



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:02 AM GMT

PDB ID : 3NOD  
Title : MURINE INDUCIBLE NITRIC OXIDE SYNTHASE OXYGENASE DIMER  
(DELTA 65) WITH TETRAHYDROBIOPTERIN AND PRODUCT ANA-  
LOGUE L-THIOCITRULLINE  
Authors : Crane, B.R.; Arvai, A.S.; Getzoff, E.D.; Stuehr, D.J.; Tainer, J.A.  
Deposited on : 1998-03-06  
Resolution : 2.70 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.

---

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

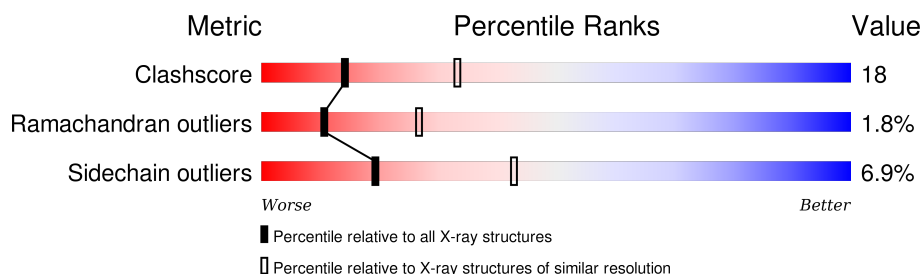
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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	423	
1	B	423	

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
4	H4B	A	902	X	-	-	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7205 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3373	2162	582	609	20			
1	B	413	Total	C	N	O	S	0	0	0
			3368	2159	581	608	20			

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



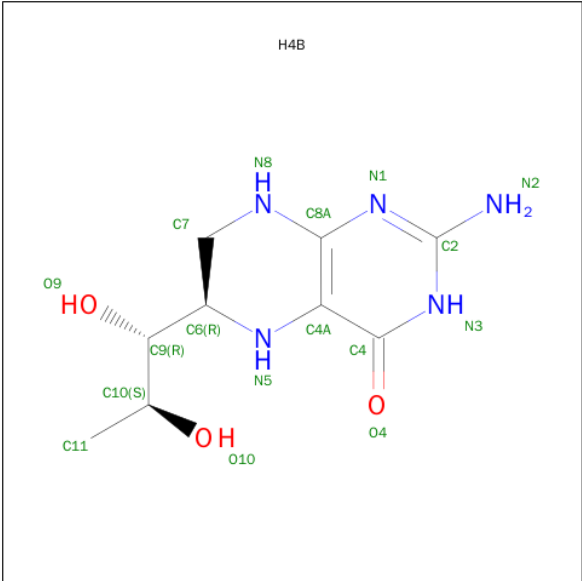
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 4 is 5,6,7,8-TETRAHYDROBIOPTERIN (three-letter code: H4B) (formula:  $C_9H_{15}N_5O_3$ ).



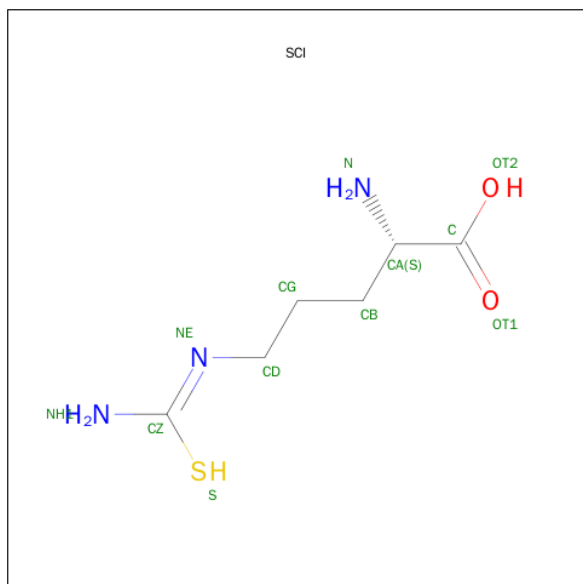
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			17	9	5	3		

Continued on next page...

*Continued from previous page...*

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

- Molecule 5 is L-THIOCITRULLINE (three-letter code: SCI) (formula:  $C_6H_{13}N_3O_2S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	3	2	1		
5	B	1	Total	C	N	O	S	0	0
			12	6	3	2	1		

- Molecule 6 is water.

