



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:11 PM GMT

PDB ID : 3WFD  
Title : Reduced and acetaldoxime-bound cytochrome c-dependent nitric oxide reductase (cNOR) from *Pseudomonas aeruginosa* in complex with antibody fragment  
Authors : Sato, N.; Ishii, S.; Hino, T.; Sugimoto, H.; Fukumori, Y.; Shiro, Y.; Tosha, T.  
Deposited on : 2013-07-18  
Resolution : 2.30 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

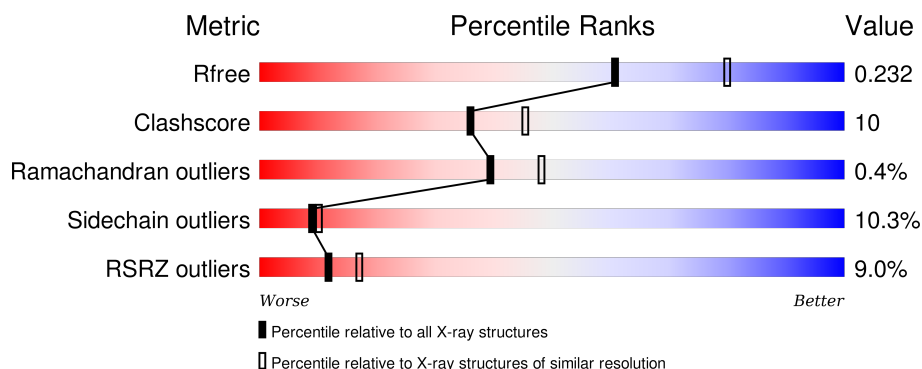
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	L	213	<div> <div>77%</div> <div>21%</div> <div>•</div> </div>
2	H	225	<div> <div>7%</div> <div>82%</div> <div>14%</div> <div>•</div> </div>
3	B	465	<div> <div>13%</div> <div>72%</div> <div>19%</div> <div>5%</div> <div>•</div> </div>
4	C	146	<div> <div>11%</div> <div>82%</div> <div>12%</div> <div>•</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	AXO	B	804	-	X	-	-
8	10M	B	805	-	-	-	X
8	10M	B	807	-	-	-	X

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 8556 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 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	DELETION	UNP Q59647

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

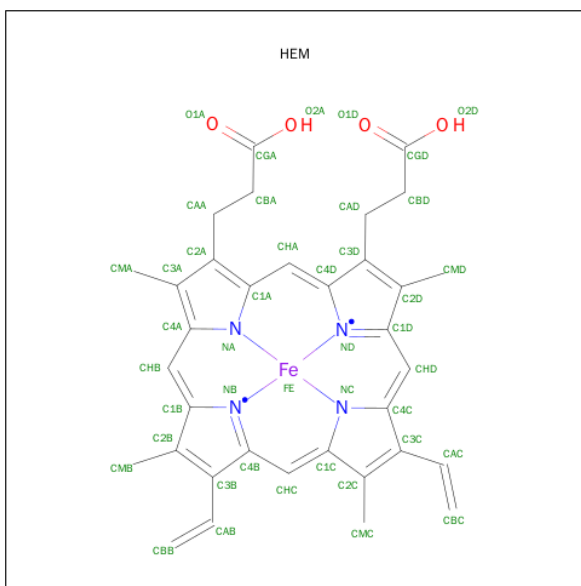
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	142	Total	C	N	O	S	0	0	0
			1123	720	195	202	6			

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

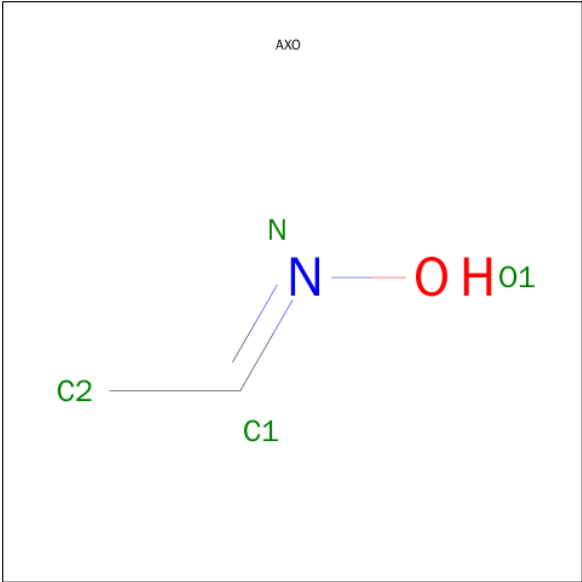


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
5	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	

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

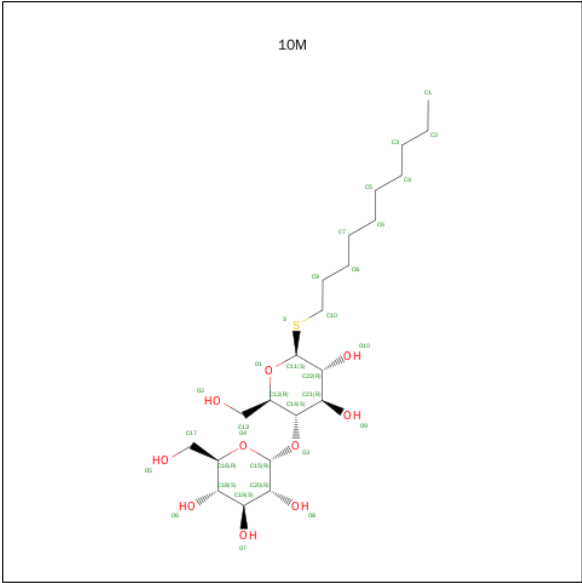
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Fe		
			1	1	0	0

- Molecule 7 is (1E)-N-HYDROXYETHANIMINE (three-letter code: AXO) (formula:  $C_2H_5NO$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			4	2	1	1		

- Molecule 8 is SUGAR (DECYL 4-O-ALPHA-D-GLUCOPYRANOSYL-1-THIO-BETA-D-GLUCOPYRANOSIDE) (three-letter code: 10M) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>10</sub>S).

