



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:32 AM GMT

PDB ID : 3O0R  
Title : Crystal structure of nitric oxide reductase from *Pseudomonas aeruginosa* in complex with antibody fragment  
Authors : Hino, T.; Matsumoto, Y.; Nagano, S.; Sugimoto, H.; Fukumori, Y.; Murata, T.; Iwata, S.; Shiro, Y.  
Deposited on : 2010-07-20  
Resolution : 2.70 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>

---

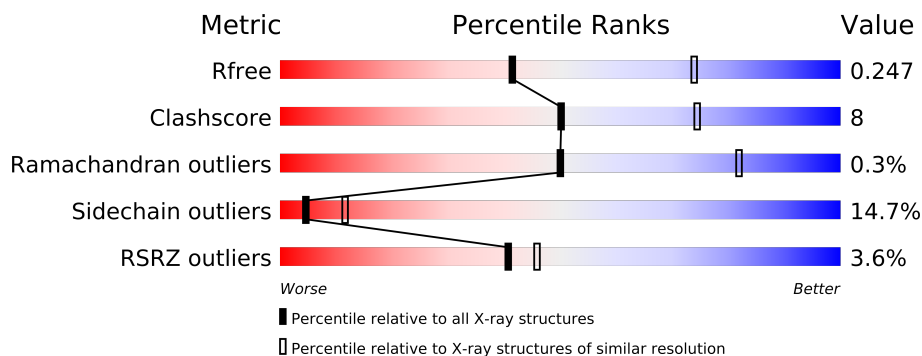
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.70 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))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (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. 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	L	213	
2	H	225	
3	B	465	
4	C	146	

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 8364 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 antibody fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1669	1047	277	338	7			

- Molecule 2 is a protein called antibody fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	225	Total	C	N	O	S	0	0	0
			1692	1065	280	338	9			

- Molecule 3 is a protein called Nitric oxide reductase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	449	Total	C	N	O	S	0	0	0
			3576	2416	563	572	25			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ARG	SEE REMARK 999	UNP Q59647

- Molecule 4 is a protein called Nitric oxide reductase subunit C.

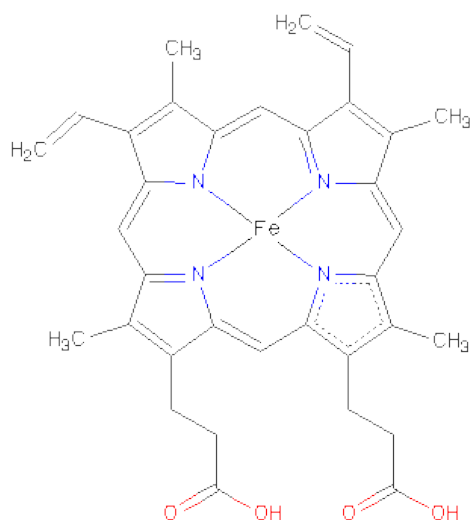
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	142	Total	C	N	O	S	0	0	0
			1123	720	195	202	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	100	LYS	ASN	CONFLICT	UNP Q59646

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (for-

mula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Fe		
			1	1	0	0

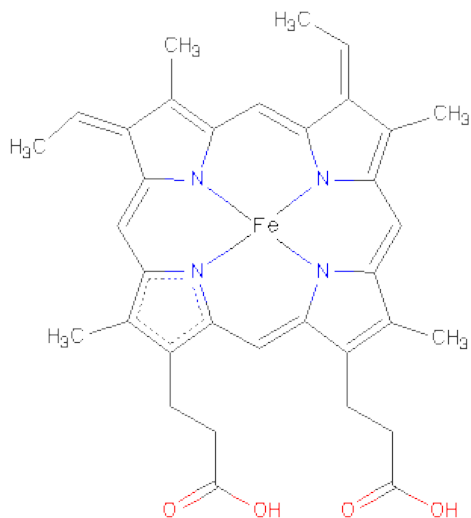
- Molecule 7 is OXYGEN ATOM (three-letter code: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	O		
			1	1	0	0

