55
1:B:139:LEU:CD1	1:B:361:GLY:HA3	2.37	0.55
1:D:372:TRP:H	4:D:550:HEM:HAB	1.72	0.55
1:D:283:ASN:O	1:D:287:THR:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:LEU:CD2	1:B:181:LEU:H	2.20	0.54
1:B:100:LEU:HB3	1:B:456:GLY:HA3	1.88	0.54
1:A:83:ARG:HB3	1:A:102:HIS:CE1	2.42	0.54
1:D:232:ARG:HH12	1:D:237:ASN:HD21	1.56	0.54
1:D:144:ILE:HG22	1:D:148:ASN:HD21	1.73	0.54
1:A:196:ASN:O	1:A:198:PRO:HD3	2.08	0.54
1:C:83:ARG:HB3	1:C:102:HIS:NE2	2.23	0.53
1:A:308:VAL:HG22	1:A:318:LEU:HD22	1.90	0.53
1:A:471:SER:OG	1:B:467:PRO:HB2	2.09	0.53
1:C:270:TYR:HB2	1:C:272:MET:HE3	1.91	0.53
1:D:354:ASN:N	1:D:354:ASN:HD22	2.08	0.52
1:D:445:LYS:HZ1	1:D:452:ARG:HH22	1.57	0.52
1:D:309:LEU:O	1:D:316:PRO:HA	2.09	0.52
1:D:380:VAL:HG22	1:D:419:ASN:HD21	1.74	0.52
1:A:413:GLN:HG2	1:B:416:VAL:HG11	1.92	0.51
1:C:194:TRP:CE3	1:C:206:TRP:HA	2.45	0.51
1:C:169:VAL:O	1:C:173:ILE:HG13	2.11	0.51
1:A:286:PHE:CE2	1:A:305:VAL:HG11	2.46	0.50
1:D:367:CYS:N	1:D:368:PRO:HD3	2.25	0.50
1:A:286:PHE:HE2	1:A:305:VAL:HG11	1.77	0.50
1:D:165:ARG:O	1:D:169:VAL:HG23	2.11	0.50
8:A:1020:HOH:O	1:B:386:VAL:HG22	2.11	0.50
1:A:194:TRP:CE3	1:A:206:TRP:HA	2.47	0.50
1:A:143:ALA:O	1:A:147:VAL:HG23	2.12	0.50
1:B:165:ARG:O	1:B:169:VAL:HG23	2.12	0.49
1:B:131:ASP:O	1:B:254:LYS:HE3	2.12	0.49
1:B:339:PHE:O	1:B:342:LEU:HB2	2.11	0.49
1:B:140:LEU:HD12	1:C:140:LEU:CD1	2.43	0.49
1:C:130:ARG:CZ	1:C:134:THR:HG22	2.43	0.49
1:B:305:VAL:CG2	1:B:306:PRO:HD2	2.41	0.49
1:C:413:GLN:HG2	1:D:416:VAL:HG11	1.95	0.49
1:C:245:THR:O	1:C:367:CYS:HA	2.13	0.49
1:D:83:ARG:HB3	1:D:102:HIS:NE2	2.28	0.49
1:C:381:ARG:HH12	5:C:602:H4B:C4	2.26	0.48
1:A:106:GLY:HA2	1:B:113:LYS:HA	1.95	0.48
1:A:155:LYS:CD	1:A:155:LYS:H	2.27	0.48
1:D:358:GLU:O	1:D:487:PRO:HA	2.13	0.48
1:D:155:LYS:H	1:D:155:LYS:HE3	1.77	0.48
1:C:248:PRO:HG2	1:C:257:PHE:CD1	2.49	0.48
1:D:140:LEU:HD11	1:D:170:THR:HG23	1.94	0.48
1:D:423:LEU:O	1:D:427:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:ASP:O	1:B:416:VAL:HG23	2.14	0.47
1:C:155:LYS:HD3	1:C:155:LYS:H	1.80	0.47
1:A:163:LEU:HA	1:A:166:VAL:HG12	1.96	0.47
1:B:333:HIS:ND1	1:B:334:PRO:HD2	2.29	0.47
1:C:270:TYR:HB2	1:C:272:MET:CE	2.44	0.47
1:A:110:CYS:HB3	1:B:110:CYS:HB3	1.96	0.47
1:D:289:LEU:O	1:D:293:LEU:HG	2.14	0.47