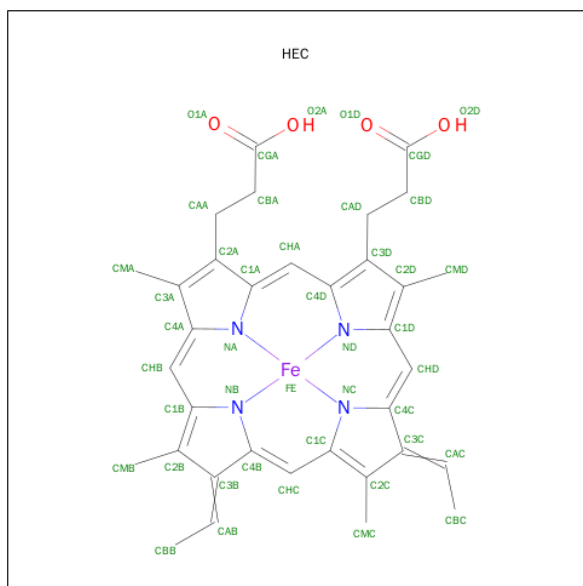


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	O	S	0	0
			33	22	10	1		
8	B	1	Total	C	O	S	0	0
			33	22	10	1		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Ca 1 1	0	0

- Molecule 10 is HEME C (three-letter code: HEC) (formula:  $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$ ).



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

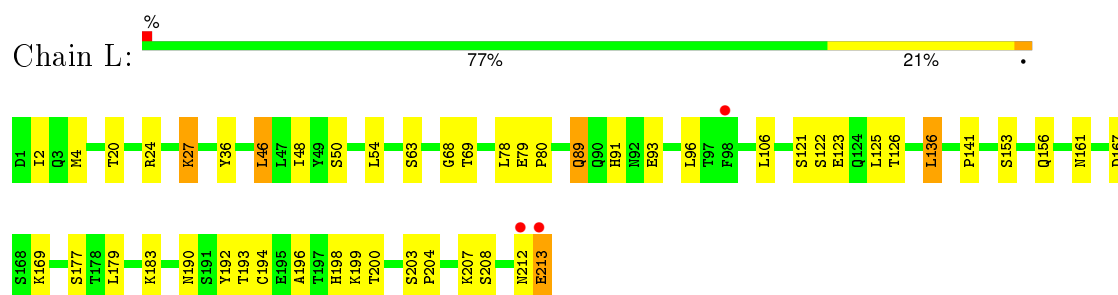
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	L	94	Total O 94 94	0	0
11	H	100	Total O 100 100	0	0
11	B	53	Total O 53 53	0	0
11	C	48	Total O 48 48	0	0

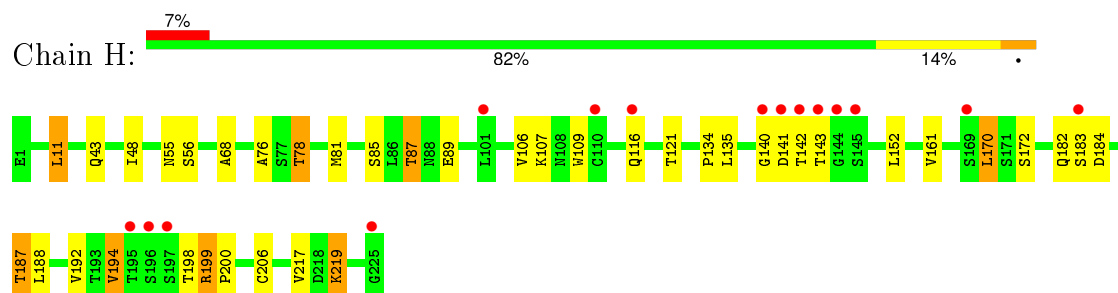
### 3 Residue-property plots [i](#)

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.

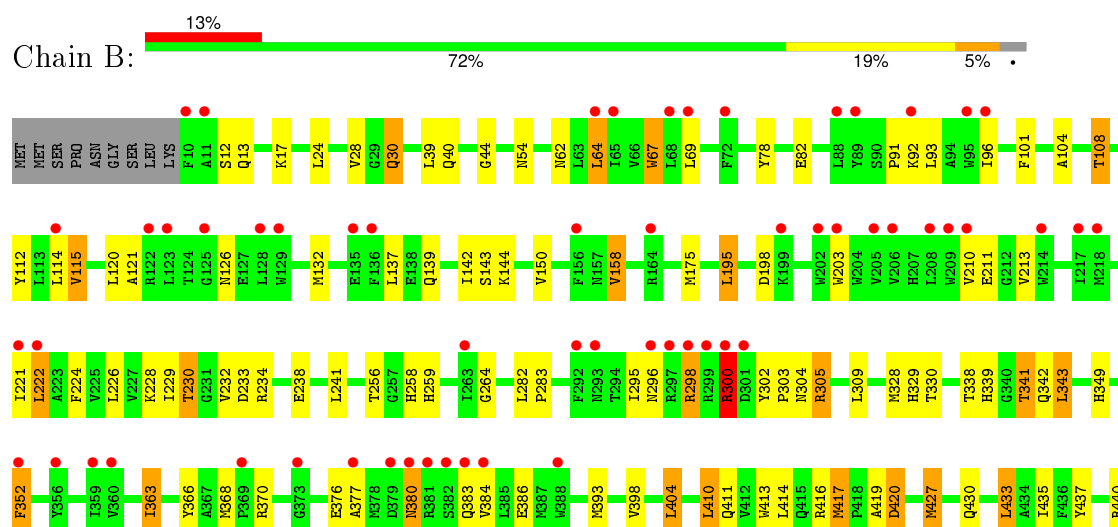
- Molecule 1: antibody fab fragment light chain



