



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 05:32 AM GMT

PDB ID : 2GC4  
Title : Structural comparison of the oxidized ternary electron transfer complex of methylamine dehydrogenase, amicyanin and cytochrome c551i from *Paracoccus denitrificans* with the substrate-reduced, copper free complex at 1.9 Å resolution.  
Authors : Chen, Z.; Durley, R.; Davidson, V.L.; Mathews, F.S.  
Deposited on : 2006-03-13  
Resolution : 1.90 Å(reported)

This is a wwPDB validation summary 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>

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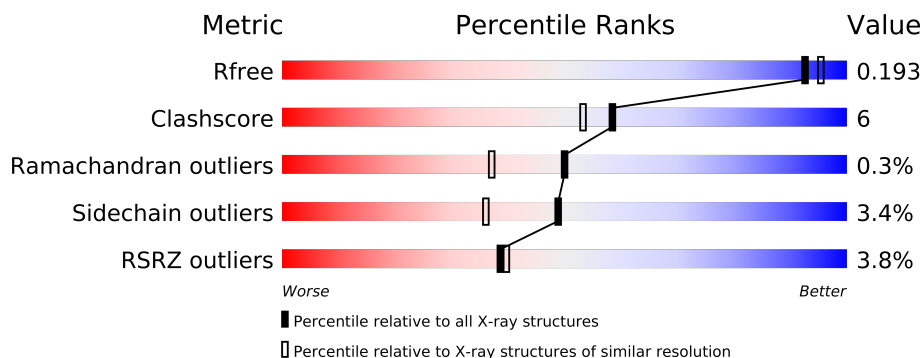
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 1.90 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	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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	A	386	
1	E	386	
1	I	386	
1	M	386	
2	B	131	
2	F	131	
2	J	131	
2	N	131	
3	C	105	
3	G	105	
3	K	105	
3	O	105	
4	D	147	
4	H	147	

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Mol	Chain	Length	Quality of chain
4	L	147	
4	P	147	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
6	NA	H	603	-	X
6	NA	L	601	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24820 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 Methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	382	Total	C	N	O	S	0	0	0
			2967	1878	509	572	8			
1	E	382	Total	C	N	O	S	0	0	0
			2967	1878	509	572	8			
1	I	382	Total	C	N	O	S	0	0	0
			2967	1878	509	572	8			
1	M	382	Total	C	N	O	S	0	0	0
			2967	1878	509	572	8			

- Molecule 2 is a protein called Methylamine dehydrogenase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	125	Total	C	N	O	S	0	0	0
			956	590	161	192	13			
2	F	125	Total	C	N	O	S	0	0	0
			956	590	161	192	13			
2	J	125	Total	C	N	O	S	0	0	0
			956	590	161	192	13			
2	N	125	Total	C	N	O	S	0	0	0
			956	590	161	192	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	57	TRQ	TRP	MODIFIED RESIDUE	UNP P22619
F	57	TRQ	TRP	MODIFIED RESIDUE	UNP P22619
J	57	TRQ	TRP	MODIFIED RESIDUE	UNP P22619
N	57	TRQ	TRP	MODIFIED RESIDUE	UNP P22619

- Molecule 3 is a protein called Amicyanin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	105	Total	C	N	O	S	0	0	0
			807	516	133	152	6			
3	G	105	Total	C	N	O	S	0	0	0
			807	516	133	152	6			
3	K	105	Total	C	N	O	S	0	0	0
			807	516	133	152	6			
3	O	105	Total	C	N	O	S	0	0	0
			807	516	133	152	6			

- Molecule 4 is a protein called Cytochrome c-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	147	Total	C	N	O	S	0	0	0
			1145	724	182	231	8			
4	H	147	Total	C	N	O	S	0	0	0
			1145	724	182	231	8			
4	L	147	Total	C	N	O	S	0	0	0
			1145	724	182	231	8			
4	P	147	Total	C	N	O	S	0	0	0
			1145	724	182	231	8			

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Cu	0	0
			1	1		
5	C	1	Total	Cu	0	0
			1	1		
5	K	1	Total	Cu	0	0
			1	1		
5	O	1	Total	Cu	0	0
			1	1		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

