



# Full wwPDB X-ray Structure Validation Report

Apr 8, 2014 – 02:45 PM EDT

PDB ID : 4LMH  
Title : Crystal structure of the outer membrane decaheme cytochrome OmcA  
Authors : Edwards, M.J.; Baiden, N.; Clarke, T.A.  
Deposited on : 2013-07-10  
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>

---

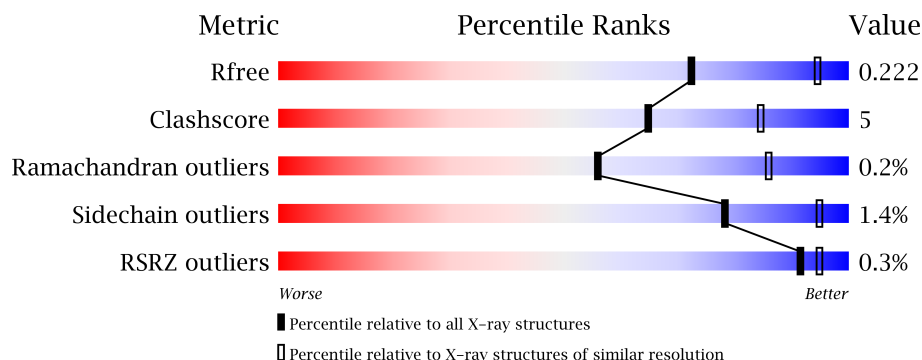
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : **FAILED**  
Xtriage (Phenix) : dev-1439  
EDS : stable22978  
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) : stable22978

# 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	A	760	
1	B	760	
1	C	760	
1	D	760	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	CA	A	812	-	X
4	DMS	A	813	-	X
4	DMS	A	814	-	X
4	DMS	A	815	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
4	DMS	B	914	-	X
4	DMS	B	915	-	X
4	DMS	C	814	-	X
4	DMS	C	815	-	X
4	DMS	C	816	-	X
4	DMS	D	814	-	X
4	DMS	D	815	-	X
4	DMS	D	816	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24443 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 Extracellular iron oxide respiratory system surface decaheme cytochrome c component OmcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	693	Total	C	N	O	S	0	0	0
			5222	3229	916	1047	30			
1	B	694	Total	C	N	O	S	0	0	0
			5231	3235	918	1048	30			
1	C	692	Total	C	N	O	S	0	0	0
			5215	3224	915	1046	30			
1	D	695	Total	C	N	O	S	0	0	0
			5235	3237	919	1049	30			

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	MET	-	INITIATING METHIONINE	UNP Q8EG33
A	7	LYS	-	EXPRESSION TAG	UNP Q8EG33
A	8	PHE	-	EXPRESSION TAG	UNP Q8EG33
A	9	LYS	-	EXPRESSION TAG	UNP Q8EG33
A	10	LEU	-	EXPRESSION TAG	UNP Q8EG33
A	11	ASN	-	EXPRESSION TAG	UNP Q8EG33
A	12	LEU	-	EXPRESSION TAG	UNP Q8EG33
A	13	ILE	-	EXPRESSION TAG	UNP Q8EG33
A	14	THR	-	EXPRESSION TAG	UNP Q8EG33
A	15	LEU	-	EXPRESSION TAG	UNP Q8EG33
A	16	ALA	-	EXPRESSION TAG	UNP Q8EG33
A	17	LEU	-	EXPRESSION TAG	UNP Q8EG33
A	18	LEU	-	EXPRESSION TAG	UNP Q8EG33
A	19	ALA	-	EXPRESSION TAG	UNP Q8EG33
A	20	ASN	-	EXPRESSION TAG	UNP Q8EG33
A	21	THR	-	EXPRESSION TAG	UNP Q8EG33
A	22	GLY	-	EXPRESSION TAG	UNP Q8EG33
A	23	LEU	-	EXPRESSION TAG	UNP Q8EG33
A	24	ALA	-	EXPRESSION TAG	UNP Q8EG33
A	25	VAL	-	EXPRESSION TAG	UNP Q8EG33