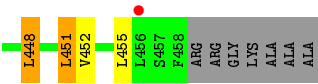
- Molecule 2: antibody fab fragment heavy chain



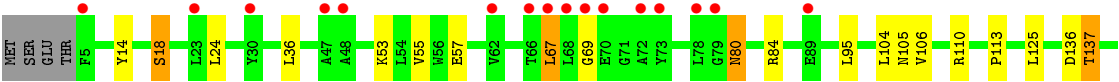
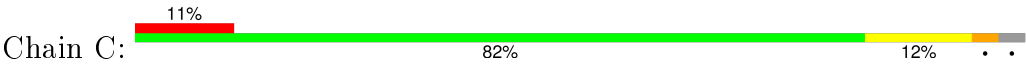
- Molecule 3: Nitric oxide reductase subunit B







● 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, $\alpha$ , $\beta$ , $\gamma$	90.93Å 106.75Å 196.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.38 – 2.30 33.36 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.1 (33.38-2.30) 96.2 (33.36-2.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.191 , 0.232 0.191 , 0.232	Depositor DCC
$R_{free}$ test set	4221 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.6	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 82815 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8556	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 10M, CA, FE, HEC, HEM, AXO

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	0.92	2/1709 (0.1%)	0.95	1/2317 (0.0%)
2	H	0.93	1/1735 (0.1%)	0.95	1/2367 (0.0%)
3	B	0.77	1/3693 (0.0%)	0.83	7/5039 (0.1%)
4	C	0.73	0/1153	0.82	0/1559
All	All	0.83	4/8290 (0.0%)	0.88	9/11282 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	63	SER	CA-CB	5.58	1.61	1.52
2	H	206	CYS	CB-SG	-5.43	1.73	1.81
1	L	194	CYS	CB-SG	-5.10	1.73	1.81
3	B	437	TYR	CE1-CZ	5.09	1.45	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	198	ASP	CB-CG-OD1	6.89	124.50	118.30
3	B	427	MET	CG-SD-CE	-5.71	91.07	100.20
3	B	198	ASP	CB-CG-OD2	-5.59	113.27	118.30
3	B	300	ARG	NE-CZ-NH1	5.49	123.05	120.30
2	H	206	CYS	CA-CB-SG	-5.38	104.31	114.00
3	B	420	ASP	CB-CG-OD1	5.13	122.92	118.30
3	B	222	LEU	CB-CG-CD2	5.05	119.59	111.00
1	L	46	LEU	CB-CG-CD2	5.03	119.55	111.00
3	B	64	LEU	CA-CB-CG	5.01	126.83	115.30

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	L	1669	0	1606	34	0
2	H	1692	0	1647	29	0
3	B	3576	0	3619	85	0
4	C	1123	0	1092	18	0
5	B	86	0	60	5	0
6	B	1	0	0	0	0
7	B	4	0	4	1	0
8	B	66	0	84	2	0
9	B	1	0	0	0	0
10	C	43	0	30	1	0
11	B	53	0	0	1	0
11	C	48	0	0	0	0
11	H	100	0	0	1	0
11	L	94	0	0	1	0
All	All	8556	0	8142	158	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 10.