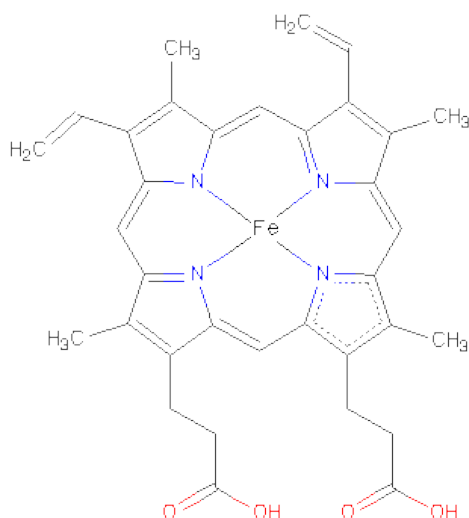
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	1	Total	Na	0	0
			1	1		
6	H	1	Total	Na	0	0
			1	1		
6	L	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Na	0	0
			1	1		

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	H	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	L	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
7	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	170	Total	O	0	0
			170	170		
8	B	54	Total	O	0	0
			54	54		
8	C	19	Total	O	0	0
			19	19		
8	D	36	Total	O	0	0
			36	36		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	160	Total 160	O 160	0	0
8	F	60	Total 60	O 60	0	0
8	G	22	Total 22	O 22	0	0
8	H	40	Total 40	O 40	0	0
8	I	155	Total 155	O 155	0	0
8	J	64	Total 64	O 64	0	0
8	K	27	Total 27	O 27	0	0
8	L	48	Total 48	O 48	0	0
8	M	173	Total 173	O 173	0	0
8	N	55	Total 55	O 55	0	0
8	O	14	Total 14	O 14	0	0
8	P	43	Total 43	O 43	0	0

### 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.

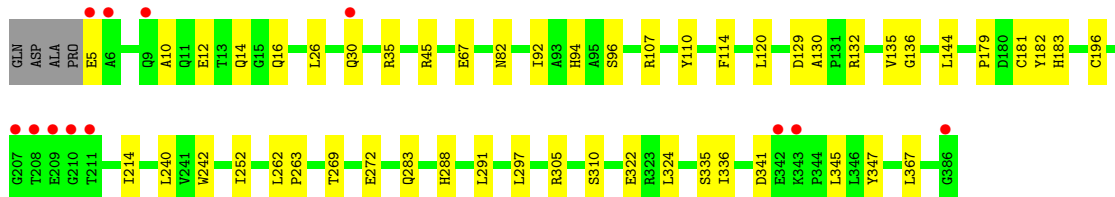
- Molecule 1: Methylamine dehydrogenase heavy chain

Chain A: 



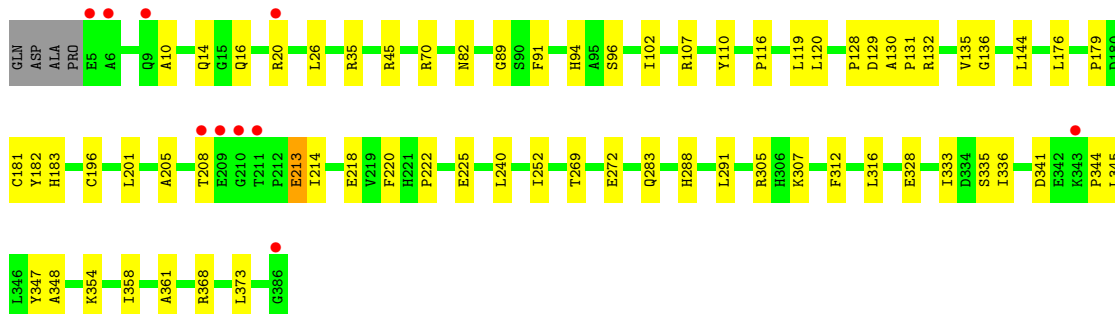
- Molecule 1: Methylamine dehydrogenase heavy chain

Chain E: 