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Ca		
			1	1	0	0

- Molecule 9 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

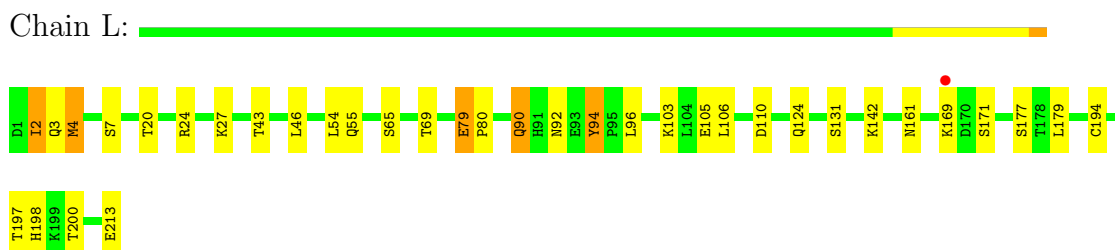
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	L	44	Total	O	0	0
			44	44		
10	H	46	Total	O	0	0
			46	46		
10	B	38	Total	O	0	0
			38	38		
10	C	44	Total	O	0	0
			44	44		

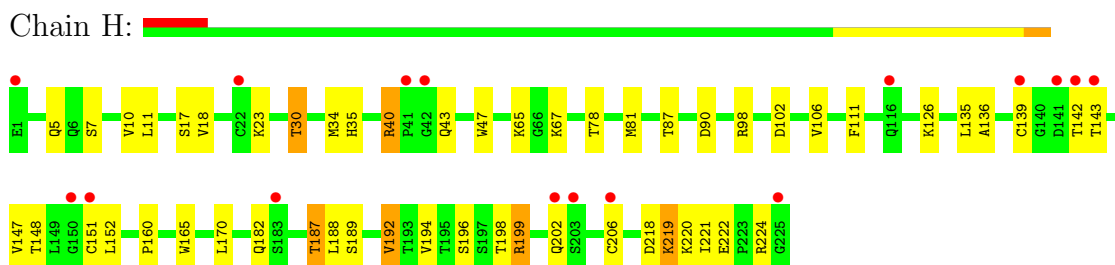
### 3 Residue-property plots

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.

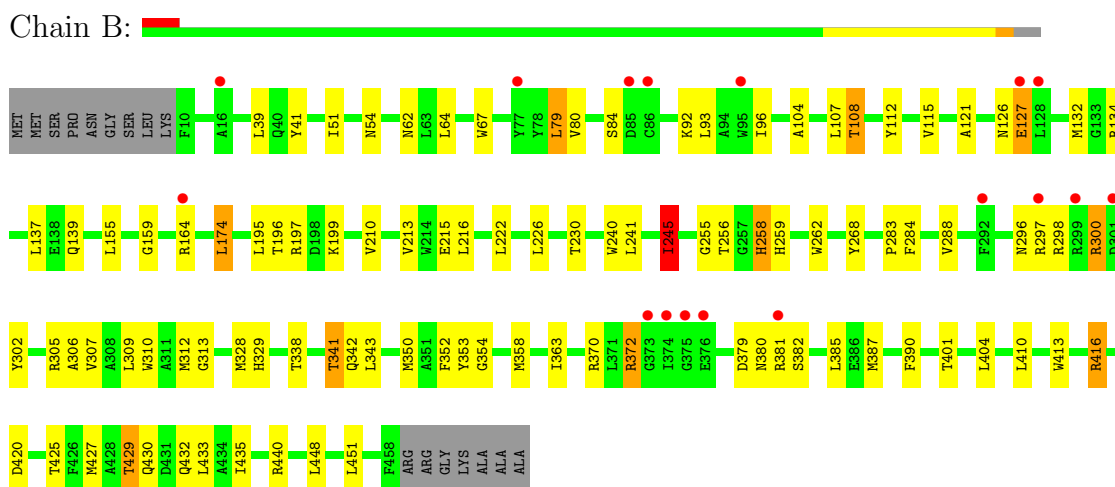
- Molecule 1: antibody fab fragment light chain



- Molecule 2: antibody fab fragment heavy chain



- Molecule 3: Nitric oxide reductase subunit B



- Molecule 4: Nitric oxide reductase subunit C





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.47Å 104.52Å 195.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-2.70) 97.5 (20.00-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.185 , 0.247 0.185 , 0.247	Depositor DCC
$R_{free}$ test set	2559 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	74.9	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 55.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 50228 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8364	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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, CA, FE, O, HEC