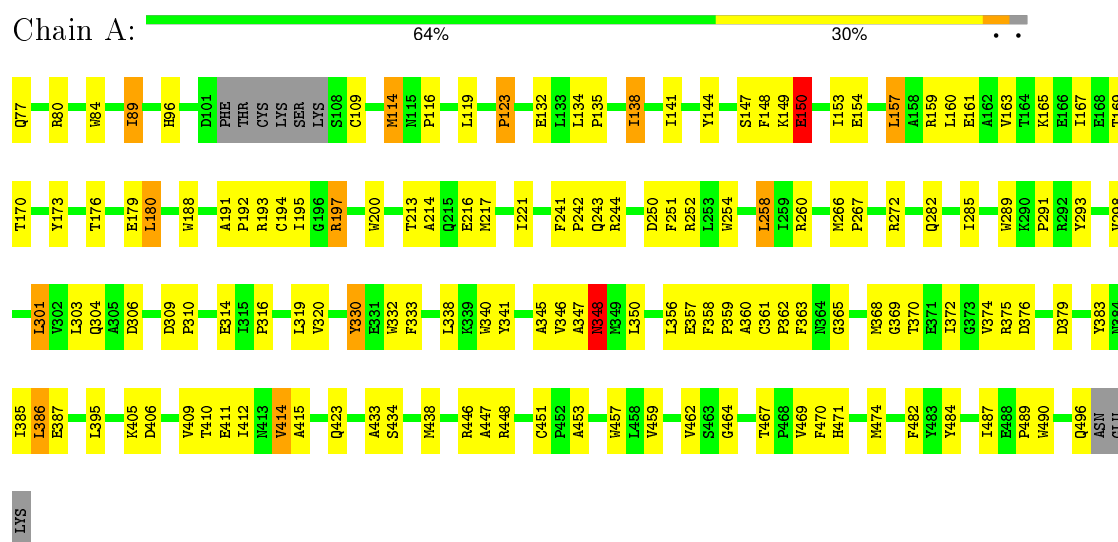
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	148	Total	O	0	0
			148	148		
6	B	167	Total	O	0	0
			167	167		

### 3 Residue-property plots

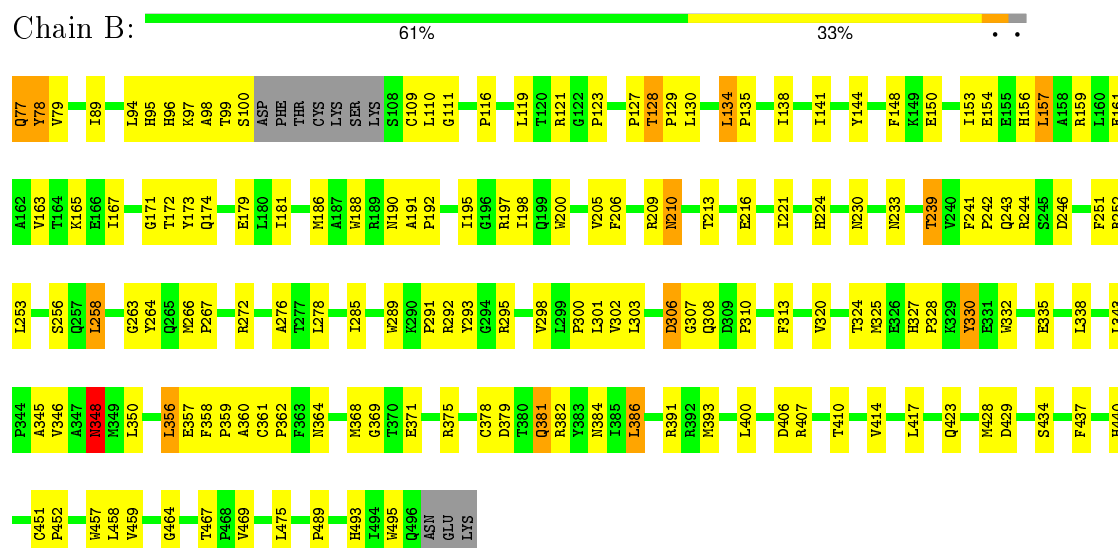
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



#### • Molecule 1: NITRIC OXIDE SYNTHASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	213.00Å 213.00Å 114.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.70	Depositor
% Data completeness (in resolution range)	95.3 (20.00-2.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.227 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	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: HEM, SCI, 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	0.35	0/3471	0.65	1/4719 (0.0%)
1	B	0.36	0/3466	0.64	0/4712
All	All	0.35	0/6937	0.65	1/9431 (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	-5.03	100.53	113.10

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	3373	0	3267	116	0
1	B	3368	0	3265	130	0
2	A	5	0	0	1	0
3	A	43	0	30	1	0
3	B	43	0	30	1	0
4	A	17	0	14	0	0
4	B	17	0	14	1	0
5	A	12	0	12	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	12	0	12	0	0
6	A	148	0	0	14	0
6	B	167	0	0	16	0
All	All	7205	0	6644	246	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 18.