1:A:255:HIS:HB3	1:A:312:ASN:HB2	1.96	0.47
1:D:445:LYS:NZ	1:D:452:ARG:NH2	2.62	0.47
1:C:385:ASP:HB2	1:C:388:ARG:HG2	1.96	0.47
1:C:293:LEU:HD12	1:C:318:LEU:HD21	1.97	0.47
1:D:140:LEU:N	1:D:141:PRO:CD	2.78	0.47
1:A:234:SER:O	1:A:240:ILE:HA	2.15	0.47
1:A:305:VAL:HG13	1:A:306:PRO:HD2	1.97	0.46
1:B:222:GLU:HA	1:B:225:GLU:OE1	2.15	0.46
1:D:158:LYS:O	1:D:160:GLU:N	2.48	0.46
1:D:173:ILE:O	1:D:177:GLY:HA2	2.15	0.46
1:A:158:LYS:O	1:A:160:GLU:N	2.48	0.46
1:C:196:ASN:O	1:C:198:PRO:HD3	2.16	0.46
1:D:374:MET:HA	1:D:434:MET:O	2.15	0.46
1:C:374:MET:HA	1:C:434:MET:O	2.16	0.46
1:B:380:VAL:O	1:B:384:CYS:HB2	2.16	0.45
1:A:215:ARG:HA	1:A:248:PRO:HD3	1.99	0.45
1:A:247:PHE:HB3	1:A:248:PRO:HD2	1.98	0.45
1:A:395:VAL:O	1:A:399:MET:HG3	2.16	0.45
1:B:263:GLN:HB2	1:B:266:ARG:HD2	1.97	0.45
1:A:308:VAL:HG22	1:A:318:LEU:CD2	2.46	0.45
1:B:340:ARG:HB3	1:B:340:ARG:HE	1.55	0.45
1:C:286:PHE:CE2	1:C:305:VAL:HG11	2.52	0.45
1:D:193:ALA:HB2	1:D:487:PRO:HB2	1.99	0.45
1:B:237:ASN:HD22	1:B:237:ASN:N	2.14	0.45
1:C:281:PRO:HA	1:C:284:VAL:HG23	1.99	0.45
1:D:498:THR:OG1	7:D:883:GOL:H32	2.17	0.45
1:C:385:ASP:HB2	1:C:388:ARG:CG	2.47	0.45
1:C:247:PHE:HB3	1:C:248:PRO:HD2	1.99	0.44
1:B:301:ARG:HH22	1:B:343:GLU:HB2	1.83	0.44
1:D:87:ILE:HG13	1:D:96:PHE:HB2	1.98	0.44
1:A:104:ALA:HA	1:A:485:LEU:HD23	2.00	0.44
1:A:260:TRP:CZ3	1:A:496:TRP:HB3	2.52	0.44
1:B:334:PRO:HG3	1:B:424:HIS:CG	2.52	0.44
1:A:148:ASN:N	1:A:148:ASN:HD22	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ILE:O	1:C:231:VAL:HG23	2.17	0.44
1:D:301:ARG:NH2	1:D:343:GLU:HB2	2.33	0.44
1:D:322:PRO:HA	1:D:323:PRO:HD3	1.88	0.44
1:D:263:GLN:HA	1:D:351:ALA:O	2.18	0.44
1:C:155:LYS:CD	1:C:155:LYS:H	2.31	0.43
1:C:308:VAL:HG22	1:C:318:LEU:HD22	2.01	0.43
1:C:486:SER:HA	1:C:487:PRO:C	2.39	0.43
1:C:106:GLY:HA2	1:D:113:LYS:HA	1.99	0.43
1:B:245:THR:O	1:B:367:CYS:HA	2.19	0.43
1:C:451:TYR:CE1	1:C:457:CYS:HB3	2.53	0.43
1:D:250:ARG:HD2	1:D:363:GLU:OE1	2.18	0.43
1:B:296:LYS:HA	1:B:297:PRO:HD2	1.89	0.43
1:D:307:LEU:HD13	1:D:321:ILE:HD11	2.00	0.43
1:A:155:LYS:H	1:A:155:LYS:HE3	1.83	0.43
1:A:130:ARG:NH1	1:A:134:THR:HG22	2.34	0.43
1:B:307:LEU:HD22	1:B:321:ILE:HG12	2.01	0.43
1:B:354:ASN:HD22	1:B:354:ASN:H	1.67	0.43
1:D:499:HIS:HA	7:D:883:GOL:O3	2.19	0.43
1:B:140:LEU:O	1:B:144:ILE:HG12	2.18	0.43