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ALA	-	EXPRESSION TAG	UNP Q8EG33
A	27	ALA	-	EXPRESSION TAG	UNP Q8EG33
A	736	LYS	-	EXPRESSION TAG	UNP Q8EG33
A	737	GLY	-	EXPRESSION TAG	UNP Q8EG33
A	738	GLU	-	EXPRESSION TAG	UNP Q8EG33
A	739	LEU	-	EXPRESSION TAG	UNP Q8EG33
A	740	LYS	-	EXPRESSION TAG	UNP Q8EG33
A	741	LEU	-	EXPRESSION TAG	UNP Q8EG33
A	742	GLU	-	EXPRESSION TAG	UNP Q8EG33
A	743	GLY	-	EXPRESSION TAG	UNP Q8EG33
A	744	LYS	-	EXPRESSION TAG	UNP Q8EG33
A	745	PRO	-	EXPRESSION TAG	UNP Q8EG33
A	746	ILE	-	EXPRESSION TAG	UNP Q8EG33
A	747	PRO	-	EXPRESSION TAG	UNP Q8EG33
A	748	ASN	-	EXPRESSION TAG	UNP Q8EG33
A	749	PRO	-	EXPRESSION TAG	UNP Q8EG33
A	750	LEU	-	EXPRESSION TAG	UNP Q8EG33
A	751	LEU	-	EXPRESSION TAG	UNP Q8EG33
A	752	GLY	-	EXPRESSION TAG	UNP Q8EG33
A	753	LEU	-	EXPRESSION TAG	UNP Q8EG33
A	754	ASP	-	EXPRESSION TAG	UNP Q8EG33
A	755	SER	-	EXPRESSION TAG	UNP Q8EG33
A	756	THR	-	EXPRESSION TAG	UNP Q8EG33
A	757	ARG	-	EXPRESSION TAG	UNP Q8EG33
A	758	THR	-	EXPRESSION TAG	UNP Q8EG33
A	759	GLY	-	EXPRESSION TAG	UNP Q8EG33
A	760	HIS	-	EXPRESSION TAG	UNP Q8EG33
A	761	HIS	-	EXPRESSION TAG	UNP Q8EG33
A	762	HIS	-	EXPRESSION TAG	UNP Q8EG33
A	763	HIS	-	EXPRESSION TAG	UNP Q8EG33
A	764	HIS	-	EXPRESSION TAG	UNP Q8EG33
A	765	HIS	-	EXPRESSION TAG	UNP Q8EG33
B	6	MET	-	INITIATING METHIONINE	UNP Q8EG33
B	7	LYS	-	EXPRESSION TAG	UNP Q8EG33
B	8	PHE	-	EXPRESSION TAG	UNP Q8EG33
B	9	LYS	-	EXPRESSION TAG	UNP Q8EG33
B	10	LEU	-	EXPRESSION TAG	UNP Q8EG33
B	11	ASN	-	EXPRESSION TAG	UNP Q8EG33
B	12	LEU	-	EXPRESSION TAG	UNP Q8EG33
B	13	ILE	-	EXPRESSION TAG	UNP Q8EG33
B	14	THR	-	EXPRESSION TAG	UNP Q8EG33
B	15	LEU	-	EXPRESSION TAG	UNP Q8EG33