All (246) 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:266:MET:SD	1:A:272:ARG:HD3	2.06	0.95
1:B:381:GLN:HE21	1:B:381:GLN:H	1.09	0.93
1:B:356:LEU:HD13	1:B:357:GLU:H	1.35	0.89
1:A:221:ILE:HG21	1:A:301:LEU:HD21	1.56	0.87
1:B:77:GLN:HE21	1:B:77:GLN:HA	1.41	0.84
1:A:195:ILE:HD12	1:A:368:MET:HE3	1.59	0.83
1:B:244:ARG:HA	6:B:1070:HOH:O	1.84	0.78
1:B:243:GLN:HB2	1:B:356:LEU:HD12	1.64	0.78
1:A:350:LEU:HD21	1:A:357:GLU:HB2	1.66	0.77
1:B:252:ARG:HH11	1:B:252:ARG:HG3	1.50	0.76
1:A:459:VAL:HG22	1:A:469:VAL:HG23	1.68	0.75
1:B:252:ARG:HD3	1:B:359:PRO:HB2	1.69	0.74
1:A:298:VAL:HG21	1:A:320:VAL:HG11	1.71	0.73
1:B:221:ILE:HD12	1:B:303:LEU:HD21	1.71	0.72
1:B:356:LEU:HD13	1:B:357:GLU:N	2.04	0.71
1:B:381:GLN:N	1:B:381:GLN:HE21	1.88	0.70
1:B:221:ILE:HG21	1:B:301:LEU:HD21	1.73	0.70
1:B:159:ARG:O	1:B:163:VAL:HG23	1.91	0.69
1:B:330:TYR:HD2	1:B:332:TRP:CZ2	2.11	0.69
1:A:134:LEU:O	1:A:138:ILE:HG12	1.94	0.68
1:B:272:ARG:NH1	1:B:295:ARG:HG3	2.10	0.67
1:A:448:ARG:HD2	2:A:907:SO4:O2	1.95	0.67
1:A:144:TYR:CE2	1:A:179:GLU:HA	2.30	0.67
1:B:188:TRP:CE3	1:B:200:TRP:HA	2.30	0.66
1:B:251:PHE:O	1:B:360:ALA:HB2	1.96	0.65
1:A:285:ILE:HD11	1:A:291:PRO:HB3	1.79	0.64
1:B:381:GLN:NE2	1:B:381:GLN:H	1.87	0.64
1:A:195:ILE:HG13	6:A:1063:HOH:O	1.98	0.64
1:A:252:ARG:HD3	1:A:359:PRO:HB2	1.78	0.63
1:B:464:GLY:O	1:B:467:THR:HB	1.98	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:VAL:O	1:A:167:ILE:HG13	1.99	0.63
1:A:197:ARG:NH2	1:A:451:CYS:SG	2.72	0.62
1:A:134:LEU:HB3	1:A:135:PRO:HD3	1.81	0.62
1:A:149:LYS:O	1:A:150:GLU:HG2	2.00	0.62
1:B:348:ASN:HB2	6:B:1123:HOH:O	2.00	0.62
1:A:346:VAL:HG23	6:A:1145:HOH:O	2.00	0.61
1:B:239:THR:HG23	1:B:362:PRO:HG2	1.81	0.61
1:A:116:PRO:HG2	1:A:119:LEU:HB2	1.83	0.61
1:B:134:LEU:O	1:B:138:ILE:HG13	2.00	0.61
1:B:209:ARG:O	1:B:242:PRO:HG3	2.01	0.61
1:B:467:THR:CG2	1:B:469:VAL:HG22	2.30	0.61
1:A:251:PHE:O	1:A:360:ALA:HB2	2.01	0.60
1:A:89:ILE:HD12	6:A:1059:HOH:O	2.00	0.60
1:B:167:ILE:HG23	1:B:171:GLY:O	2.01	0.60
1:A:252:ARG:NH2	1:A:489:PRO:HD3	2.17	0.60
1:B:467:THR:HG22	1:B:469:VAL:HG22	1.83	0.59
1:A:266:MET:HB3	1:A:267:PRO:HD2	1.84	0.59
1:A:195:ILE:HD12	1:A:368:MET:CE	2.31	0.59
1:B:459:VAL:HG22	1:B:469:VAL:HG23	1.85	0.58
1:B:243:GLN:HB2	1:B:356:LEU:CD1	2.33	0.58
1:A:141:ILE:HD11	1:A:163:VAL:HG21	1.85	0.58
1:A:304:GLN:O	1:A:304:GLN:HG3	2.02	0.58
1:B:243:GLN:HB3	1:B:358:PHE:CE2	2.38	0.57
1:A:360:ALA:HA	6:A:1038:HOH:O	2.04	0.57
1:B:127:PRO:HG3	1:B:246:ASP:HA	1.86	0.57
1:B:110:LEU:HB2	6:B:1193:HOH:O	2.03	0.57
1:A:405:LYS:O	1:A:409:VAL:HG23	2.04	0.57
1:B:134:LEU:HB3	1:B:135:PRO:HD3	1.85	0.57
1:B:327:HIS:ND1	1:B:328:PRO:HD2	2.20	0.57
1:B:144:TYR:CE1	1:B:179:GLU:HA	2.40	0.56
1:B:276:ALA:HB2	1:B:382:ARG:HD2	1.88	0.56
1:B:360:ALA:HA	6:B:1096:HOH:O	2.05	0.56