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	L	0.95	2/1709 (0.1%)	0.94	1/2317 (0.0%)
2	H	0.92	1/1735 (0.1%)	0.95	4/2367 (0.2%)
3	B	0.81	0/3693	0.86	6/5039 (0.1%)
4	C	0.94	2/1153 (0.2%)	0.89	1/1559 (0.1%)
All	All	0.88	5/8290 (0.1%)	0.90	12/11282 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	73	TYR	CE1-CZ	6.88	1.47	1.38
1	L	194	CYS	CB-SG	-6.17	1.71	1.82
4	C	94	PHE	CD2-CE2	5.57	1.50	1.39
2	H	151	CYS	CB-SG	-5.54	1.72	1.81
1	L	105	GLU	CG-CD	5.06	1.59	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	416	ARG	NE-CZ-NH2	-7.17	116.71	120.30
3	B	416	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	L	110	ASP	CB-CG-OD1	6.56	124.20	118.30
3	B	79	LEU	CA-CB-CG	6.45	130.14	115.30
2	H	218	ASP	CB-CG-OD1	6.06	123.76	118.30
3	B	420	ASP	CB-CG-OD2	-5.79	113.09	118.30
3	B	245	ILE	CB-CA-C	-5.70	100.20	111.60
4	C	110	ARG	NE-CZ-NH2	-5.70	117.45	120.30
3	B	174	LEU	CA-CB-CG	5.65	128.30	115.30
2	H	192	VAL	CB-CA-C	-5.36	101.21	111.40
2	H	199	ARG	CG-CD-NE	-5.33	100.60	111.80
2	H	81	MET	CG-SD-CE	-5.28	91.75	100.20