1:D:87:ILE:CG1	1:D:96:PHE:HB2	2.49	0.43
1:A:156:GLU:HB3	1:A:157:ALA:H	1.66	0.42
1:A:127:ARG:HD3	1:A:127:ARG:HA	1.85	0.42
1:A:248:PRO:HG2	1:A:257:PHE:CG	2.54	0.42
4:D:550:HEM:HBC2	4:D:550:HEM:HMC1	2.00	0.42
1:B:181:LEU:CD2	1:B:181:LEU:N	2.83	0.42
1:B:342:LEU:HA	1:B:342:LEU:HD12	1.87	0.42
1:D:296:LYS:HD3	1:D:296:LYS:N	2.35	0.42
1:A:459:ALA:HB3	1:A:480:MET:HB2	2.00	0.42
1:B:200:CYS:HB2	4:B:550:HEM:ND	2.35	0.42
1:C:148:ASN:N	1:C:148:ASN:HD22	2.16	0.42
1:C:375:GLY:HA3	1:C:423:LEU:HD11	2.02	0.42
1:D:244:ILE:HG12	1:D:245:THR:N	2.33	0.42
1:D:426:PHE:CD2	1:D:433:ILE:HB	2.55	0.42
1:D:268:ALA:HB1	1:D:287:THR:HG21	2.01	0.42
1:C:193:ALA:HB2	1:C:487:PRO:HB2	2.01	0.42
1:A:87:ILE:HD13	1:A:87:ILE:HA	1.77	0.42
1:B:249:GLN:HB3	1:B:364:PHE:CE2	2.54	0.42
1:B:159:ILE:HG22	1:C:159:ILE:HG22	2.01	0.42
1:B:181:LEU:HD23	1:B:181:LEU:N	2.35	0.42
1:C:270:TYR:CE1	1:C:299:TYR:HA	2.55	0.42
1:D:133:PRO:HB3	1:D:251:SER:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:LYS:H	1:B:155:LYS:HE3	1.85	0.42
1:D:155:LYS:NZ	1:D:156:GLU:HG3	2.35	0.42
1:C:289:LEU:O	1:C:293:LEU:HG	2.20	0.42
1:D:337:GLU:HB3	2:D:923:SO4:O2	2.19	0.42
1:C:412:ASP:O	1:C:415:VAL:HG12	2.20	0.41
1:B:155:LYS:NZ	1:B:156:GLU:HG3	2.35	0.41
1:B:309:LEU:HD23	1:B:319:PHE:CD1	2.55	0.41
1:D:215:ARG:O	1:D:248:PRO:HG3	2.20	0.41
1:C:234:SER:O	1:C:240:ILE:HA	2.20	0.41
1:B:162:HIS:O	1:B:166:VAL:HG23	2.20	0.41
1:C:110:CYS:O	1:C:111:ARG:HD3	2.20	0.41
1:D:181:LEU:HD22	1:D:362:LEU:CD1	2.51	0.41
1:C:322:PRO:HA	1:C:323:PRO:HD2	1.91	0.41
1:A:374:MET:HA	1:A:434:MET:O	2.21	0.41
1:C:367:CYS:SG	1:C:367:CYS:O	2.79	0.41
1:C:437:HIS:O	1:C:441:GLU:HG3	2.21	0.41
1:C:219:THR:OG1	1:C:222:GLU:HG3	2.21	0.41
1:A:457:CYS:HA	1:A:458:PRO:HD2	1.96	0.41
1:B:110:CYS:C	1:B:111:ARG:HD2	2.40	0.41
1:D:127:ARG:HB2	1:D:490:TYR:CB	2.50	0.41
1:C:307:LEU:HD13	1:C:321:ILE:HD11	2.02	0.41
1:B:144:ILE:HG22	1:B:148:ASN:ND2	2.32	0.41
1:B:354:ASN:ND2	1:B:354:ASN:N	2.65	0.41
1:B:309:LEU:O	1:B:316:PRO:HA	2.21	0.41
1:A:272:MET:HE1	1:A:299:TYR:CD1	2.56	0.41
1:C:472:ILE:HG13	1:D:415:VAL:HG21	2.03	0.41
1:B:354:ASN:ND2	1:B:354:ASN:H	2.19	0.41
1:D:192:GLN:HG3	1:D:196:ASN:HD21	1.86	0.41
1:D:279:GLY:O	1:D:281:PRO:HD3	2.21	0.40
1:A:322:PRO:HA	1:A:323:PRO:HD2	1.86	0.40