All (158) 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)
2:H:199:ARG:CG	2:H:199:ARG:HH11	1.52	1.22
2:H:199:ARG:NH1	2:H:199:ARG:HG3	1.48	1.11
3:B:126:ASN:HB2	3:B:132:MET:HE2	1.20	1.10
3:B:121:ALA:HA	3:B:132:MET:HE1	1.26	1.08
3:B:126:ASN:HB2	3:B:132:MET:CE	1.88	1.02
3:B:126:ASN:CB	3:B:132:MET:HE2	1.89	1.02
3:B:300:ARG:HG3	3:B:300:ARG:HH11	1.23	1.00
2:H:48:ILE:HG21	2:H:81:MET:CE	1.97	0.94
2:H:199:ARG:HH11	2:H:199:ARG:HG3	0.77	0.94
2:H:48:ILE:HG21	2:H:81:MET:HE3	1.51	0.92
1:L:121:SER:HB2	1:L:123:GLU:OE1	1.71	0.90
3:B:338:THR:O	3:B:341:THR:HB	1.78	0.83
3:B:126:ASN:CB	3:B:132:MET:CE	2.52	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:104:ALA:O	3:B:108:THR:HG23	1.82	0.80
2:H:183:SER:OG	2:H:184:ASP:N	2.13	0.80
1:L:192:TYR:O	1:L:208:SER:HB2	1.82	0.79
3:B:137:LEU:HA	3:B:139:GLN:HE22	1.47	0.78
3:B:121:ALA:HA	3:B:132:MET:CE	2.12	0.77
3:B:393:MET:HE1	3:B:451:LEU:HD23	1.66	0.77
3:B:121:ALA:CA	3:B:132:MET:HE1	2.11	0.77
1:L:2:ILE:HD11	1:L:93:GLU:OE1	1.86	0.75
3:B:13:GLN:HE22	3:B:82:GLU:HB2	1.52	0.75
1:L:79:GLU:HG3	1:L:80:PRO:HD2	1.67	0.74
3:B:430:GLN:HE21	4:C:110:ARG:HH22	1.36	0.73
3:B:139:GLN:HE21	3:B:144:LYS:HE3	1.54	0.72
1:L:198:HIS:HD2	1:L:200:THR:OG1	1.73	0.71
3:B:28:VAL:HG22	3:B:451:LEU:CD1	2.21	0.70
2:H:199:ARG:CG	2:H:199:ARG:NH1	2.20	0.70
1:L:27:LYS:HD3	11:L:344:HOH:O	1.91	0.69
2:H:107:LYS:HB3	11:H:322:HOH:O	1.93	0.68
3:B:300:ARG:CG	3:B:300:ARG:HH11	2.04	0.68
1:L:2:ILE:HD11	1:L:93:GLU:CD	2.15	0.66
3:B:341:THR:CG2	3:B:343:LEU:H	2.10	0.64
3:B:126:ASN:CG	3:B:132:MET:HE2	2.18	0.63
4:C:137:THR:HG21	4:C:140:TRP:O	1.99	0.63
2:H:87:THR:CG2	2:H:89:GLU:H	2.11	0.63
3:B:300:ARG:NH1	3:B:300:ARG:HG3	2.02	0.62
3:B:108:THR:HG21	3:B:143:SER:OG	1.99	0.62
1:L:50:SER:H	1:L:91:HIS:HE1	1.48	0.62
2:H:194:VAL:HG13	2:H:198:THR:HB	1.82	0.61
4:C:80:ASN:HD22	4:C:80:ASN:H	1.49	0.61
3:B:142:ILE:HG12	11:B:924:HOH:O	1.99	0.61
3:B:13:GLN:NE2	3:B:82:GLU:HB2	2.14	0.61
3:B:430:GLN:HE21	4:C:110:ARG:NH2	1.99	0.60
3:B:195:LEU:HD11	4:C:67:LEU:HD13	1.83	0.60
3:B:229:ILE:HD11	3:B:366:TYR:CD1	2.37	0.60
3:B:230:THR:HG23	3:B:232:VAL:H	1.67	0.60
2:H:48:ILE:HG21	2:H:81:MET:HE1	1.80	0.58
2:H:87:THR:HG22	2:H:89:GLU:H	1.67	0.57
1:L:79:GLU:HG3	1:L:80:PRO:CD	2.34	0.57
1:L:161:ASN:HD22	1:L:177:SER:HA	1.69	0.57
1:L:2:ILE:HD12	1:L:2:ILE:N	2.20	0.57
2:H:48:ILE:CG2	2:H:81:MET:HE3	2.31	0.57
1:L:167:ASP:OD2	1:L:169:LYS:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:123:GLU:CD	1:L:123:GLU:H	2.09	0.56
4:C:80:ASN:ND2	4:C:84:ARG:HH12	2.04	0.56
3:B:28:VAL:HG22	3:B:451:LEU:HD11	1.87	0.55
4:C:80:ASN:HD21	4:C:84:ARG:HH12	1.53	0.55
3:B:224:PHE:CE1	3:B:228:LYS:HE2	2.42	0.55
3:B:210:VAL:HG13	5:B:802:HEM:C2B	2.42	0.54
3:B:264:GLY:HA2	4:C:136:ASP:O	2.06	0.54
2:H:76:ALA:O	2:H:78:THR:HG22	2.06	0.54
3:B:413:TRP:HA	3:B:417:MET:HG3	1.90	0.54
3:B:430:GLN:NE2	4:C:110:ARG:HH22	2.02	0.54
3:B:229:ILE:HD11	3:B:366:TYR:HD1	1.71	0.53
3:B:234:ARG:O	3:B:238:GLU:HG3	2.08	0.53
1:L:50:SER:H	1:L:91:HIS:CE1	2.26	0.53
3:B:158:VAL:CG1	3:B:175:MET:SD	2.97	0.53
3:B:341:THR:HG22	3:B:343:LEU:H	1.74	0.53
3:B:137:LEU:HA	3:B:139:GLN:NE2	2.21	0.53
3:B:230:THR:CG2	3:B:232:VAL:H	2.22	0.53
3:B:341:THR:HG23	3:B:343:LEU:H	1.74	0.52
2:H:134:PRO:HD3	2:H:219:LYS:HG3	1.91	0.52
3:B:230:THR:HG23	3:B:232:VAL:HG23	1.90	0.52
1:L:136:LEU:CD1	1:L:196:ALA:HB2	2.40	0.52
1:L:36:TYR:HE2	1:L:89:GLN:HE21	1.57	0.52
2:H:55:ASN:O	2:H:56:SER:HB2	2.09	0.52
3:B:230:THR:CG2	3:B:232:VAL:HB	2.40	0.51
3:B:305:ARG:HH12	3:B:380:ASN:HD21	1.58	0.51
3:B:221:ILE:HG23	3:B:363:ILE:HG12	1.93	0.51
3:B:295:ILE:O	3:B:298:ARG:HG3	2.11	0.51
3:B:210:VAL:CG1	5:B:802:HEM:C2B	2.93	0.51
3:B:349:HIS:CD2	5:B:801:HEM:NC	2.78	0.51