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	L	1669	0	17	9	0
2	H	1692	0	116	11	0
3	B	3576	0	0	34	0
4	C	1123	0	0	12	0
5	B	86	0	0	3	0
6	B	1	0	0	0	0
7	B	1	0	0	0	0
8	C	1	0	0	0	0
9	C	43	0	30	2	0
10	B	38	0	0	4	0
10	C	44	0	0	3	0
10	H	46	0	0	2	0
10	L	44	0	0	1	0
All	All	8364	0	163	63	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (63) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:C:201:HEC:CGA	10:C:332:HOH:O	2.31	0.78
1:L:79:GLU:CG	1:L:80:PRO:CD	2.66	0.73
3:B:104:ALA:O	3:B:108:THR:CG2	2.36	0.73
2:H:30:THR:CB	10:H:338:HOH:O	2.37	0.73
3:B:262:TRP:N	10:B:916:HOH:O	2.24	0.70
3:B:302:TYR:OH	3:B:370:ARG:NH1	2.26	0.68
1:L:198:HIS:CD2	1:L:200:THR:OG1	2.49	0.66
3:B:226:LEU:O	3:B:230:THR:CG2	2.45	0.65
2:H:165:TRP:CZ3	2:H:221:ILE:HD11	2.33	0.64
3:B:127:GLU:OE2	3:B:127:GLU:CA	2.46	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:220:LYS:HE3	2:H:222:GLU:OE2	2.00	0.61
3:B:425:THR:O	3:B:429:THR:CG2	2.49	0.61
4:C:84:ARG:NH1	9:C:201:HEC:O2A	2.35	0.59
4:C:137:THR:CG2	4:C:140:TRP:O	2.52	0.58
3:B:372:ARG:CG	3:B:372:ARG:NH1	2.68	0.57
4:C:85:ARG:NE	10:C:332:HOH:O	2.38	0.57
3:B:350:MET:O	3:B:354:GLY:N	2.41	0.53
1:L:161:ASN:ND2	1:L:177:SER:OG	2.41	0.53
3:B:121:ALA:CA	3:B:132:MET:CE	2.86	0.53
2:H:40:ARG:NH1	10:H:319:HOH:O	2.43	0.52
3:B:197:ARG:CD	4:C:33:GLU:OE2	2.57	0.52
3:B:300:ARG:CG	3:B:300:ARG:NH1	2.74	0.50
1:L:4:MET:CE	1:L:4:MET:CA	2.89	0.50
3:B:155:LEU:O	3:B:159:GLY:N	2.44	0.50
3:B:80:VAL:O	3:B:84:SER:N	2.45	0.50
3:B:255:GLY:O	3:B:258:HIS:N	2.45	0.50
1:L:4:MET:N	1:L:4:MET:CE	2.76	0.49
3:B:342:GLN:OE1	10:B:935:HOH:O	2.20	0.49
1:L:90:GLN:OE1	1:L:92:ASN:N	2.46	0.49
3:B:390:PHE:CD1	3:B:390:PHE:C	2.86	0.49
2:H:182:GLN:NE2	2:H:187:THR:CG2	2.76	0.48
3:B:258:HIS:CD2	3:B:259:HIS:CD2	3.02	0.47
2:H:67:LYS:NZ	2:H:90:ASP:OD2	2.47	0.47
5:B:802:HEM:O1A	10:B:906:HOH:O	2.20	0.47
2:H:35:HIS:ND1	2:H:47:TRP:NE1	2.63	0.47
4:C:25:PHE:O	4:C:29:THR:CG2	2.62	0.47
3:B:353:TYR:N	5:B:801:HEM:CBC	2.80	0.45
3:B:126:ASN:CB	3:B:132:MET:CE	2.95	0.45
3:B:306:ALA:O	3:B:310:TRP:CD1	2.70	0.45
3:B:215:GLU:OE2	3:B:284:PHE:CZ	2.70	0.45
3:B:430:GLN:NE2	4:C:110:ARG:NH1	2.65	0.45
3:B:338:THR:O	3:B:341:THR:CB	2.65	0.45
2:H:206:CYS:N	2:H:219:LYS:O	2.50	0.44
3:B:62:ASN:ND2	3:B:112:TYR:OH	2.50	0.44
1:L:94:TYR:C	1:L:94:TYR:CD1	2.90	0.44
3:B:51:ILE:O	3:B:51:ILE:CG2	2.66	0.44
4:C:88:GLU:CG	4:C:89:GLU:N	2.81	0.44
4:C:58:GLN:NE2	10:C:345:HOH:O	2.51	0.43
3:B:197:ARG:NE	4:C:33:GLU:OE2	2.53	0.42
2:H:198:THR:O	2:H:202:GLN:N	2.52	0.42
2:H:102:ASP:OD2	2:H:102:ASP:N	2.52	0.42
3:B:312:MET:O	3:B:313:GLY:C	2.57	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:B:216:LEU:CD1	3:B:245:ILE:CG2	2.97	0.42
3:B:268:TYR:OH	4:C:31:HIS:CD2	2.73	0.42
3:B:134:ARG:O	3:B:137:LEU:N	2.54	0.41
3:B:432:GLN:NE2	10:B:466:HOH:O	2.53	0.41
1:L:124:GLN:OE1	1:L:131:SER:N	2.54	0.41
3:B:379:ASP:O	3:B:382:SER:N	2.54	0.41
1:L:2:ILE:N	10:L:305:HOH:O	2.54	0.41
2:H:136:ALA:O	2:H:224:ARG:NH1	2.54	0.41
3:B:199:LYS:NZ	4:C:70:GLU:OE1	2.54	0.40
3:B:41:TYR:OH	5:B:801:HEM:O1A	2.40	0.40
4:C:84:ARG:O	4:C:84:ARG:CG	2.69	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	211/213 (99%)	202 (96%)	9 (4%)	0	100	100
2	H	223/225 (99%)	210 (94%)	12 (5%)	1 (0%)	43	76
3	B	447/465 (96%)	411 (92%)	34 (8%)	2 (0%)	43	76
4	C	140/146 (96%)	132 (94%)	8 (6%)	0	100	100
All	All	1021/1049 (97%)	955 (94%)	63 (6%)	3 (0%)	50	82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	256	THR
3	B	380	ASN
2	H	196	SER

### 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	L	189/189 (100%)	164 (87%)	25 (13%)	6	14
2	H	192/192 (100%)	158 (82%)	34 (18%)	3	7
3	B	360/371 (97%)	304 (84%)	56 (16%)	4	10
4	C	116/120 (97%)	105 (90%)	11 (10%)	12	28
All	All	857/872 (98%)	731 (85%)	126 (15%)	4	11