1:C:286:PHE:HE2	1:C:305:VAL:HG11	1.87	0.40
1:C:83:ARG:NH1	1:C:83:ARG:HG2	2.36	0.40
1:C:139:LEU:HD12	1:C:361:GLY:HA3	2.02	0.40
1:D:413:GLN:O	1:D:417:GLU:HG2	2.21	0.40
1:D:104:ALA:CB	1:D:483:TYR:HB2	2.51	0.40
1:C:163:LEU:HA	1:C:166:VAL:HG12	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	418/431 (97%)	388 (93%)	28 (7%)	2 (0%)	34	54
1	B	418/431 (97%)	383 (92%)	30 (7%)	5 (1%)	16	27
1	C	418/431 (97%)	386 (92%)	29 (7%)	3 (1%)	26	44
1	D	418/431 (97%)	381 (91%)	32 (8%)	5 (1%)	16	27
All	All	1672/1724 (97%)	1538 (92%)	119 (7%)	15 (1%)	21	36

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	ILE
1	B	299	TYR
1	D	159	ILE
1	B	159	ILE
1	C	159	ILE
1	C	312	ASN
1	B	156	GLU
1	B	453	SER
1	A	312	ASN
1	B	128	GLY
1	D	156	GLU
1	C	106	GLY
1	D	375	GLY
1	D	106	GLY
1	D	360	GLY

### 5.3.2 Protein sidechains [i](#)

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	366/376 (97%)	358 (98%)	8 (2%)	60	83
1	B	366/376 (97%)	347 (95%)	19 (5%)	29	49
1	C	366/376 (97%)	360 (98%)	6 (2%)	70	89
1	D	366/376 (97%)	353 (96%)	13 (4%)	42	67
All	All	1464/1504 (97%)	1418 (97%)	46 (3%)	47	73

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ARG
1	A	87	ILE
1	A	116	LEU
1	A	155	LYS
1	A	390	ASN
1	A	398	ARG
1	A	433	ILE
1	A	480	MET
1	B	83	ARG
1	B	111	ARG
1	B	116	LEU
1	B	134	THR
1	B	140	LEU
1	B	155	LYS
1	B	167	GLU
1	B	181	LEU
1	B	208	ASN
1	B	219	THR
1	B	278	ARG
1	B	288	GLN
1	B	309	LEU
1	B	337	GLU
1	B	342	LEU
1	B	354	ASN
1	B	390	ASN
1	B	444	MET
1	B	452	ARG
1	C	87	ILE
1	C	116	LEU
1	C	148	ASN
1	C	155	LYS

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Mol	Chain	Res	Type
1	C	433	ILE
1	C	482	ASN
1	D	83	ARG
1	D	116	LEU
1	D	155	LYS
1	D	181	LEU
1	D	208	ASN
1	D	232	ARG
1	D	252	ASP
1	D	278	ARG
1	D	296	LYS
1	D	320	GLU
1	D	354	ASN
1	D	390	ASN
1	D	444	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	162	HIS
1	A	205	GLN
1	A	390	ASN
1	A	482	ASN
1	B	148	ASN
1	B	192	GLN
1	B	205	GLN
1	B	208	ASN
1	B	237	ASN
1	B	249	GLN
1	B	263	GLN
1	B	310	GLN
1	B	312	ASN
1	B	354	ASN
1	B	390	ASN
1	B	424	HIS
1	B	427	GLN
1	B	482	ASN
1	B	502	GLN
1	C	192	GLN
1	C	205	GLN
1	C	390	ASN

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Mol	Chain	Res	Type
1	C	427	GLN
1	C	482	ASN
1	D	142	GLN
1	D	148	ASN
1	D	192	GLN
1	D	205	GLN
1	D	208	ASN