4:C:137:THR:CG2	4:C:140:TRP:O	2.59	0.50
1:L:212:ASN:OD1	1:L:213:GLU:N	2.35	0.50
3:B:411:GLN:HB2	3:B:433:LEU:HD21	1.94	0.49
1:L:193:THR:HA	1:L:208:SER:HB3	1.94	0.49
3:B:295:ILE:O	3:B:298:ARG:CG	2.61	0.49
1:L:122:SER:O	1:L:126:THR:HG23	2.13	0.49
3:B:101:PHE:HB2	3:B:150:VAL:HG11	1.94	0.49
3:B:211:GLU:OE2	7:B:804:AXO:H1	2.12	0.49
3:B:210:VAL:HG13	5:B:802:HEM:C3B	2.48	0.48
4:C:14:TYR:O	4:C:18:SER:OG	2.28	0.48
1:L:141:PRO:O	1:L:198:HIS:HE1	1.97	0.48
3:B:126:ASN:HD21	3:B:132:MET:H	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:303:PRO:HG2	3:B:376:GLU:OE1	2.14	0.48
2:H:87:THR:HG22	2:H:89:GLU:N	2.29	0.48
3:B:24:LEU:HB3	3:B:455:LEU:HD21	1.96	0.47
3:B:304:ASN:HB2	3:B:377:ALA:HB2	1.96	0.47
1:L:125:LEU:O	1:L:183:LYS:HD2	2.14	0.47
3:B:420:ASP:OD1	4:C:143:ASN:HB2	2.14	0.47
3:B:300:ARG:CG	3:B:300:ARG:NH1	2.72	0.47
3:B:226:LEU:O	3:B:230:THR:HB	2.14	0.47
3:B:352:PHE:HB3	5:B:801:HEM:HBC1	1.97	0.47
1:L:192:TYR:O	1:L:208:SER:CB	2.58	0.47
4:C:113:PRO:HD3	10:C:201:HEC:HBC2	1.97	0.46
1:L:91:HIS:HD2	2:H:109:TRP:CE3	2.34	0.46
3:B:30:GLN:NE2	3:B:67:TRP:HE1	2.13	0.46
3:B:40:GLN:O	3:B:44:GLY:HA2	2.16	0.46
2:H:183:SER:HG	2:H:184:ASP:H	1.59	0.46
4:C:80:ASN:HD22	4:C:80:ASN:N	2.09	0.45
3:B:305:ARG:HG3	3:B:383:GLN:NE2	2.31	0.45
3:B:12:SER:HB2	3:B:91:PRO:HG3	1.98	0.45
2:H:11:LEU:HD12	2:H:121:THR:HB	1.99	0.45
1:L:2:ILE:CD1	1:L:2:ILE:N	2.80	0.45
3:B:305:ARG:NH1	3:B:380:ASN:HD21	2.15	0.45
3:B:62:ASN:ND2	3:B:112:TYR:OH	2.50	0.45
1:L:190:ASN:HD21	1:L:212:ASN:H	1.65	0.44
4:C:53:LYS:NZ	4:C:57:GLU:OE2	2.49	0.44
4:C:55:VAL:HG11	4:C:125:LEU:HG	1.99	0.44
1:L:121:SER:CB	1:L:123:GLU:OE1	2.55	0.44
3:B:126:ASN:CG	3:B:132:MET:CE	2.83	0.44
2:H:199:ARG:HH11	2:H:199:ARG:HG2	1.68	0.43
3:B:339:HIS:CD2	4:C:69:GLY:HA3	2.53	0.43
1:L:203:SER:HA	1:L:204:PRO:HD3	1.83	0.43
2:H:170:LEU:HD13	2:H:192:VAL:HG21	2.00	0.43
2:H:199:ARG:HD2	2:H:200:PRO:HA	2.01	0.43
3:B:115:VAL:HG22	3:B:120:LEU:HB2	2.01	0.43
3:B:282:LEU:N	3:B:283:PRO:HD2	2.33	0.43
3:B:28:VAL:CG2	3:B:451:LEU:HD11	2.49	0.43
3:B:342:GLN:H	3:B:411:GLN:NE2	2.17	0.43
1:L:4:MET:HB3	1:L:4:MET:HE2	1.69	0.43
1:L:2:ILE:HG13	1:L:27:LYS:HG3	2.02	0.42
1:L:161:ASN:ND2	1:L:177:SER:OG	2.52	0.42
3:B:417:MET:O	8:B:805:10M:C13	2.67	0.42
3:B:203:TRP:CE2	3:B:259:HIS:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:82:GLU:OE1	3:B:228:LYS:HE3	2.19	0.42
1:L:36:TYR:OH	1:L:89:GLN:NE2	2.52	0.42
3:B:230:THR:HG23	3:B:232:VAL:CG2	2.49	0.42
2:H:219:LYS:HD2	2:H:219:LYS:HA	1.67	0.42
3:B:69:LEU:HA	3:B:69:LEU:HD23	1.89	0.42
2:H:199:ARG:HG2	2:H:199:ARG:NH1	2.23	0.42
3:B:158:VAL:HG13	3:B:175:MET:SD	2.59	0.42
2:H:182:GLN:NE2	2:H:187:THR:HG21	2.35	0.41
3:B:302:TYR:OH	3:B:370:ARG:NH1	2.54	0.41
3:B:448:LEU:O	3:B:452:VAL:HG23	2.20	0.41
1:L:156:GLN:HE21	1:L:156:GLN:HB3	1.68	0.41
3:B:419:ALA:HB2	8:B:805:10M:H17A	2.01	0.41
3:B:410:LEU:HD22	3:B:414:LEU:CD1	2.50	0.41
1:L:78:LEU:HD23	1:L:78:LEU:HA	1.91	0.41
4:C:104:LEU:O	4:C:105:ASN:HB2	2.20	0.41
3:B:121:ALA:CB	3:B:132:MET:CE	2.98	0.41
2:H:76:ALA:O	2:H:78:THR:CG2	2.68	0.41
3:B:404:LEU:HD13	3:B:440:ARG:HG3	2.03	0.41
2:H:68:ALA:HB1	2:H:81:MET:CE	2.52	0.40
1:L:48:ILE:HD13	1:L:54:LEU:HD23	2.03	0.40
2:H:68:ALA:HB1	2:H:81:MET:HE2	2.04	0.40
3:B:13:GLN:NE2	3:B:78:TYR:O	2.55	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	L	211/213 (99%)	206 (98%)	4 (2%)	1 (0%)	34	41
2	H	223/225 (99%)	210 (94%)	11 (5%)	2 (1%)	21	24
3	B	447/465 (96%)	434 (97%)	12 (3%)	1 (0%)	52	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	140/146 (96%)	136 (97%)	4 (3%)	0	100	100
All	All	1021/1049 (97%)	986 (97%)	31 (3%)	4 (0%)	39	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	256	THR
2	H	140	GLY
2	H	141	ASP
1	L	68	GLY