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	ILE
1	L	3	GLN
1	L	4	MET
1	L	7	SER
1	L	20	THR
1	L	24	ARG
1	L	27	LYS
1	L	43	THR
1	L	46	LEU
1	L	54	LEU
1	L	55	GLN
1	L	65	SER
1	L	69	THR
1	L	79	GLU
1	L	90	GLN
1	L	94	TYR
1	L	96	LEU
1	L	103	LYS
1	L	106	LEU
1	L	142	LYS
1	L	169	LYS
1	L	171	SER
1	L	179	LEU
1	L	197	THR
1	L	213	GLU
2	H	5	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	H	7	SER
2	H	10	VAL
2	H	11	LEU
2	H	17	SER
2	H	18	VAL
2	H	23	LYS
2	H	30	THR
2	H	34	MET
2	H	40	ARG
2	H	43	GLN
2	H	65	LYS
2	H	78	THR
2	H	87	THR
2	H	98	ARG
2	H	106	VAL
2	H	111	PHE
2	H	126	LYS
2	H	135	LEU
2	H	139	CYS
2	H	142	THR
2	H	143	THR
2	H	147	VAL
2	H	148	THR
2	H	152	LEU
2	H	160	PRO
2	H	170	LEU
2	H	187	THR
2	H	188	LEU
2	H	189	SER
2	H	192	VAL
2	H	194	VAL
2	H	199	ARG
2	H	219	LYS
3	B	39	LEU
3	B	54	ASN
3	B	64	LEU
3	B	67	TRP
3	B	79	LEU
3	B	92	LYS
3	B	93	LEU
3	B	96	ILE
3	B	107	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	B	108	THR
3	B	115	VAL
3	B	127	GLU
3	B	139	GLN
3	B	164	ARG
3	B	174	LEU
3	B	195	LEU
3	B	196	THR
3	B	210	VAL
3	B	213	VAL
3	B	222	LEU
3	B	240	TRP
3	B	241	LEU
3	B	245	ILE
3	B	258	HIS
3	B	283	PRO
3	B	288	VAL
3	B	296	ASN
3	B	297	ARG
3	B	298	ARG
3	B	300	ARG
3	B	305	ARG
3	B	307	VAL
3	B	309	LEU
3	B	328	MET
3	B	329	HIS
3	B	341	THR
3	B	343	LEU
3	B	352	PHE
3	B	358	MET
3	B	363	ILE
3	B	372	ARG
3	B	381	ARG
3	B	385	LEU
3	B	387	MET
3	B	401	THR
3	B	404	LEU
3	B	410	LEU
3	B	413	TRP
3	B	416	ARG
3	B	427	MET
3	B	429	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	B	433	LEU
3	B	435	ILE
3	B	440	ARG
3	B	448	LEU
3	B	451	LEU
4	C	9	MET
4	C	24	LEU
4	C	29	THR
4	C	33	GLU
4	C	38	GLU
4	C	67	LEU
4	C	80	ASN
4	C	95	LEU
4	C	106	VAL
4	C	137	THR
4	C	144	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\# Z  > 2$
5	HEM	B	801	8,3	49,50,50	2.19	15 (30%)	46,82,82	2.96	14 (30%)
5	HEM	B	802	8,3,7	49,50,50	2.26	13 (26%)	46,82,82	2.10	12 (26%)
9	HEC	C	201	4	50,50,50	2.84	12 (24%)	56,82,82	2.14	17 (30%)

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
5	HEM	B	801	8,3	-	0/14/114/114	0/0/8/8
5	HEM	B	802	8,3,7	-	0/14/114/114	0/0/8/8
9	HEC	C	201	4	-	0/10/54/54	0/0/8/8