- Molecule 1: Methylamine dehydrogenase heavy chain

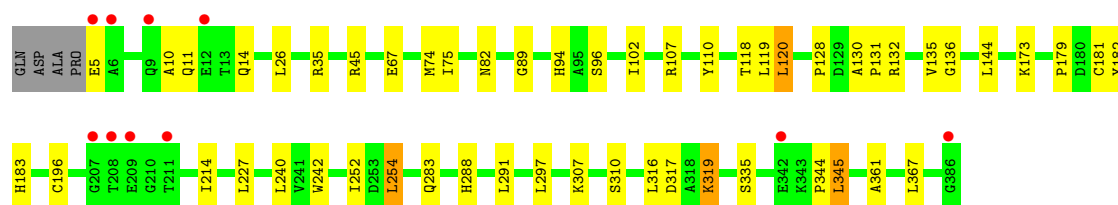
Chain I: 



- Molecule 1: Methylamine dehydrogenase heavy chain

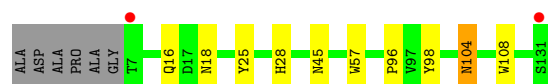
Chain M: 





- Molecule 2: Methylamine dehydrogenase light chain

Chain B:



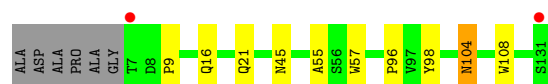
- Molecule 2: Methylamine dehydrogenase light chain

Chain F:



- Molecule 2: Methylamine dehydrogenase light chain

Chain J:



- Molecule 2: Methylamine dehydrogenase light chain

Chain N:



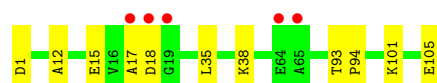
- Molecule 3: Amicyanin

Chain C:



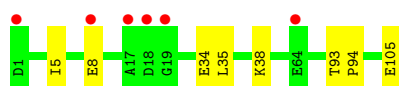
- Molecule 3: Amicyanin

Chain G:



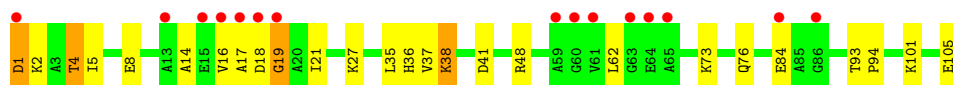
- Molecule 3: Amicyanin

Chain K:



- Molecule 3: Amicyanin

Chain O:



- Molecule 4: Cytochrome c-L

Chain D:



- Molecule 4: Cytochrome c-L

Chain H:



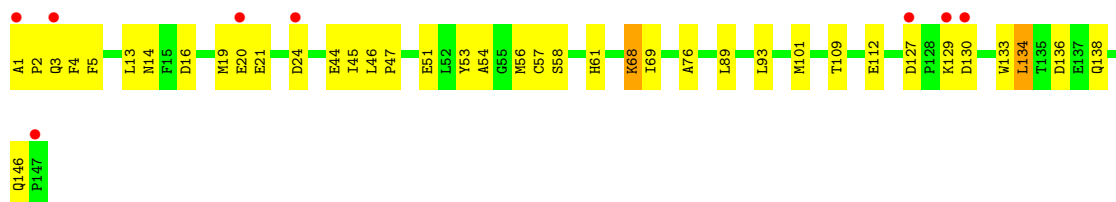
- Molecule 4: Cytochrome c-L

Chain L:



- Molecule 4: Cytochrome c-L

Chain P:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.37Å 188.98Å 128.84Å 90.00° 99.74° 90.00°	Depositor
Resolution (Å)	29.95 – 1.90 29.95 – 1.84	Depositor EDS
% Data completeness (in resolution range)	84.3 (29.95-1.90) 79.8 (29.95-1.84)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 1.84Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.173 , 0.197 0.171 , 0.193	Depositor DCC
$R_{free}$ test set	21022 reflections (8.69%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.8	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 263090 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	24820	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.20 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3668e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: TRQ, HEM, CU, NA