1	D	237	ASN
1	D	249	GLN
1	D	263	GLN
1	D	271	GLN
1	D	312	ASN
1	D	354	ASN
1	D	390	ASN
1	D	427	GLN
1	D	482	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](#)

Of 27 ligands modelled in this entry, 2 are monoatomic - leaving 25 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	550	1	30,50,50	3.06	7 (23%)	24,82,82	2.09	7 (29%)
5	H4B	A	600	-	13,18,18	1.79	3 (23%)	11,26,26	4.13	6 (54%)
6	ARG	A	700	-	5,11,11	0.22	0	3,13,13	0.05	0
7	GOL	A	880	-	5,5,5	0.32	0	5,5,5	0.30	0
2	SO4	A	910	-	4,4,4	0.83	0	6,6,6	0.29	0
2	SO4	A	920	-	4,4,4	1.01	0	6,6,6	0.27	0
2	SO4	A	930	-	4,4,4	0.89	0	6,6,6	0.22	0
4	HEM	B	550	1	30,50,50	2.81	8 (26%)	24,82,82	2.24	8 (33%)
5	H4B	B	601	-	13,18,18	1.90	3 (23%)	11,26,26	4.12	6 (54%)
6	ARG	B	701	-	5,11,11	0.27	0	3,13,13	0.10	0
7	GOL	B	881	-	5,5,5	0.24	0	5,5,5	0.31	0
2	SO4	B	911	-	4,4,4	0.99	0	6,6,6	0.29	0
2	SO4	B	921	-	4,4,4	0.95	0	6,6,6	0.37	0
4	HEM	C	550	1	30,50,50	3.11	9 (30%)	24,82,82	2.33	8 (33%)
5	H4B	C	602	-	13,18,18	1.88	3 (23%)	11,26,26	4.23	6 (54%)
6	ARG	C	702	-	5,11,11	0.26	0	3,13,13	0.28	0
7	GOL	C	882	-	5,5,5	0.34	0	5,5,5	0.29	0
2	SO4	C	912	-	4,4,4	0.87	0	6,6,6	0.22	0
2	SO4	C	922	-	4,4,4	0.96	0	6,6,6	0.24	0
4	HEM	D	550	1	30,50,50	2.87	6 (20%)	24,82,82	2.23	7 (29%)
5	H4B	D	603	-	13,18,18	1.92	3 (23%)	11,26,26	4.16	6 (54%)
6	ARG	D	703	-	5,11,11	0.22	0	3,13,13	0.17	0
7	GOL	D	883	-	5,5,5	0.31	0	5,5,5	0.25	0
2	SO4	D	913	-	4,4,4	0.97	0	6,6,6	0.20	0
2	SO4	D	923	-	4,4,4	1.00	0	6,6,6	0.26	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
4	HEM	A	550	1	-	0/10/54/54	0/0/8/8
5	H4B	A	600	-	-	0/8/17/17	0/2/2/2
6	ARG	A	700	-	-	0/5/11/11	0/0/0/0
7	GOL	A	880	-	-	0/4/4/4	0/0/0/0
2	SO4	A	910	-	-	0/0/0/0	0/0/0/0
2	SO4	A	920	-	-	0/0/0/0	0/0/0/0
2	SO4	A	930	-	-	0/0/0/0	0/0/0/0
4	HEM	B	550	1	-	0/10/54/54	0/0/8/8
5	H4B	B	601	-	-	0/8/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ARG	B	701	-	-	0/5/11/11	0/0/0/0
7	GOL	B	881	-	-	0/4/4/4	0/0/0/0
2	SO4	B	911	-	-	0/0/0/0	0/0/0/0
2	SO4	B	921	-	-	0/0/0/0	0/0/0/0
4	HEM	C	550	1	-	0/10/54/54	0/0/8/8
5	H4B	C	602	-	-	0/8/17/17	0/2/2/2
6	ARG	C	702	-	-	0/5/11/11	0/0/0/0
7	GOL	C	882	-	-	0/4/4/4	0/0/0/0
2	SO4	C	912	-	-	0/0/0/0	0/0/0/0
2	SO4	C	922	-	-	0/0/0/0	0/0/0/0
4	HEM	D	550	1	-	0/10/54/54	0/0/8/8