1:A:188:TRP:CE3	1:A:200:TRP:HA	2.41	0.56
1:A:258:LEU:HB2	1:A:345:ALA:HB3	1.86	0.56
1:B:213:THR:OG1	1:B:216:GLU:HB2	2.07	0.55
1:B:361:CYS:SG	1:B:361:CYS:O	2.64	0.55
1:A:213:THR:OG1	1:A:216:GLU:HB2	2.06	0.55
1:A:153:ILE:O	1:A:157:LEU:HD13	2.06	0.55
1:B:493:HIS:HD2	1:B:495:TRP:CD1	2.25	0.55
1:B:378:CYS:SG	1:B:386:LEU:HD23	2.47	0.55
1:A:303:LEU:O	1:A:310:PRO:HA	2.07	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:TYR:HE2	1:A:179:GLU:HA	1.71	0.54
1:A:144:TYR:O	1:A:147:SER:HB3	2.07	0.54
1:B:289:TRP:O	1:B:291:PRO:HD3	2.07	0.54
1:A:132:GLU:O	1:A:135:PRO:HD2	2.07	0.54
1:A:180:LEU:HB2	6:A:1109:HOH:O	2.08	0.54
1:A:453:ALA:HB3	1:A:474:MET:HB2	1.90	0.54
1:A:340:TRP:HZ3	1:A:383:TYR:CE1	2.26	0.53
1:A:217:MET:HA	1:A:241:PHE:HE2	1.72	0.53
1:A:191:ALA:O	1:A:197:ARG:NH1	2.39	0.53
1:A:411:GLU:HA	1:A:414:VAL:HG23	1.91	0.53
1:B:285:ILE:HD11	1:B:291:PRO:HB3	1.90	0.53
1:B:252:ARG:NH1	1:B:252:ARG:HG3	2.22	0.53
1:B:230:ASN:HB3	1:B:233:ASN:O	2.08	0.53
1:B:417:LEU:HD21	1:B:429:ASP:HB3	1.91	0.53
1:B:191:ALA:O	1:B:197:ARG:HD3	2.08	0.53
1:B:197:ARG:NH2	1:B:452:PRO:O	2.42	0.53
1:B:330:TYR:HD2	1:B:332:TRP:HZ2	1.57	0.53
1:A:260:ARG:HD2	1:A:341:TYR:OH	2.09	0.52
1:A:80:ARG:NH2	6:A:1059:HOH:O	2.42	0.52
1:B:190:ASN:O	1:B:192:PRO:HD3	2.09	0.52
1:B:77:GLN:NE2	1:B:77:GLN:HA	2.19	0.52
1:A:464:GLY:O	1:A:467:THR:HB	2.10	0.52
3:B:901:HEM:HMC2	3:B:901:HEM:HBC2	1.91	0.52
1:A:176:THR:OG1	1:A:179:GLU:HG3	2.09	0.52
1:B:379:ASP:HB3	1:B:381:GLN:HG2	1.91	0.52
1:A:370:THR:HA	1:A:374:VAL:HG23	1.92	0.51
1:A:387:GLU:HB3	6:A:1084:HOH:O	2.09	0.51
1:A:254:TRP:CZ3	1:A:490:TRP:HB3	2.44	0.51
1:A:252:ARG:HD2	1:A:359:PRO:O	2.11	0.51
1:B:303:LEU:O	1:B:310:PRO:HA	2.11	0.51
1:A:482:PHE:HB3	1:A:484:TYR:CE1	2.46	0.51
1:B:252:ARG:HH22	1:B:489:PRO:HD3	1.76	0.51
1:B:303:LEU:HD12	1:B:303:LEU:N	2.26	0.51
1:A:217:MET:HE3	1:A:303:LEU:HB3	1.92	0.51
1:B:285:ILE:CD1	1:B:291:PRO:HB3	2.41	0.51
1:B:330:TYR:N	1:B:330:TYR:HD1	2.09	0.50
1:A:330:TYR:HD2	1:A:332:TRP:CZ2	2.29	0.50
1:A:176:THR:O	1:A:179:GLU:HB2	2.11	0.50
1:A:250:ASP:HA	6:A:1018:HOH:O	2.11	0.50
1:B:457:TRP:HA	4:B:902:H4B:N1	2.27	0.50
1:B:302:VAL:C	1:B:303:LEU:HD12	2.31	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:TYR:N	1:B:330:TYR:CD1	2.79	0.50
1:B:423:GLN:HB3	6:B:1102:HOH:O	2.12	0.50
1:B:195:ILE:HG13	6:B:1137:HOH:O	2.11	0.50
1:B:356:LEU:HB2	6:B:1203:HOH:O	2.10	0.50
1:B:346:VAL:HG23	6:B:1210:HOH:O	2.11	0.50
1:A:316:PRO:HD2	1:A:319:LEU:HD12	1.93	0.50
1:B:258:LEU:HB2	1:B:345:ALA:HB3	1.94	0.49
1:A:217:MET:CE	1:A:303:LEU:HB3	2.43	0.49
1:B:276:ALA:HB2	1:B:382:ARG:CD	2.42	0.49
1:A:194:CYS:HB2	3:A:901:HEM:ND	2.26	0.49
1:A:244:ARG:HA	6:A:1019:HOH:O	2.12	0.49
1:A:291:PRO:HB2	1:A:293:TYR:CE2	2.47	0.49