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	16	ALA	-	EXPRESSION TAG	UNP Q8EG33
B	17	LEU	-	EXPRESSION TAG	UNP Q8EG33
B	18	LEU	-	EXPRESSION TAG	UNP Q8EG33
B	19	ALA	-	EXPRESSION TAG	UNP Q8EG33
B	20	ASN	-	EXPRESSION TAG	UNP Q8EG33
B	21	THR	-	EXPRESSION TAG	UNP Q8EG33
B	22	GLY	-	EXPRESSION TAG	UNP Q8EG33
B	23	LEU	-	EXPRESSION TAG	UNP Q8EG33
B	24	ALA	-	EXPRESSION TAG	UNP Q8EG33
B	25	VAL	-	EXPRESSION TAG	UNP Q8EG33
B	26	ALA	-	EXPRESSION TAG	UNP Q8EG33
B	27	ALA	-	EXPRESSION TAG	UNP Q8EG33
B	736	LYS	-	EXPRESSION TAG	UNP Q8EG33
B	737	GLY	-	EXPRESSION TAG	UNP Q8EG33
B	738	GLU	-	EXPRESSION TAG	UNP Q8EG33
B	739	LEU	-	EXPRESSION TAG	UNP Q8EG33
B	740	LYS	-	EXPRESSION TAG	UNP Q8EG33
B	741	LEU	-	EXPRESSION TAG	UNP Q8EG33
B	742	GLU	-	EXPRESSION TAG	UNP Q8EG33
B	743	GLY	-	EXPRESSION TAG	UNP Q8EG33
B	744	LYS	-	EXPRESSION TAG	UNP Q8EG33
B	745	PRO	-	EXPRESSION TAG	UNP Q8EG33
B	746	ILE	-	EXPRESSION TAG	UNP Q8EG33
B	747	PRO	-	EXPRESSION TAG	UNP Q8EG33
B	748	ASN	-	EXPRESSION TAG	UNP Q8EG33
B	749	PRO	-	EXPRESSION TAG	UNP Q8EG33
B	750	LEU	-	EXPRESSION TAG	UNP Q8EG33
B	751	LEU	-	EXPRESSION TAG	UNP Q8EG33
B	752	GLY	-	EXPRESSION TAG	UNP Q8EG33
B	753	LEU	-	EXPRESSION TAG	UNP Q8EG33
B	754	ASP	-	EXPRESSION TAG	UNP Q8EG33
B	755	SER	-	EXPRESSION TAG	UNP Q8EG33
B	756	THR	-	EXPRESSION TAG	UNP Q8EG33
B	757	ARG	-	EXPRESSION TAG	UNP Q8EG33
B	758	THR	-	EXPRESSION TAG	UNP Q8EG33
B	759	GLY	-	EXPRESSION TAG	UNP Q8EG33
B	760	HIS	-	EXPRESSION TAG	UNP Q8EG33
B	761	HIS	-	EXPRESSION TAG	UNP Q8EG33
B	762	HIS	-	EXPRESSION TAG	UNP Q8EG33
B	763	HIS	-	EXPRESSION TAG	UNP Q8EG33
B	764	HIS	-	EXPRESSION TAG	UNP Q8EG33
B	765	HIS	-	EXPRESSION TAG	UNP Q8EG33

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	6	MET	-	INITIATING METHIONINE	UNP Q8EG33
C	7	LYS	-	EXPRESSION TAG	UNP Q8EG33
C	8	PHE	-	EXPRESSION TAG	UNP Q8EG33
C	9	LYS	-	EXPRESSION TAG	UNP Q8EG33
C	10	LEU	-	EXPRESSION TAG	UNP Q8EG33
C	11	ASN	-	EXPRESSION TAG	UNP Q8EG33
C	12	LEU	-	EXPRESSION TAG	UNP Q8EG33
C	13	ILE	-	EXPRESSION TAG	UNP Q8EG33
C	14	THR	-	EXPRESSION TAG	UNP Q8EG33
C	15	LEU	-	EXPRESSION TAG	UNP Q8EG33
C	16	ALA	-	EXPRESSION TAG	UNP Q8EG33
C	17	LEU	-	EXPRESSION TAG	UNP Q8EG33
C	18	LEU	-	EXPRESSION TAG	UNP Q8EG33
C	19	ALA	-	EXPRESSION TAG	UNP Q8EG33
C	20	ASN	-	EXPRESSION TAG	UNP Q8EG33
C	21	THR	-	EXPRESSION TAG	UNP Q8EG33
C	22	GLY	-	EXPRESSION TAG	UNP Q8EG33
C	23	LEU	-	EXPRESSION TAG	UNP Q8EG33
C	24	ALA	-	EXPRESSION TAG	UNP Q8EG33
C	25	VAL	-	EXPRESSION TAG	UNP Q8EG33
C	26	ALA	-	EXPRESSION TAG	UNP Q8EG33
C	27	ALA	-	EXPRESSION TAG	UNP Q8EG33
C	736	LYS	-	EXPRESSION TAG	UNP Q8EG33
C	737	GLY	-	EXPRESSION TAG	UNP Q8EG33
C	738	GLU	-	EXPRESSION TAG	UNP Q8EG33
C	739	LEU	-	EXPRESSION TAG	UNP Q8EG33
C	740	LYS	-	EXPRESSION TAG	UNP Q8EG33
C	741	LEU	-	EXPRESSION TAG	UNP Q8EG33
C	742	GLU	-	EXPRESSION TAG	UNP Q8EG33
C	743	GLY	-	EXPRESSION TAG	UNP Q8EG33
C	744	LYS	-	EXPRESSION TAG	UNP Q8EG33
C	745	PRO	-	EXPRESSION TAG	UNP Q8EG33
C	746	ILE	-	EXPRESSION TAG	UNP Q8EG33
C	747	PRO	-	EXPRESSION TAG	UNP Q8EG33
C	748	ASN	-	EXPRESSION TAG	UNP Q8EG33
C	749	PRO	-	EXPRESSION TAG	UNP Q8EG33
C	750	LEU	-	EXPRESSION TAG	UNP Q8EG33
C	751	LEU	-	EXPRESSION TAG	UNP Q8EG33
C	752	GLY	-	EXPRESSION TAG	UNP Q8EG33
C	753	LEU	-	EXPRESSION TAG	UNP Q8EG33
C	754	ASP	-	EXPRESSION TAG	UNP Q8EG33
C	755	SER	-	EXPRESSION TAG	UNP Q8EG33