### 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%)	175 (93%)	14 (7%)	17	21
2	H	192/192 (100%)	172 (90%)	20 (10%)	9	10
3	B	360/371 (97%)	314 (87%)	46 (13%)	5	5
4	C	116/120 (97%)	108 (93%)	8 (7%)	19	24
All	All	857/872 (98%)	769 (90%)	88 (10%)	9	10

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	20	THR
1	L	24	ARG
1	L	27	LYS
1	L	46	LEU
1	L	69	THR
1	L	89	GLN
1	L	96	LEU
1	L	106	LEU
1	L	136	LEU
1	L	153	SER

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Mol	Chain	Res	Type
1	L	179	LEU
1	L	199	LYS
1	L	207	LYS
1	L	213	GLU
2	H	11	LEU
2	H	43	GLN
2	H	78	THR
2	H	85	SER
2	H	87	THR
2	H	106	VAL
2	H	116	GLN
2	H	135	LEU
2	H	142	THR
2	H	143	THR
2	H	152	LEU
2	H	161	VAL
2	H	170	LEU
2	H	172	SER
2	H	187	THR
2	H	188	LEU
2	H	194	VAL
2	H	199	ARG
2	H	217	VAL
2	H	219	LYS
3	B	17	LYS
3	B	30	GLN
3	B	39	LEU
3	B	54	ASN
3	B	64	LEU
3	B	67	TRP
3	B	92	LYS
3	B	93	LEU
3	B	96	ILE
3	B	108	THR
3	B	114	LEU
3	B	115	VAL
3	B	158	VAL
3	B	195	LEU
3	B	213	VAL
3	B	222	LEU
3	B	230	THR
3	B	233	ASP

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Mol	Chain	Res	Type
3	B	241	LEU
3	B	258	HIS
3	B	296	ASN
3	B	298	ARG
3	B	300	ARG
3	B	305	ARG
3	B	309	LEU
3	B	328	MET
3	B	329	HIS
3	B	330	THR
3	B	341	THR
3	B	343	LEU
3	B	352	PHE
3	B	363	ILE
3	B	368	MET
3	B	380	ASN
3	B	384	VAL
3	B	386	GLU
3	B	398	VAL
3	B	404	LEU
3	B	410	LEU
3	B	416	ARG
3	B	417	MET
3	B	427	MET
3	B	433	LEU
3	B	435	ILE
3	B	448	LEU
3	B	451	LEU
4	C	18	SER
4	C	24	LEU
4	C	36	LEU
4	C	67	LEU
4	C	80	ASN
4	C	95	LEU
4	C	106	VAL
4	C	137	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	89	GLN
1	L	91	HIS

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Mol	Chain	Res	Type
1	L	137	ASN
1	L	156	GLN
1	L	161	ASN
1	L	198	HIS
2	H	182	GLN
3	B	13	GLN
3	B	30	GLN
3	B	54	ASN
3	B	62	ASN
3	B	126	ASN
3	B	139	GLN
3	B	296	ASN
3	B	380	ASN
3	B	383	GLN
3	B	411	GLN
3	B	430	GLN
4	C	31	HIS
4	C	60	ASN
4	C	80	ASN
4	C	96	GLN
4	C	102	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](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	9,3	30,50,50	2.24	7 (23%)	24,82,82	5.58	14 (58%)
5	HEM	B	802	9,3,7	30,50,50	2.21	5 (16%)	24,82,82	3.29	12 (50%)
7	AXO	B	804	5,6	3,3,3	3.10	2 (66%)	1,2,2	12.44	1 (100%)
8	10M	B	805	-	34,34,34	1.31	5 (14%)	43,45,45	1.52	8 (18%)
8	10M	B	807	-	34,34,34	1.31	3 (8%)	43,45,45	1.03	3 (6%)
10	HEC	C	201	4	24,50,50	2.68	9 (37%)	19,82,82	2.50	5 (26%)