1:A:213:THR:HB	6:A:1032:HOH:O	2.13	0.48
1:A:243:GLN:HB3	1:A:358:PHE:CE2	2.48	0.48
1:A:375:ARG:NH1	1:A:379:ASP:OD2	2.46	0.48
1:A:84:TRP:NE1	1:A:114:MET:HG3	2.28	0.48
1:A:320:VAL:HB	6:A:1037:HOH:O	2.13	0.48
1:B:198:ILE:HA	1:B:440:HIS:ND1	2.28	0.48
1:A:309:ASP:HB3	1:A:310:PRO:HD2	1.96	0.48
1:B:272:ARG:HH11	1:B:295:ARG:HG3	1.76	0.48
1:B:188:TRP:O	1:B:197:ARG:HD2	2.13	0.48
1:B:154:GLU:HA	1:B:157:LEU:HD12	1.95	0.48
1:A:385:ILE:HD11	1:A:412:ILE:HD13	1.95	0.48
1:A:149:LYS:C	1:A:150:GLU:HG2	2.34	0.48
1:A:372:ILE:HA	1:A:376:ASP:HB2	1.95	0.48
1:B:195:ILE:HG12	1:B:458:LEU:HD22	1.96	0.48
1:B:141:ILE:HD13	1:B:163:VAL:HG21	1.96	0.47
1:A:374:VAL:HG11	1:A:462:VAL:HG13	1.96	0.47
1:B:343:LEU:HD11	1:B:364:ASN:ND2	2.28	0.47
1:B:381:GLN:HA	6:B:1148:HOH:O	2.14	0.47
1:B:252:ARG:CD	1:B:359:PRO:HB2	2.40	0.47
1:B:163:VAL:O	1:B:167:ILE:HG13	2.14	0.47
1:B:258:LEU:HD22	1:B:345:ALA:HB1	1.97	0.47
1:B:161:GLU:HG2	1:B:165:LYS:HE3	1.96	0.47
1:A:221:ILE:HD12	1:A:303:LEU:HD21	1.96	0.47
1:B:89:ILE:HD12	6:B:1125:HOH:O	2.15	0.47
1:A:266:MET:SD	1:A:272:ARG:CD	2.93	0.47
1:B:213:THR:HB	6:B:1089:HOH:O	2.15	0.47
1:A:314:GLU:HG3	6:A:1144:HOH:O	2.15	0.47
1:B:161:GLU:O	1:B:165:LYS:HG3	2.15	0.47
1:B:330:TYR:HE2	1:B:393:MET:HG2	1.80	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ARG:O	1:A:163:VAL:HG23	2.14	0.46
1:B:384:ASN:HA	6:B:1118:HOH:O	2.15	0.46
1:B:356:LEU:HA	1:B:356:LEU:HD22	1.73	0.46
1:A:214:ALA:O	1:A:217:MET:HB2	2.15	0.46
1:B:77:GLN:O	1:B:96:HIS:HE1	1.99	0.45
1:B:241:PHE:HB3	1:B:242:PRO:CD	2.47	0.45
1:A:77:GLN:O	1:A:96:HIS:HE1	1.99	0.45
1:A:241:PHE:HB3	1:A:242:PRO:CD	2.47	0.45
1:B:306:ASP:HB3	1:B:307:GLY:H	1.62	0.45
1:A:193:ARG:HB3	1:A:457:TRP:CE3	2.52	0.45
1:B:128:THR:HA	1:B:129:PRO:HD2	1.85	0.45
1:B:96:HIS:C	1:B:98:ALA:H	2.20	0.45
1:B:153:ILE:O	1:B:156:HIS:HB3	2.17	0.45
1:A:446:ARG:HH11	1:A:446:ARG:HG2	1.82	0.45
1:A:434:SER:HB3	1:A:469:VAL:HG13	1.99	0.45
1:B:153:ILE:HG22	1:B:154:GLU:N	2.31	0.45
1:B:134:LEU:CD1	1:B:138:ILE:HD11	2.47	0.45
1:B:161:GLU:CG	1:B:165:LYS:HE3	2.46	0.45
1:A:423:GLN:HB3	6:A:1043:HOH:O	2.17	0.45
1:B:79:VAL:HG23	1:B:95:HIS:NE2	2.31	0.45
1:B:188:TRP:CZ3	1:B:200:TRP:HA	2.51	0.45
1:A:191:ALA:O	1:A:197:ARG:HD3	2.17	0.45
1:B:174:GLN:HA	6:B:1054:HOH:O	2.17	0.45
1:B:172:THR:OG1	1:B:173:TYR:N	2.50	0.44
1:A:289:TRP:O	1:A:291:PRO:HD3	2.18	0.44
1:A:434:SER:CB	1:A:467:THR:HG23	2.48	0.44
1:B:253:LEU:HD21	1:B:362:PRO:HG3	2.00	0.44
1:B:99:THR:CG2	1:B:100:SER:N	2.80	0.44
1:B:263:GLY:O	1:B:278:LEU:HD23	2.17	0.44
1:B:266:MET:HB3	1:B:267:PRO:HD2	1.98	0.44
1:B:368:MET:HA	1:B:428:MET:O	2.17	0.44
1:A:266:MET:CB	1:A:267:PRO:HD2	2.45	0.44
1:A:188:TRP:CZ3	1:A:200:TRP:HA	2.52	0.44
1:B:350:LEU:HD21	1:B:357:GLU:HB2	1.98	0.44
1:B:252:ARG:NH2	1:B:489:PRO:HD3	2.32	0.44