*Continued on next page...*



*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	756	THR	-	EXPRESSION TAG	UNP Q8EG33
C	757	ARG	-	EXPRESSION TAG	UNP Q8EG33
C	758	THR	-	EXPRESSION TAG	UNP Q8EG33
C	759	GLY	-	EXPRESSION TAG	UNP Q8EG33
C	760	HIS	-	EXPRESSION TAG	UNP Q8EG33
C	761	HIS	-	EXPRESSION TAG	UNP Q8EG33
C	762	HIS	-	EXPRESSION TAG	UNP Q8EG33
C	763	HIS	-	EXPRESSION TAG	UNP Q8EG33
C	764	HIS	-	EXPRESSION TAG	UNP Q8EG33
C	765	HIS	-	EXPRESSION TAG	UNP Q8EG33
D	6	MET	-	INITIATING METHIONINE	UNP Q8EG33
D	7	LYS	-	EXPRESSION TAG	UNP Q8EG33
D	8	PHE	-	EXPRESSION TAG	UNP Q8EG33
D	9	LYS	-	EXPRESSION TAG	UNP Q8EG33
D	10	LEU	-	EXPRESSION TAG	UNP Q8EG33
D	11	ASN	-	EXPRESSION TAG	UNP Q8EG33
D	12	LEU	-	EXPRESSION TAG	UNP Q8EG33
D	13	ILE	-	EXPRESSION TAG	UNP Q8EG33
D	14	THR	-	EXPRESSION TAG	UNP Q8EG33
D	15	LEU	-	EXPRESSION TAG	UNP Q8EG33
D	16	ALA	-	EXPRESSION TAG	UNP Q8EG33
D	17	LEU	-	EXPRESSION TAG	UNP Q8EG33
D	18	LEU	-	EXPRESSION TAG	UNP Q8EG33
D	19	ALA	-	EXPRESSION TAG	UNP Q8EG33
D	20	ASN	-	EXPRESSION TAG	UNP Q8EG33
D	21	THR	-	EXPRESSION TAG	UNP Q8EG33
D	22	GLY	-	EXPRESSION TAG	UNP Q8EG33
D	23	LEU	-	EXPRESSION TAG	UNP Q8EG33
D	24	ALA	-	EXPRESSION TAG	UNP Q8EG33
D	25	VAL	-	EXPRESSION TAG	UNP Q8EG33
D	26	ALA	-	EXPRESSION TAG	UNP Q8EG33
D	27	ALA	-	EXPRESSION TAG	UNP Q8EG33
D	736	LYS	-	EXPRESSION TAG	UNP Q8EG33
D	737	GLY	-	EXPRESSION TAG	UNP Q8EG33
D	738	GLU	-	EXPRESSION TAG	UNP Q8EG33
D	739	LEU	-	EXPRESSION TAG	UNP Q8EG33
D	740	LYS	-	EXPRESSION TAG	UNP Q8EG33
D	741	LEU	-	EXPRESSION TAG	UNP Q8EG33
D	742	GLU	-	EXPRESSION TAG	UNP Q8EG33
D	743	GLY	-	EXPRESSION TAG	UNP Q8EG33
D	744	LYS	-	EXPRESSION TAG	UNP Q8EG33
D	745	PRO	-	EXPRESSION TAG	UNP Q8EG33