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	9,3	-	0/10/54/54	0/0/8/8
5	HEM	B	802	9,3,7	-	0/10/54/54	0/0/8/8
7	AXO	B	804	5,6	-	0/0/1/1	0/0/0/0
8	10M	B	805	-	-	0/19/59/59	0/2/2/2
8	10M	B	807	-	-	0/19/59/59	0/2/2/2
10	HEC	C	201	4	-	0/6/54/54	0/0/8/8

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	802	HEM	C3B-C4B	-8.48	1.44	1.51
5	B	801	HEM	C3B-C4B	-7.69	1.45	1.51
10	C	201	HEC	C3B-C2B	-7.01	1.33	1.40
10	C	201	HEC	C3C-C2C	-6.34	1.34	1.40
5	B	801	HEM	C3D-C4D	-5.87	1.44	1.51
7	B	804	AXO	O1-N	-4.38	1.30	1.40
5	B	802	HEM	C3D-C4D	-4.32	1.46	1.51
5	B	802	HEM	C2C-C1C	-3.39	1.46	1.52
7	B	804	AXO	C1-N	-3.11	1.23	1.26
5	B	801	HEM	C2C-C1C	-2.77	1.47	1.52
5	B	801	HEM	C2D-C1D	-2.15	1.44	1.51
8	B	805	10M	O3-C14	2.05	1.49	1.43
10	C	201	HEC	C1A-NA	2.10	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	201	HEC	C3C-C4C	2.12	1.47	1.42
8	B	805	10M	C11-S	2.12	1.84	1.80
5	B	802	HEM	C3C-CAC	2.17	1.55	1.51
8	B	805	10M	O4-C15	2.19	1.47	1.41
5	B	802	HEM	CAA-C2A	2.20	1.55	1.52
10	C	201	HEC	CMC-C2C	2.22	1.56	1.51
10	C	201	HEC	CMA-C3A	2.23	1.56	1.51
10	C	201	HEC	C4C-NC	2.30	1.39	1.36
5	B	801	HEM	C3B-CAB	2.33	1.55	1.51
5	B	801	HEM	C3C-CAC	2.36	1.55	1.51
8	B	805	10M	C10-S	2.53	1.84	1.81
8	B	807	10M	C10-S	3.01	1.85	1.81
8	B	807	10M	C11-S	3.07	1.85	1.80
8	B	805	10M	O3-C15	3.12	1.50	1.41
5	B	801	HEM	C1C-NC	3.47	1.40	1.36
10	C	201	HEC	C4A-NA	3.85	1.41	1.36
10	C	201	HEC	C3D-C2D	4.91	1.52	1.37
8	B	807	10M	O1-C11	5.09	1.51	1.42