1:B:325:MET:HB2	1:B:338:LEU:HB2	1.99	0.44
1:A:217:MET:HG2	1:A:241:PHE:CE2	2.52	0.43
1:A:163:VAL:HG13	1:A:173:TYR:CD2	2.53	0.43
1:B:332:TRP:O	1:B:335:GLU:HB2	2.18	0.43
1:B:303:LEU:HD13	1:B:313:PHE:HD2	1.83	0.43
1:B:206:PHE:HE2	1:B:224:HIS:HA	1.83	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:THR:CG2	1:B:362:PRO:HG2	2.47	0.43
1:A:348:ASN:HB2	6:A:1091:HOH:O	2.18	0.43
1:A:157:LEU:HA	1:A:160:LEU:HD12	2.00	0.43
1:B:195:ILE:HG22	1:B:195:ILE:O	2.17	0.43
1:B:298:VAL:HG21	1:B:320:VAL:HG11	1.99	0.43
1:A:285:ILE:CD1	1:A:291:PRO:HB3	2.48	0.43
1:B:233:ASN:ND2	6:B:1068:HOH:O	2.52	0.43
1:A:241:PHE:HB3	1:A:242:PRO:HD2	2.00	0.43
1:A:293:TYR:CD2	1:B:267:PRO:HB3	2.53	0.43
1:A:165:LYS:HB2	1:A:165:LYS:HE3	1.79	0.43
1:A:188:TRP:O	1:A:197:ARG:HD2	2.19	0.42
1:B:195:ILE:HG23	1:B:437:PHE:HB2	2.00	0.42
1:B:121:ARG:HD3	1:B:121:ARG:HA	1.82	0.42
1:B:141:ILE:HD11	1:B:163:VAL:HG11	2.01	0.42
1:A:346:VAL:HB	1:A:363:PHE:CZ	2.53	0.42
1:B:78:TYR:CD1	1:B:78:TYR:C	2.92	0.42
1:B:239:THR:O	1:B:361:CYS:HA	2.19	0.42
1:B:116:PRO:HG2	1:B:119:LEU:HB2	2.02	0.42
1:B:437:PHE:CE2	1:B:458:LEU:HD13	2.55	0.42
1:B:241:PHE:HB3	1:B:242:PRO:HD2	2.01	0.42
1:A:368:MET:HE2	1:A:433:ALA:HB1	2.02	0.42
1:B:210:ASN:C	1:B:210:ASN:HD22	2.24	0.42
1:A:192:PRO:HA	1:A:197:ARG:HH12	1.85	0.42
1:B:348:ASN:C	1:B:348:ASN:HD22	2.22	0.42
1:B:95:HIS:HE1	6:B:1129:HOH:O	2.03	0.42
1:A:386:LEU:HA	1:A:386:LEU:HD23	1.91	0.42
1:A:368:MET:HE2	1:A:433:ALA:CB	2.50	0.41
1:B:434:SER:CB	1:B:467:THR:HG23	2.50	0.41
1:B:382:ARG:NH2	6:B:1192:HOH:O	2.52	0.41
1:A:123:PRO:HD3	1:A:487:ILE:HD12	2.02	0.41
1:A:250:ASP:O	1:A:304:GLN:NE2	2.53	0.41
1:A:467:THR:CG2	1:A:469:VAL:HG22	2.51	0.41
1:B:301:LEU:HD12	1:B:301:LEU:HA	1.90	0.41
1:A:148:PHE:HD1	1:A:149:LYS:O	2.03	0.41
1:A:347:ALA:HA	1:A:362:PRO:HB3	2.02	0.41
1:B:371:GLU:O	1:B:375:ARG:HB2	2.21	0.41
1:A:438:MET:CE	1:A:469:VAL:HG12	2.51	0.41
1:B:242:PRO:HB2	1:B:251:PHE:CE1	2.55	0.41
1:A:254:TRP:N	1:A:254:TRP:CD1	2.89	0.41
1:A:282:GLN:O	1:A:285:ILE:HB	2.21	0.41
1:A:410:THR:O	1:A:414:VAL:HG22	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:GLU:H	1:A:154:GLU:CD	2.24	0.41
1:B:410:THR:O	1:B:414:VAL:HG22	2.21	0.41
1:A:153:ILE:H	1:A:153:ILE:HG13	1.55	0.41
1:B:289:TRP:CE2	1:B:300:PRO:HD3	2.56	0.41
1:B:181:ILE:HA	1:B:205:VAL:HG21	2.03	0.41
1:A:252:ARG:CD	1:A:359:PRO:HB2	2.50	0.40
1:A:361:CYS:O	1:A:361:CYS:SG	2.79	0.40
1:A:467:THR:HG22	1:A:469:VAL:H	1.86	0.40
1:A:333:PHE:CE2	1:A:415:ALA:HB1	2.56	0.40
1:A:470:PHE:HD1	1:A:471:HIS:CD2	2.39	0.40
1:A:438:MET:HE2	1:A:469:VAL:HG12	2.03	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	410/423 (97%)	347 (85%)	57 (14%)	6 (2%)	13	32
1	B	409/423 (97%)	355 (87%)	45 (11%)	9 (2%)	8	22
All	All	819/846 (97%)	702 (86%)	102 (12%)	15 (2%)	11	27