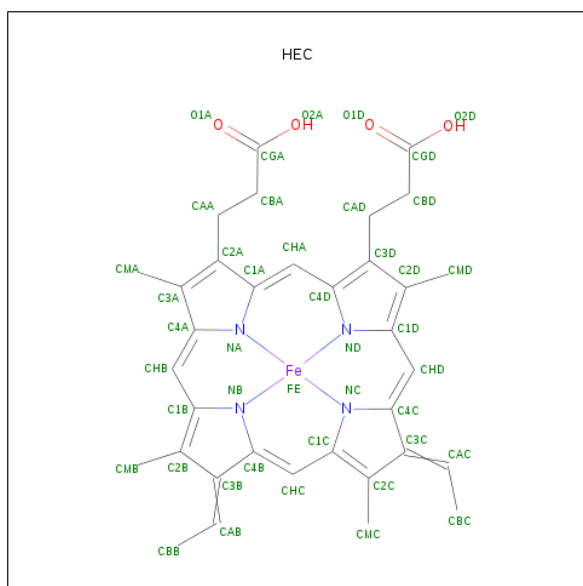
*Continued on next page...*



Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	746	ILE	-	EXPRESSION TAG	UNP Q8EG33
D	747	PRO	-	EXPRESSION TAG	UNP Q8EG33
D	748	ASN	-	EXPRESSION TAG	UNP Q8EG33
D	749	PRO	-	EXPRESSION TAG	UNP Q8EG33
D	750	LEU	-	EXPRESSION TAG	UNP Q8EG33
D	751	LEU	-	EXPRESSION TAG	UNP Q8EG33
D	752	GLY	-	EXPRESSION TAG	UNP Q8EG33
D	753	LEU	-	EXPRESSION TAG	UNP Q8EG33
D	754	ASP	-	EXPRESSION TAG	UNP Q8EG33
D	755	SER	-	EXPRESSION TAG	UNP Q8EG33
D	756	THR	-	EXPRESSION TAG	UNP Q8EG33
D	757	ARG	-	EXPRESSION TAG	UNP Q8EG33
D	758	THR	-	EXPRESSION TAG	UNP Q8EG33
D	759	GLY	-	EXPRESSION TAG	UNP Q8EG33
D	760	HIS	-	EXPRESSION TAG	UNP Q8EG33
D	761	HIS	-	EXPRESSION TAG	UNP Q8EG33
D	762	HIS	-	EXPRESSION TAG	UNP Q8EG33
D	763	HIS	-	EXPRESSION TAG	UNP Q8EG33
D	764	HIS	-	EXPRESSION TAG	UNP Q8EG33
D	765	HIS	-	EXPRESSION TAG	UNP Q8EG33

- Molecule 2 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



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

Continued on next page...

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

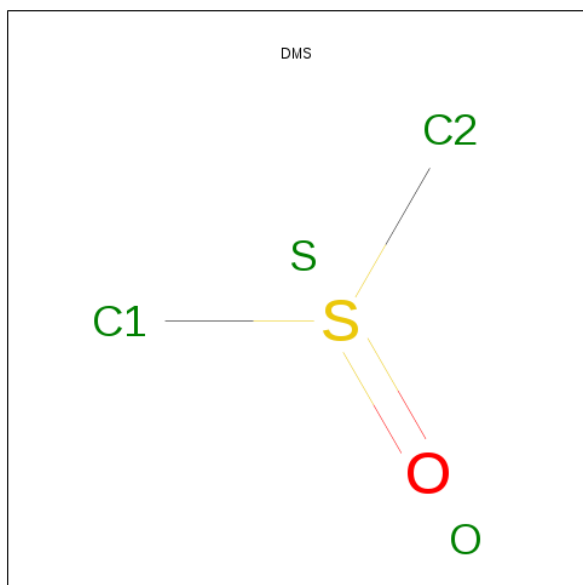
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Ca 2	0	0
3	D	2	Total 2	Ca 2	0	0
3	C	2	Total 2	Ca 2	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	397	Total O 397 397	0	0
5	B	420	Total O 420 420	0	0
5	C	380	Total O 380 380	0	0
5	D	551	Total O 551 551	0	0