5	H4B	D	603	-	-	0/8/17/17	0/2/2/2
6	ARG	D	703	-	-	0/5/11/11	0/0/0/0
7	GOL	D	883	-	-	0/4/4/4	0/0/0/0
2	SO4	D	913	-	-	0/0/0/0	0/0/0/0
2	SO4	D	923	-	-	0/0/0/0	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	550	HEM	C2D-C3D	-7.99	1.30	1.54
4	D	550	HEM	C3B-C4B	-7.80	1.44	1.51
4	A	550	HEM	C3B-CAB	-7.58	1.37	1.51
4	B	550	HEM	C3B-C4B	-7.57	1.45	1.51
4	D	550	HEM	C2D-C3D	-7.45	1.32	1.54
4	A	550	HEM	C3B-C4B	-7.44	1.45	1.51
4	C	550	HEM	C3B-C4B	-7.19	1.45	1.51
4	A	550	HEM	C2D-C3D	-6.94	1.33	1.54
4	A	550	HEM	C3C-CAC	-6.71	1.38	1.51
4	D	550	HEM	C3B-CAB	-6.56	1.39	1.51
4	C	550	HEM	C3C-CAC	-6.39	1.39	1.51
4	B	550	HEM	C2D-C3D	-6.38	1.35	1.54
4	C	550	HEM	C3D-C4D	-6.30	1.43	1.51
4	C	550	HEM	C3B-CAB	-6.30	1.39	1.51
4	B	550	HEM	C3B-CAB	-6.30	1.39	1.51
4	B	550	HEM	C3D-C4D	-5.81	1.44	1.51
4	D	550	HEM	C3C-CAC	-5.41	1.41	1.51
4	B	550	HEM	C3C-CAC	-5.27	1.41	1.51
4	A	550	HEM	C3D-C4D	-5.18	1.44	1.51
4	D	550	HEM	C3D-C4D	-4.57	1.45	1.51
4	C	550	HEM	C2C-C1C	-4.16	1.44	1.52
4	D	550	HEM	C2C-C1C	-3.99	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	550	HEM	C2C-C1C	-3.61	1.45	1.52
4	B	550	HEM	C2C-C1C	-3.42	1.46	1.52
4	C	550	HEM	C2D-C1D	-2.70	1.43	1.51
4	C	550	HEM	CAD-C3D	-2.61	1.48	1.54
4	C	550	HEM	C2B-C1B	-2.51	1.43	1.51
4	B	550	HEM	C2D-C1D	-2.37	1.44	1.51
4	B	550	HEM	C2B-C1B	-2.26	1.44	1.51
5	D	603	H4B	C6-N5	2.82	1.51	1.45
5	B	601	H4B	C6-N5	2.85	1.51	1.45
5	C	602	H4B	C6-N5	3.01	1.51	1.45
5	A	600	H4B	C6-N5	3.03	1.51	1.45
4	A	550	HEM	C4C-NC	3.07	1.39	1.36
5	A	600	H4B	C4A-N5	3.11	1.45	1.38
5	B	601	H4B	C4A-N5	3.13	1.45	1.38
5	C	602	H4B	C4A-N5	3.15	1.45	1.38
5	D	603	H4B	C4A-N5	3.39	1.45	1.38
5	A	600	H4B	C4-N3	4.06	1.40	1.33
5	C	602	H4B	C4-N3	4.39	1.41	1.33
5	D	603	H4B	C4-N3	4.45	1.41	1.33
5	B	601	H4B	C4-N3	4.46	1.41	1.33

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	602	H4B	N3-C2-N1	-4.46	118.22	125.53
5	B	601	H4B	N3-C2-N1	-4.42	118.29	125.53
5	A	600	H4B	N3-C2-N1	-4.37	118.37	125.53
5	D	603	H4B	N3-C2-N1	-4.37	118.37	125.53
4	D	550	HEM	CBD-CAD-C3D	-3.43	103.58	113.55
4	B	550	HEM	CAA-C2A-C1A	2.04	129.23	127.01
4	B	550	HEM	C2D-C3D-C4D	2.34	105.46	101.50
4	A	550	HEM	CMD-C2D-C3D	2.51	125.44	114.35
4	A	550	HEM	C3C-CAC-CBC	2.55	128.37	124.46
4	B	550	HEM	CMD-C2D-C3D	2.67	126.17	114.35