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	369	GLY
1	B	111	GLY
1	B	308	GLN
1	B	150	GLU
1	B	293	TYR
1	B	369	GLY
1	A	197	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	447	ALA
1	B	97	LYS
1	B	348	ASN
1	A	150	GLU
1	A	123	PRO
1	A	348	ASN
1	B	451	CYS
1	B	123	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	361/371 (97%)	339 (94%)	22 (6%)	23	49
1	B	361/371 (97%)	333 (92%)	28 (8%)	16	35
All	All	722/742 (97%)	672 (93%)	50 (7%)	19	43

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ILE
1	A	109	CYS
1	A	114	MET
1	A	138	ILE
1	A	150	GLU
1	A	157	LEU
1	A	161	GLU
1	A	169	THR
1	A	170	THR
1	A	180	LEU
1	A	258	LEU
1	A	301	LEU
1	A	306	ASP
1	A	330	TYR
1	A	338	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	348	ASN
1	A	356	LEU
1	A	386	LEU
1	A	395	LEU
1	A	406	ASP
1	A	414	VAL
1	A	496	GLN
1	B	77	GLN
1	B	78	TYR
1	B	94	LEU
1	B	109	CYS
1	B	128	THR
1	B	130	LEU
1	B	134	LEU
1	B	148	PHE
1	B	157	LEU
1	B	186	MET
1	B	210	ASN
1	B	239	THR
1	B	256	SER
1	B	258	LEU
1	B	264	TYR
1	B	292	ARG
1	B	306	ASP
1	B	324	THR
1	B	330	TYR
1	B	348	ASN
1	B	356	LEU
1	B	381	GLN
1	B	386	LEU
1	B	391	ARG
1	B	400	LEU
1	B	406	ASP
1	B	407	ARG
1	B	475	LEU