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	201	HEC	C3B-CAB	9.65	1.55	1.35
9	C	201	HEC	C3C-CAC	9.50	1.55	1.35
5	B	801	HEM	C3B-C2B	-6.50	1.32	1.43
5	B	802	HEM	C3D-C2D	5.70	1.53	1.43
5	B	801	HEM	C3C-C2C	-5.62	1.33	1.43
5	B	802	HEM	C3B-C2B	-5.53	1.34	1.43
5	B	802	HEM	C2B-C1B	5.50	1.45	1.44
9	C	201	HEC	C3B-C4B	5.33	1.48	1.41
9	C	201	HEC	C1C-C2C	5.26	1.46	1.40
5	B	802	HEM	C3C-C2C	-5.16	1.34	1.43
9	C	201	HEC	C1D-C2D	5.10	1.46	1.40
9	C	201	HEC	C3D-C2D	5.00	1.52	1.37
5	B	801	HEM	C4A-C3A	4.50	1.45	1.40
5	B	802	HEM	C3C-CAC	4.43	1.54	1.40
5	B	802	HEM	C3B-CAB	4.32	1.54	1.40
9	C	201	HEC	C3B-C2B	-4.26	1.32	1.41
9	C	201	HEC	FE-ND	4.20	2.10	1.92
5	B	801	HEM	C3D-C2D	4.17	1.51	1.43
5	B	802	HEM	C4A-C3A	4.05	1.45	1.40
5	B	801	HEM	FE-NC	3.98	2.12	1.97
5	B	801	HEM	C3C-CAC	3.95	1.52	1.40
9	C	201	HEC	C3C-C2C	-3.92	1.33	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	801	HEM	C3B-CAB	3.85	1.52	1.40
9	C	201	HEC	C1B-C2B	3.36	1.44	1.40
9	C	201	HEC	FE-NA	3.09	2.05	1.92
5	B	802	HEM	FE-ND	3.07	2.09	1.97
5	B	802	HEM	C3D-C4D	2.97	1.45	1.44
9	C	201	HEC	C3C-C4C	2.74	1.45	1.41
5	B	801	HEM	C1A-C2A	2.62	1.48	1.43
5	B	801	HEM	CMB-C2B	2.60	1.55	1.47
5	B	801	HEM	CHB-C1B	2.58	1.39	1.35
5	B	801	HEM	CMC-C2C	2.56	1.55	1.47
5	B	801	HEM	FE-NA	2.50	2.03	1.92
5	B	802	HEM	CMC-C2C	2.30	1.54	1.47
5	B	802	HEM	CMB-C2B	2.30	1.54	1.47
5	B	802	HEM	CMD-C2D	2.23	1.54	1.47
5	B	802	HEM	FE-NA	2.17	2.01	1.92
5	B	801	HEM	CBA-CGA	2.03	1.55	1.50
5	B	801	HEM	CMD-C2D	2.02	1.53	1.47
5	B	801	HEM	FE-ND	2.01	2.05	1.97