4	C	550	HEM	C3B-CAB-CBB	2.72	128.63	124.46
4	C	550	HEM	CMD-C2D-C3D	2.79	126.68	114.35
4	C	550	HEM	C3C-CAC-CBC	2.90	128.90	124.46
5	A	600	H4B	N2-C2-N1	2.95	122.09	117.20
4	D	550	HEM	C2D-C3D-C4D	3.00	106.59	101.50
5	B	601	H4B	N2-C2-N1	3.08	122.30	117.20
5	C	602	H4B	N2-C2-N1	3.08	122.30	117.20
5	D	603	H4B	N2-C2-N1	3.19	122.47	117.20

*Continued on next page...*



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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	600	H4B	C2-N1-C8A	3.40	122.18	114.54
5	B	601	H4B	C2-N1-C8A	3.45	122.29	114.54
5	D	603	H4B	C2-N1-C8A	3.47	122.33	114.54
5	C	602	H4B	C2-N1-C8A	3.47	122.34	114.54
4	A	550	HEM	C2D-C3D-C4D	3.51	107.45	101.50
4	D	550	HEM	CMB-C2B-C3B	3.52	125.31	116.53
4	C	550	HEM	CAD-C3D-C2D	3.52	123.35	113.22
4	A	550	HEM	CMB-C2B-C3B	3.56	125.42	116.53
5	B	601	H4B	C4A-C8A-N8	3.73	122.82	118.43
4	D	550	HEM	C3C-CAC-CBC	3.75	130.20	124.46
4	C	550	HEM	CMB-C2B-C3B	3.84	126.12	116.53
4	D	550	HEM	CAD-C3D-C2D	3.93	124.51	113.22
5	D	603	H4B	C4A-C8A-N8	4.02	123.16	118.43
5	A	600	H4B	C4A-C8A-N8	4.02	123.17	118.43
5	C	602	H4B	C4A-C8A-N8	4.04	123.19	118.43
4	B	550	HEM	CMB-C2B-C3B	4.09	126.75	116.53
4	C	550	HEM	CAD-C3D-C4D	4.11	126.97	112.47
4	A	550	HEM	CAD-C3D-C2D	4.15	125.14	113.22
4	A	550	HEM	CAD-C3D-C4D	4.17	127.16	112.47
4	B	550	HEM	CAD-C3D-C4D	4.20	127.29	112.47
4	B	550	HEM	C3C-CAC-CBC	4.29	131.04	124.46
4	D	550	HEM	CAD-C3D-C4D	4.43	128.11	112.47
4	B	550	HEM	CMC-C2C-C3C	4.55	127.88	116.53
4	B	550	HEM	CAD-C3D-C2D	4.56	126.34	113.22
4	D	550	HEM	CMC-C2C-C3C	4.59	127.99	116.53
4	C	550	HEM	C2D-C3D-C4D	4.61	109.32	101.50
4	A	550	HEM	CMC-C2C-C3C	4.76	128.41	116.53
4	C	550	HEM	CMC-C2C-C3C	4.87	128.69	116.53
5	B	601	H4B	C4-N3-C2	6.50	124.97	115.94
5	C	602	H4B	C4-N3-C2	6.53	125.00	115.94
5	D	603	H4B	C4-N3-C2	6.55	125.04	115.94
5	A	600	H4B	C4-N3-C2	6.78	125.35	115.94
5	A	600	H4B	C4-C4A-C8A	9.08	122.78	114.56
5	B	601	H4B	C4-C4A-C8A	9.25	122.93	114.56
5	D	603	H4B	C4-C4A-C8A	9.31	122.99	114.56
5	C	602	H4B	C4-C4A-C8A	9.62	123.27	114.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	550	HEM	1	0
4	B	550	HEM	2	0
5	C	602	H4B	1	0
4	D	550	HEM	2	0
7	D	883	GOL	3	0
2	D	923	SO4	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.