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.64Å 245.38Å 135.63Å 90.00° 97.89° 90.00°	Depositor
Resolution (Å)	50.97 – 2.70 52.54 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.4 (50.97-2.70) 98.4 (52.54-2.70)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.193 , 0.230 0.184 , 0.222	Depositor DCC
$R_{free}$ test set	8077 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.2	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 18.2	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 161255 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	24443	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.51% 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: CA, DMS, 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	A	0.27	0/5337	0.44	0/7254
1	B	0.27	0/5346	0.44	0/7265
1	C	0.27	0/5330	0.43	0/7244
1	D	0.28	0/5350	0.44	0/7270
All	All	0.27	0/21363	0.44	0/29033

There are no bond length outliers.

There are no bond angle outliers.

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	5222	0	4957	50	0
1	B	5231	0	4971	59	0
1	C	5215	0	4948	48	0
1	D	5235	0	4974	47	0
2	A	430	0	301	24	0
2	B	430	0	302	35	0
2	C	430	0	301	17	0
2	D	430	0	302	28	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	16	0	24	3	0
4	B	16	0	24	1	0
4	C	16	0	24	2	0
4	D	16	0	24	1	0
5	A	397	0	0	5	0
5	B	420	0	0	2	0
5	C	380	0	0	2	0
5	D	551	0	0	0	0
All	All	24443	0	21152	222	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 5.