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	801	HEM	C3B-C4B-NB	-12.40	105.13	114.00
5	B	802	HEM	CBA-CAA-C2A	-8.36	97.96	112.69
5	B	801	HEM	CHC-C4B-NB	7.68	130.97	124.58
9	C	201	HEC	CBD-CAD-C3D	-6.82	100.67	112.69
5	B	801	HEM	CHD-C4C-NC	6.46	130.34	124.73
9	C	201	HEC	CBC-CAC-C3C	-6.03	111.46	128.44
5	B	802	HEM	C3B-C4B-NB	-5.29	110.21	114.00
9	C	201	HEC	CBB-CAB-C3B	-5.10	114.09	128.44
5	B	802	HEM	C4D-ND-C1D	4.81	110.08	105.16
5	B	801	HEM	C4D-ND-C1D	4.78	110.06	105.16
9	C	201	HEC	CBA-CAA-C2A	-4.35	104.21	112.35
5	B	801	HEM	CAD-C3D-C4D	3.61	131.02	124.53
5	B	801	HEM	C4C-NC-C1C	3.60	109.27	105.53
5	B	801	HEM	CHC-C1C-NC	-3.59	121.61	124.73
5	B	801	HEM	CBD-CAD-C3D	-3.57	106.58	114.37
5	B	802	HEM	CAD-C3D-C4D	3.31	130.47	124.53
9	C	201	HEC	C4B-CHC-C1C	-3.29	123.15	127.47
5	B	801	HEM	C2D-C1D-ND	-3.27	109.07	112.93
9	C	201	HEC	C4D-C3D-C2D	-3.02	103.79	106.92
9	C	201	HEC	C2C-C1C-NC	-2.88	107.24	109.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	201	HEC	CHB-C1B-NB	2.85	129.34	124.58
9	C	201	HEC	CMB-C2B-C1B	-2.84	124.26	128.62
9	C	201	HEC	CMA-C3A-C2A	2.79	130.20	124.94
5	B	802	HEM	C2D-C1D-ND	-2.76	109.67	112.93
5	B	802	HEM	CHD-C4C-NC	2.74	127.12	124.73
9	C	201	HEC	C3C-C2C-C1C	2.63	108.82	107.07
5	B	801	HEM	C1B-NB-C4B	2.60	107.83	105.16
9	C	201	HEC	C3B-C4B-NB	-2.49	107.93	111.52
5	B	802	HEM	CHD-C1D-ND	2.48	126.64	124.58
9	C	201	HEC	C2B-C1B-CHB	-2.44	121.37	126.00
9	C	201	HEC	O2A-CGA-O1A	-2.32	117.38	123.30
5	B	801	HEM	CHB-C1B-NB	2.31	127.47	124.31
5	B	802	HEM	CHA-C1A-NA	2.26	128.35	124.58
5	B	801	HEM	O1D-CGD-CBD	-2.26	115.26	123.03
5	B	802	HEM	C1A-CHA-C4D	-2.21	124.56	127.47
5	B	802	HEM	CAD-CBD-CGD	-2.15	106.78	113.48
5	B	801	HEM	C4B-CHC-C1C	-2.12	121.00	126.57
5	B	802	HEM	C1A-C2A-C3A	2.11	109.10	106.92
5	B	801	HEM	CAD-CBD-CGD	2.11	120.05	113.48
9	C	201	HEC	C3B-C2B-C1B	2.06	108.44	107.07
5	B	802	HEM	CHC-C4B-NB	2.04	126.28	124.58
9	C	201	HEC	C1D-C2D-C3D	-2.03	105.59	107.00
9	C	201	HEC	O2A-CGA-CBA	2.00	121.30	114.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	L	213/213 (100%)	-0.49	1 (0%) 88 92	48, 72, 99, 121	1 (0%)
2	H	225/225 (100%)	-0.19	16 (7%) 16 17	48, 70, 107, 134	3 (1%)
3	B	449/465 (96%)	-0.30	17 (3%) 38 43	57, 89, 141, 179	0
4	C	142/146 (97%)	-0.43	3 (2%) 60 67	49, 78, 114, 137	0
All	All	1029/1049 (98%)	-0.34	37 (3%) 41 46	48, 79, 129, 179	4 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	225	GLY	6.7
3	B	381	ARG	4.7
2	H	206	CYS	4.4
2	H	141	ASP	4.3
3	B	299	ARG	4.1
4	C	5	PHE	3.9
4	C	139	GLN	3.6
2	H	202	GLN	3.5
3	B	77	TYR	3.4
2	H	143	THR	3.4
3	B	85	ASP	3.4
3	B	373	GLY	3.2
3	B	374	ILE	3.2
3	B	164	ARG	3.1
2	H	151	CYS	3.0
3	B	297	ARG	3.0
3	B	301	ASP	2.8
3	B	375	GLY	2.8
3	B	86	CYS	2.5
2	H	41	PRO	2.5
2	H	42	GLY	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	B	95	TRP	2.3
2	H	183	SER	2.3
2	H	150	GLY	2.3
2	H	116	GLN	2.3
3	B	127	GLU	2.3
2	H	142	THR	2.2
2	H	139	CYS	2.2
3	B	128	LEU	2.2
3	B	16	ALA	2.2
1	L	169	LYS	2.2
2	H	203	SER	2.2
4	C	43	ALA	2.1
3	B	292	PHE	2.1
3	B	376	GLU	2.1
2	H	22	CYS	2.1
2	H	1	GLU	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
9	HEC	C	201	43/43	0.14	0.57	50,58,64,70	0
5	HEM	B	801	43/43	0.14	0.54	51,59,68,76	0
5	HEM	B	802	43/43	0.13	0.32	57,66,73,83	0
7	O	B	805	1/1	0.16	0.09	60,60,60,60	0
6	FE	B	803	1/1	0.12	-0.31	64,64,64,64	0
8	CA	C	804	1/1	0.04	-3.22	60,60,60,60	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.