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	0.32	0/3044	0.64	0/4148
1	E	0.31	0/3044	0.63	0/4148
1	I	0.32	0/3044	0.64	0/4148
1	M	0.32	0/3044	0.64	0/4148
2	B	0.32	0/964	0.61	0/1315
2	F	0.32	0/964	0.61	0/1315
2	J	0.33	0/964	0.61	0/1315
2	N	0.31	0/964	0.61	0/1315
3	C	0.32	0/828	0.55	0/1124
3	G	0.32	0/828	0.58	0/1124
3	K	0.33	0/828	0.60	0/1124
3	O	0.30	0/828	0.57	0/1124
4	D	0.33	0/1180	0.63	1/1605 (0.1%)
4	H	0.37	1/1180 (0.1%)	0.65	1/1605 (0.1%)
4	L	0.35	1/1180 (0.1%)	0.63	1/1605 (0.1%)
4	P	0.34	1/1180 (0.1%)	0.61	1/1605 (0.1%)
All	All	0.32	3/24064 (0.0%)	0.62	4/32768 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	61	HIS	CE1-NE2	5.26	1.44	1.32
4	H	61	HIS	CE1-NE2	5.25	1.44	1.32
4	P	61	HIS	CE1-NE2	5.05	1.44	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	61	HIS	ND1-CG-CD2	8.05	120.07	108.80
4	H	61	HIS	ND1-CG-CD2	8.04	120.06	108.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	61	HIS	ND1-CG-CD2	7.98	119.97	108.80
4	D	61	HIS	ND1-CG-CD2	7.97	119.95	108.80

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	A	2967	0	2845	39	0
1	E	2967	0	2845	31	0
1	I	2967	0	2845	39	0
1	M	2967	0	2845	41	0
2	B	956	0	857	11	0
2	F	956	0	857	10	0
2	J	956	0	857	12	0
2	N	956	0	857	12	0
3	C	807	0	794	9	0
3	G	807	0	794	4	0
3	K	807	0	794	6	0
3	O	807	0	794	19	0
4	D	1145	0	1038	17	0
4	H	1145	0	1038	21	0
4	L	1145	0	1038	18	0
4	P	1145	0	1038	23	0
5	C	1	0	0	0	0
5	G	1	0	0	0	0
5	K	1	0	0	0	0
5	O	1	0	0	0	0
6	D	1	0	0	0	0
6	H	1	0	0	0	0
6	L	1	0	0	0	0
6	P	1	0	0	0	0
7	D	43	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	43	0	30	3	0
7	L	43	0	30	1	0
7	P	43	0	30	2	0
8	A	170	0	0	4	0
8	B	54	0	0	0	0
8	C	19	0	0	1	0
8	D	36	0	0	0	0
8	E	160	0	0	1	0
8	F	60	0	0	1	0
8	G	22	0	0	0	0
8	H	40	0	0	1	0
8	I	155	0	0	1	0
8	J	64	0	0	1	0
8	K	27	0	0	0	0
8	L	48	0	0	0	0
8	M	173	0	0	2	0
8	N	55	0	0	0	0
8	O	14	0	0	1	0
8	P	43	0	0	0	0
All	All	24820	0	22256	284	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 6.

The worst 5 of 284 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:J:21:GLN:HE22	1:M:11:GLN:HG3	1.28	0.92
2:J:57:TRQ:HB2	2:J:108:TRP:NE1	1.89	0.88
2:B:57:TRQ:HB2	2:B:108:TRP:NE1	1.87	0.88
2:J:21:GLN:NE2	1:M:11:GLN:HG3	1.89	0.88
2:N:57:TRQ:HB2	2:N:108:TRP:NE1	1.88	0.88

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	A	380/386 (98%)	367 (97%)	12 (3%)	1 (0%)	50	37
1	E	380/386 (98%)	367 (97%)	13 (3%)	0	100	100
1	I	380/386 (98%)	364 (96%)	15 (4%)	1 (0%)	50	37
1	M	380/386 (98%)	366 (96%)	13 (3%)	1 (0%)	50	37
2	B	122/131 (93%)	118 (97%)	4 (3%)	0	100	100
2	F	122/131 (93%)	119 (98%)	3 (2%)	0	100	100
2	J	122/131 (93%)	119 (98%)	3 (2%)	0	100	100
2	N	122/131 (93%)	119 (98%)	3 (2%)	0	100	100
3	C	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
3	G	103/105 (98%)	98 (95%)	4 (4%)	1 (1%)	22	8
3	K	103/105 (98%)	101 (98%)	2 (2%)	0	100	100
3	O	103/105 (98%)	92 (89%)	9 (9%)	2 (2%)	12	2
4	D	145/147 (99%)	142 (98%)	2 (1%)	1 (1%)	30	15
4	H	145/147 (99%)	140 (97%)	4 (3%)	1 (1%)	30	15
4	L	145/147 (99%)	142 (98%)	2 (1%)	1 (1%)	30	15
4	P	145/147 (99%)	142 (98%)	2 (1%)	1 (1%)	30	15
All	All	3000/3076 (98%)	2897 (97%)	93 (3%)	10 (0%)	50	37