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	96	HIS
1	A	231	ASN
1	A	233	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	243	GLN
1	A	348	ASN
1	A	471	HIS
1	A	486	GLN
1	B	77	GLN
1	B	91	HIS
1	B	96	HIS
1	B	210	ASN
1	B	231	ASN
1	B	233	ASN
1	B	348	ASN
1	B	364	ASN
1	B	381	GLN
1	B	486	GLN
1	B	493	HIS
1	B	496	GLN

### 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](#)

7 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	HEM	A	901	1	30,50,50	2.83	9 (30%)	24,82,82	2.52	10 (41%)
4	H4B	A	902	-	13,18,18	1.65	2 (15%)	11,26,26	2.24	6 (54%)
5	SCI	A	906	-	6,11,11	0.44	0	5,13,13	1.74	1 (20%)
2	SO4	A	907	-	4,4,4	0.50	0	6,6,6	0.23	0
3	HEM	B	901	1	30,50,50	3.09	9 (30%)	24,82,82	2.41	10 (41%)
4	H4B	B	902	-	13,18,18	1.77	2 (15%)	11,26,26	2.12	5 (45%)
5	SCI	B	906	-	6,11,11	0.46	0	5,13,13	1.85	1 (20%)

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	HEM	A	901	1	-	0/10/54/54	0/0/8/8
4	H4B	A	902	-	1/1/3/5	0/8/17/17	0/2/2/2
5	SCI	A	906	-	-	0/5/11/11	0/0/0/0
2	SO4	A	907	-	-	0/0/0/0	0/0/0/0
3	HEM	B	901	1	-	0/10/54/54	0/0/8/8
4	H4B	B	902	-	-	0/8/17/17	0/2/2/2
5	SCI	B	906	-	-	0/5/11/11	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	HEM	C3B-C4B	-7.64	1.45	1.51
3	B	901	HEM	C3B-CAB	-7.09	1.38	1.51
3	B	901	HEM	C3D-C4D	-6.88	1.42	1.51
3	A	901	HEM	C2D-C3D	-6.87	1.33	1.54
3	B	901	HEM	C2D-C3D	-6.79	1.34	1.54
3	A	901	HEM	C3B-C4B	-6.16	1.46	1.51
3	A	901	HEM	C3D-C4D	-5.98	1.43	1.51
3	B	901	HEM	C3C-CAC	-5.66	1.40	1.51
4	B	902	H4B	C7-N8	-5.60	1.38	1.46
3	A	901	HEM	C3B-CAB	-5.60	1.40	1.51
3	A	901	HEM	C3C-CAC	-5.53	1.40	1.51
4	A	902	H4B	C7-N8	-5.29	1.39	1.46
3	A	901	HEM	C2C-C1C	-4.40	1.44	1.52
3	B	901	HEM	C2C-C1C	-3.99	1.45	1.52
3	A	901	HEM	C2B-C1B	-2.85	1.42	1.51
3	A	901	HEM	CAD-C3D	-2.72	1.48	1.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	901	HEM	CAD-C3D	-2.56	1.49	1.54
3	B	901	HEM	C2B-C1B	-2.50	1.43	1.51
4	B	902	H4B	C4A-N5	-2.31	1.32	1.38
4	A	902	H4B	C4A-N5	-2.23	1.32	1.38
3	B	901	HEM	C2D-C1D	-2.16	1.44	1.51
3	A	901	HEM	FE-NC	2.05	2.03	1.95

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	901	HEM	CBA-CAA-C2A	-3.91	105.52	112.53
3	B	901	HEM	CBA-CAA-C2A	-2.46	108.11	112.53
4	B	902	H4B	N3-C2-N1	-2.39	121.62	125.53
4	A	902	H4B	N3-C2-N1	-2.34	121.70	125.53
3	B	901	HEM	CMA-C3A-C4A	-2.27	124.61	128.36
3	A	901	HEM	C3B-C4B-CHC	2.01	125.99	123.16
4	A	902	H4B	C8A-C4A-N5	2.04	121.42	118.85
3	B	901	HEM	C3C-CAC-CBC	2.20	127.84	124.46
3	A	901	HEM	C3C-CAC-CBC	2.23	127.88	124.46
3	B	901	HEM	CMD-C2D-C3D	2.44	125.14	114.35
4	B	902	H4B	C4-C4A-C8A	2.49	116.81	114.56
3	A	901	HEM	CMD-C2D-C3D	2.58	125.75	114.35
3	B	901	HEM	C3B-C4B-CHC	2.64	126.88	123.16
4	A	902	H4B	C2-N1-C8A	2.76	120.74	114.54
4	A	902	H4B	C4-C4A-C8A	2.94	117.22	114.56
4	B	902	H4B	C7-C6-N5	2.95	116.58	110.45
4	B	902	H4B	C2-N1-C8A	3.13	121.57	114.54
4	B	902	H4B	C4-N3-C2	3.27	120.48	115.94
3	A	901	HEM	C3B-CAB-CBB	3.33	129.56	124.46
5	A	906	SCI	CD-NE-CZ	3.36	123.43	117.86
4	A	902	H4B	C4-N3-C2	3.41	120.67	115.94
4	A	902	H4B	C7-C6-N5	3.42	117.55	110.45
3	A	901	HEM	CAD-C3D-C4D	3.61	125.21	112.47
5	B	906	SCI	CD-NE-CZ	3.73	124.04	117.86
3	B	901	HEM	CAD-C3D-C2D	3.86	124.31	113.22
3	B	901	HEM	CAD-C3D-C4D	3.86	126.08	112.47
3	B	901	HEM	CMB-C2B-C3B	3.94	126.37	116.53
3	A	901	HEM	CAD-C3D-C2D	4.17	125.21	113.22
3	A	901	HEM	CMB-C2B-C3B	4.33	127.33	116.53
3	A	901	HEM	C2D-C3D-C4D	4.75	109.56	101.50
3	B	901	HEM	C2D-C3D-C4D	4.77	109.58	101.50
3	A	901	HEM	CMC-C2C-C3C	5.27	129.68	116.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	901	HEM	CMC-C2C-C3C	5.31	129.78	116.53

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	902	H4B	C6

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	HEM	1	0
2	A	907	SO4	1	0
3	B	901	HEM	1	0
4	B	902	H4B	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.