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	801	HEM	C3C-CAC-CBC	-22.84	89.42	124.46
7	B	804	AXO	O1-N-C1	-12.44	99.75	111.69
10	C	201	HEC	CBB-CAB-C3B	-7.61	110.44	127.35
5	B	802	HEM	CBA-CAA-C2A	-6.66	100.58	112.53
5	B	802	HEM	C3B-CAB-CBB	-5.87	115.46	124.46
5	B	801	HEM	CAA-CBA-CGA	-5.41	102.83	112.75
5	B	801	HEM	CAA-C2A-C1A	-5.11	121.46	127.01
5	B	801	HEM	CMA-C3A-C4A	-4.84	120.35	128.36
10	C	201	HEC	CBD-CAD-C3D	-4.55	104.38	112.53
5	B	801	HEM	CBD-CAD-C3D	-4.20	101.34	113.55
5	B	802	HEM	C3C-CAC-CBC	-4.12	118.14	124.46
10	C	201	HEC	CMB-C2B-C1B	-3.83	122.02	128.36
5	B	802	HEM	CAA-CBA-CGA	-3.08	107.09	112.75
5	B	801	HEM	C3B-CAB-CBB	-2.93	119.97	124.46
5	B	802	HEM	C4B-CHC-C1C	-2.78	121.17	125.82
8	B	805	10M	C15-O3-C14	-2.59	111.25	118.01
8	B	807	10M	O3-C14-C21	-2.31	101.20	107.17
10	C	201	HEC	CBA-CAA-C2A	-2.30	108.40	112.53
10	C	201	HEC	CMC-C2C-C1C	-2.17	124.78	128.36
5	B	802	HEM	C2C-C1C-NC	-2.16	106.57	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	801	HEM	C3B-C4B-NB	-2.08	107.66	111.63
5	B	802	HEM	CMD-C2D-C3D	2.16	123.92	114.35
8	B	807	10M	C11-O1-C12	2.22	116.98	112.74
8	B	807	10M	O4-C16-C17	2.28	112.12	106.36
8	B	805	10M	C19-C18-C16	2.29	114.19	110.20
5	B	802	HEM	CAD-C3D-C2D	2.34	119.95	113.22
5	B	802	HEM	C2D-C3D-C4D	2.43	105.62	101.50
5	B	801	HEM	C2C-C1C-NC	2.53	114.48	110.21
8	B	805	10M	C21-C14-C12	2.66	116.86	110.84
8	B	805	10M	O4-C16-C18	2.75	114.85	109.68
8	B	805	10M	C15-C20-C19	3.05	115.97	109.97
8	B	805	10M	O3-C15-C20	3.07	115.58	108.10
5	B	801	HEM	CMD-C2D-C3D	3.18	128.41	114.35
5	B	801	HEM	CMB-C2B-C3B	3.20	124.51	116.53
8	B	805	10M	C18-C19-C20	3.20	116.76	110.79
5	B	801	HEM	CMC-C2C-C3C	3.41	125.05	116.53
8	B	805	10M	C22-C21-C14	3.42	117.11	109.60
5	B	801	HEM	CAD-C3D-C4D	3.56	125.03	112.47
5	B	801	HEM	CMA-C3A-C2A	4.14	133.90	125.24
5	B	802	HEM	CMC-C2C-C3C	5.12	129.30	116.53
5	B	802	HEM	CAD-C3D-C4D	6.23	134.43	112.47
5	B	801	HEM	CAD-C3D-C2D	6.37	131.53	113.22
5	B	802	HEM	CMB-C2B-C3B	7.22	134.56	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	801	HEM	2	0
5	B	802	HEM	3	0
7	B	804	AXO	1	0
8	B	805	10M	2	0
10	C	201	HEC	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	L	213/213 (100%)	-0.20	3 (1%) 78 83	37, 49, 70, 118	0
2	H	225/225 (100%)	0.06	15 (6%) 21 29	37, 49, 79, 148	0
3	B	449/465 (96%)	0.44	59 (13%) 5 7	40, 63, 102, 137	0
4	C	142/146 (97%)	0.49	16 (11%) 7 10	40, 61, 85, 109	0
All	All	1029/1049 (98%)	0.23	93 (9%) 12 17	37, 57, 92, 148	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	299	ARG	8.1
3	B	381	ARG	7.7
3	B	206	VAL	5.8
3	B	296	ASN	5.4
2	H	143	THR	5.2
2	H	225	GLY	5.1
4	C	67	LEU	5.0
3	B	388	TRP	4.9
3	B	297	ARG	4.8
3	B	95	TRP	4.8
4	C	68	LEU	4.8
3	B	129	TRP	4.8
3	B	65	ILE	4.7
3	B	136	PHE	4.7
2	H	142	THR	4.5
3	B	68	LEU	4.3
4	C	5	PHE	4.3
4	C	30	TYR	4.3
3	B	202	TRP	4.2
3	B	300	ARG	4.1
3	B	352	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
4	C	89	GLU	4.0
3	B	72	PHE	3.9
4	C	66	THR	3.9
3	B	11	ALA	3.9
3	B	69	LEU	3.8
3	B	384	VAL	3.8
3	B	356	TYR	3.7
3	B	263	ILE	3.6
3	B	209	TRP	3.6
2	H	144	GLY	3.5
4	C	78	LEU	3.5
3	B	301	ASP	3.4
3	B	210	VAL	3.4
3	B	164	ARG	3.4
3	B	214	TRP	3.3
3	B	89	TYR	3.3
3	B	203	TRP	3.2
3	B	382	SER	3.2
3	B	292	PHE	3.2
3	B	379	ASP	3.2
3	B	298	ARG	3.2
3	B	96	ILE	3.2
3	B	128	LEU	3.1
3	B	156	PHE	3.1
1	L	213	GLU	3.0
3	B	88	LEU	3.0
1	L	212	ASN	3.0
4	C	69	GLY	3.0
2	H	195	THR	2.9
4	C	73	TYR	2.9
4	C	23	LEU	2.9
3	B	360	VAL	2.8
4	C	62	VAL	2.8
3	B	373	GLY	2.8
3	B	199	LYS	2.7
3	B	217	ILE	2.7
3	B	380	ASN	2.7
3	B	64	LEU	2.6
3	B	92	LYS	2.6
2	H	101	LEU	2.5
2	H	145	SER	2.5
3	B	218	MET	2.4

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Mol	Chain	Res	Type	RSRZ
4	C	70	GLU	2.4
3	B	135	GLU	2.4
3	B	10	PHE	2.4
3	B	122	ARG	2.3
2	H	140	GLY	2.3
3	B	114	LEU	2.3
3	B	383	GLN	2.3
1	L	98	PHE	2.3
3	B	125	GLY	2.3
3	B	377	ALA	2.3
3	B	293	ASN	2.3
3	B	369	PRO	2.3
2	H	196	SER	2.3
2	H	183	SER	2.2
4	C	48	ALA	2.2
3	B	221	ILE	2.2
2	H	169	SER	2.2
2	H	116	GLN	2.2
4	C	79	GLY	2.2
3	B	123	LEU	2.2
3	B	456	LEU	2.2
3	B	359	ILE	2.1
4	C	47	ALA	2.1
3	B	205	VAL	2.1
3	B	208	LEU	2.1
2	H	141	ASP	2.1
3	B	222	LEU	2.1
2	H	110	CYS	2.0
2	H	197	SER	2.0
4	C	72	ALA	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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
8	10M	B	805	33/33	0.81	0.37	6.94	87,119,132,133	0
8	10M	B	807	33/33	0.94	0.25	3.40	63,84,105,114	0
10	HEC	C	201	43/43	0.98	0.19	0.74	40,44,46,50	0
5	HEM	B	801	43/43	0.96	0.19	0.23	41,47,55,68	0
5	HEM	B	802	43/43	0.98	0.20	-0.07	41,45,50,51	0
7	AXO	B	804	4/4	0.99	0.18	-0.54	45,47,49,53	0
9	CA	B	806	1/1	0.99	0.23	-0.68	52,52,52,52	0
6	FE	B	803	1/1	0.99	0.15	-	48,48,48,48	0

## 6.5 Other polymers

There are no such residues in this entry.