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	17	ALA
3	O	18	ASP
4	H	68	LYS
3	O	19	GLY
4	P	68	LYS

### 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	308/311 (99%)	296 (96%)	12 (4%)	43	30
1	E	308/311 (99%)	299 (97%)	9 (3%)	55	44
1	I	308/311 (99%)	296 (96%)	12 (4%)	43	30
1	M	308/311 (99%)	298 (97%)	10 (3%)	51	39
2	B	104/106 (98%)	102 (98%)	2 (2%)	69	63
2	F	104/106 (98%)	102 (98%)	2 (2%)	69	63
2	J	104/106 (98%)	102 (98%)	2 (2%)	69	63
2	N	104/106 (98%)	102 (98%)	2 (2%)	69	63
3	C	85/85 (100%)	83 (98%)	2 (2%)	61	53
3	G	85/85 (100%)	81 (95%)	4 (5%)	36	22
3	K	85/85 (100%)	84 (99%)	1 (1%)	82	80
3	O	85/85 (100%)	79 (93%)	6 (7%)	21	9
4	D	118/118 (100%)	114 (97%)	4 (3%)	49	36
4	H	118/118 (100%)	114 (97%)	4 (3%)	49	36
4	L	118/118 (100%)	114 (97%)	4 (3%)	49	36
4	P	118/118 (100%)	110 (93%)	8 (7%)	22	10
All	All	2460/2480 (99%)	2376 (97%)	84 (3%)	49	36

5 of 84 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	H	134	LEU
1	I	316	LEU
4	P	51	GLU
1	I	26	LEU
1	I	144	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 57 such sidechains are listed below:

Mol	Chain	Res	Type
2	F	45	ASN
1	I	9	GLN
2	N	45	ASN
2	F	104	ASN
4	H	14	ASN



### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	TRQ	B	57	2	17,17,18	5.44	6 (35%)	20,24,26	3.28	4 (20%)
2	TRQ	F	57	2	17,17,18	5.44	6 (35%)	20,24,26	3.22	4 (20%)
2	TRQ	J	57	2	17,17,18	5.50	6 (35%)	20,24,26	3.16	4 (20%)
2	TRQ	N	57	2	17,17,18	5.46	6 (35%)	20,24,26	3.29	4 (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
2	TRQ	B	57	2	-	0/4/19/21	0/0/2/2
2	TRQ	F	57	2	-	0/4/19/21	0/0/2/2
2	TRQ	J	57	2	-	0/4/19/21	0/0/2/2
2	TRQ	N	57	2	-	0/4/19/21	0/0/2/2

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	57	TRQ	O-C	17.79	1.23	1.11
2	B	57	TRQ	O-C	17.64	1.23	1.11
2	F	57	TRQ	O-C	17.42	1.23	1.11
2	N	57	TRQ	O-C	17.36	1.23	1.11
2	N	57	TRQ	CE2-CZ2	-11.87	1.40	1.50

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	57	TRQ	C-CA-N	-12.04	101.81	113.83
2	J	57	TRQ	C-CA-N	-11.89	101.95	113.83
2	B	57	TRQ	C-CA-N	-11.83	102.01	113.83
2	F	57	TRQ	C-CA-N	-11.66	102.18	113.83
2	B	57	TRQ	O7-CZ2-CH2	6.20	126.61	119.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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
7	HEM	D	200	4	49,50,50	3.06	22 (44%)	46,82,82	1.45	5 (10%)
7	HEM	H	200	4	49,50,50	4.21	19 (38%)	46,82,82	1.50	5 (10%)
7	HEM	L	200	4	49,50,50	3.67	22 (44%)	46,82,82	1.49	5 (10%)
7	HEM	P	200	4	49,50,50	3.64	21 (42%)	46,82,82	1.44	5 (10%)

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
7	HEM	D	200	4	-	0/14/114/114	0/0/8/8
7	HEM	H	200	4	-	0/14/114/114	0/0/8/8

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	HEM	L	200	4	-	0/14/114/114	0/0/8/8
7	HEM	P	200	4	-	0/14/114/114	0/0/8/8

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	200	HEM	C3D-C4D	15.99	1.48	1.44
7	L	200	HEM	C2B-C1B	15.44	1.48	1.44
7	P	200	HEM	C3D-C4D	15.25	1.48	1.44
7	H	200	HEM	C2D-C1D	13.39	1.47	1.44
7	H	200	HEM	C2B-C1B	12.54	1.47	1.44

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	200	HEM	C3B-C4B-NB	-5.50	110.06	114.00
7	P	200	HEM	C3B-C4B-NB	-5.29	110.21	114.00
7	H	200	HEM	C3B-C4B-NB	-5.12	110.34	114.00
7	L	200	HEM	CBD-CAD-C3D	-5.08	103.27	114.37
7	L	200	HEM	C3B-C4B-NB	-5.02	110.41	114.00

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	A	382/386 (98%)	-0.27	10 (2%)	53	55	21, 29, 49, 87	0
1	E	382/386 (98%)	-0.23	12 (3%)	47	48	21, 30, 51, 89	0
1	I	382/386 (98%)	-0.25	10 (2%)	53	55	21, 29, 53, 88	0
1	M	382/386 (98%)	-0.26	10 (2%)	53	55	20, 29, 50, 89	0
2	B	125/131 (95%)	-0.23	2 (1%)	68	70	22, 28, 48, 86	0
2	F	125/131 (95%)	-0.19	2 (1%)	68	70	20, 26, 46, 86	0
2	J	125/131 (95%)	-0.19	2 (1%)	68	70	19, 24, 45, 86	0
2	N	125/131 (95%)	-0.21	5 (4%)	36	37	22, 28, 49, 85	0
3	C	105/105 (100%)	0.33	9 (8%)	11	10	28, 42, 69, 81	0
3	G	105/105 (100%)	-0.01	5 (4%)	29	30	25, 38, 60, 81	0
3	K	105/105 (100%)	-0.16	6 (5%)	23	23	24, 35, 57, 77	0
3	O	105/105 (100%)	0.75	15 (14%)	3	3	32, 51, 76, 88	0
4	D	147/147 (100%)	-0.15	6 (4%)	35	36	24, 35, 62, 76	0
4	H	147/147 (100%)	0.03	7 (4%)	29	30	25, 38, 68, 78	0
4	L	147/147 (100%)	-0.18	8 (5%)	25	25	24, 33, 59, 74	0
4	P	147/147 (100%)	0.09	8 (5%)	25	25	25, 38, 68, 79	0
All	All	3036/3076 (98%)	-0.14	117 (3%)	38	38	19, 31, 61, 89	0

The worst 5 of 117 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	131	SER	13.6
2	B	131	SER	11.8
2	F	131	SER	11.7
1	E	5	GLU	10.7
2	N	131	SER	8.7

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

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
2	TRQ	B	57	16/17	0.09	-0.22	23,25,27,29	0
2	TRQ	F	57	16/17	0.10	-0.31	20,23,26,27	0
2	TRQ	J	57	16/17	0.10	-0.47	20,23,26,27	0
2	TRQ	N	57	16/17	0.09	-0.49	21,26,29,29	0

## 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
6	NA	L	601	1/1	0.10	4.29	23,23,23,23	0
6	NA	H	603	1/1	0.12	3.16	27,27,27,27	0
6	NA	P	602	1/1	0.11	1.72	28,28,28,28	0
7	HEM	P	200	43/43	0.10	0.35	23,28,31,34	0
7	HEM	D	200	43/43	0.10	0.18	21,25,29,34	0
7	HEM	L	200	43/43	0.08	-0.19	20,24,29,33	0
7	HEM	H	200	43/43	0.09	-0.33	25,29,34,36	0
5	CU	K	107	1/1	0.09	-1.18	29,29,29,29	0
5	CU	G	107	1/1	0.06	-2.40	32,32,32,32	0
6	NA	D	604	1/1	0.03	-2.88	32,32,32,32	0
5	CU	O	107	1/1	0.06	-3.05	39,39,39,39	0
5	CU	C	107	1/1	0.05	-3.70	33,33,33,33	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.