All (222) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:253:CYS:SG	2:D:802:HEC:HAC	1.35	1.63
1:D:350:CYS:SG	2:D:804:HEC:HAC	1.53	1.47
1:C:350:CYS:SG	2:C:804:HEC:HAC	1.56	1.44
1:A:350:CYS:SG	2:A:804:HEC:HAC	1.64	1.34
1:B:586:CYS:SG	2:B:908:HEC:HAC	1.70	1.25
1:A:350:CYS:HG	2:A:804:HEC:HAC	0.95	1.02
1:D:569:CYS:SG	2:D:806:HEC:C3C	2.69	0.80
1:C:350:CYS:SG	2:C:804:HEC:C3C	2.70	0.80
1:D:350:CYS:SG	2:D:804:HEC:C3C	2.69	0.79
1:B:569:CYS:SG	2:B:907:HEC:C3C	2.72	0.77
1:D:239:LEU:HD13	2:D:802:HEC:HMB2	1.65	0.77
1:D:586:CYS:SG	2:D:807:HEC:C3C	2.73	0.76
1:A:350:CYS:SG	2:A:804:HEC:C3C	2.73	0.75
1:A:576:HIS:HE1	2:A:807:HEC:ND	1.83	0.75
1:C:239:LEU:HD13	2:C:802:HEC:HMB2	1.69	0.74
1:B:586:CYS:SG	2:B:908:HEC:C3C	2.76	0.73
1:D:85:THR:HG23	1:D:87:ASP:H	1.53	0.72
1:A:407:LYS:HD3	1:A:412:THR:HG21	1.73	0.71
1:B:239:LEU:HD13	2:B:903:HEC:HMB2	1.71	0.71
1:B:576:HIS:HE1	2:B:908:HEC:ND	1.88	0.71
1:D:253:CYS:SG	2:D:802:HEC:C3C	2.81	0.69
1:B:724:HIS:HA	1:B:728:GLN:HG2	1.75	0.68
1:A:557:ARG:NH2	2:A:808:HEC:O1D	2.28	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:239:LEU:HD13	2:A:802:HEC:HMB2	1.76	0.67
1:B:557:ARG:NH2	2:B:909:HEC:O1D	2.29	0.65
2:D:810:HEC:HBD2	2:D:810:HEC:HHA	1.78	0.65
1:A:661:LEU:HD11	1:A:671:VAL:HG13	1.80	0.64
1:B:43:VAL:N	5:B:1357:HOH:O	2.31	0.64
1:A:697:ILE:HG22	1:A:702:GLY:HA3	1.79	0.64
1:B:73:LEU:HD11	1:B:84:LEU:HD22	1.84	0.60
2:B:904:HEC:HBB2	2:B:905:HEC:C4C	2.32	0.60
1:A:719:SER:O	1:A:722:THR:OG1	2.21	0.59
1:C:44:GLY:N	5:C:1113:HOH:O	2.34	0.59
1:A:652:LEU:HD23	1:A:720:CYS:HB2	1.84	0.58
1:B:377:THR:OG1	1:B:378:GLY:N	2.36	0.58
1:D:149:ASN:OD1	1:D:150:LYS:NZ	2.36	0.58
1:B:600:PRO:HB2	1:B:665:ILE:HB	1.86	0.57
1:A:491:LEU:HD21	1:A:493:LEU:HD13	1.87	0.57
1:A:244:ARG:NH2	2:A:802:HEC:HBC2	2.20	0.57
1:C:73:LEU:HD11	1:C:84:LEU:HD22	1.85	0.56
1:B:382:LYS:NZ	1:B:520:GLU:O	2.39	0.56
1:C:404:ILE:HD12	1:C:550:THR:HG21	1.87	0.56
1:D:557:ARG:NH2	2:D:808:HEC:O1D	2.39	0.55
1:D:660:TRP:CD1	1:D:679:GLY:HA3	2.41	0.55
1:D:89:ASP:OD2	1:D:243:ARG:NH1	2.40	0.55
1:D:244:ARG:NH2	2:D:802:HEC:HBC2	2.21	0.55
1:C:351:HIS:HB3	1:C:355:PRO:HB3	1.89	0.55
1:C:312:HIS:N	5:C:973:HOH:O	2.30	0.54
1:B:371:THR:OG1	1:B:372:LYS:N	2.41	0.53
1:B:384:HIS:CE1	2:B:904:HEC:HBB3	2.43	0.53
1:B:312:HIS:HB2	4:B:915:DMS:H22	1.91	0.53
1:C:59:ASN:OD1	1:C:70:ASN:ND2	2.42	0.53
1:B:313:TYR:CE1	2:B:902:HEC:HBC2	2.43	0.53
1:C:711:ASP:OD1	1:C:715:ARG:NH1	2.40	0.52
1:D:403:ASN:ND2	1:D:414:ASP:OD2	2.35	0.52
2:C:806:HEC:HMA2	2:C:807:HEC:HMA1	1.92	0.52
1:C:733:HIS:CD2	2:C:809:HEC:ND	2.77	0.52
1:D:576:HIS:HE1	2:D:807:HEC:ND	2.05	0.51
1:A:198:GLN:OE1	1:A:198:GLN:N	2.44	0.51
1:A:244:ARG:CZ	2:A:802:HEC:HBC2	2.40	0.51
1:B:661:LEU:HD11	1:B:671:VAL:HG13	1.91	0.51
2:A:802:HEC:HBC3	2:A:802:HEC:HMC1	1.92	0.51
1:C:244:ARG:NH2	2:C:802:HEC:HBC2	2.26	0.51
1:D:253:CYS:CB	2:D:802:HEC:CAC	2.89	0.51
1:B:278:LYS:HE2	2:B:905:HEC:HMD3	1.92	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:577:TYR:CE2	2:A:807:HEC:HBC2	2.47	0.50
1:D:491:LEU:HD21	1:D:493:LEU:HD13	1.93	0.50
1:B:444:SER:OG	1:B:463:ARG:NH2	2.44	0.50
1:B:244:ARG:NH2	2:B:903:HEC:HBC2	2.27	0.50
1:C:244:ARG:CZ	2:C:802:HEC:HBC2	2.42	0.50
1:B:437:THR:HG23	1:B:577:TYR:CZ	2.47	0.50
1:B:557:ARG:HH22	2:B:909:HEC:CGD	2.25	0.50
1:D:449:LYS:O	1:D:557:ARG:HD2	2.12	0.49
1:D:736:LYS:HG2	1:D:737:GLY:H	1.77	0.49
2:B:911:HEC:HHA	2:B:911:HEC:HBD2	1.93	0.49
1:C:509:ALA:HA	1:C:535:TYR:HA	1.92	0.49
1:C:724:HIS:HA	1:C:728:GLN:HG2	1.93	0.49
1:C:285:PHE:O	1:C:354:LYS:HD3	2.12	0.49
1:C:661:LEU:HD11	1:C:671:VAL:HG13	1.94	0.49
1:A:262:GLU:HB2	1:A:299:ILE:HB	1.94	0.49
2:D:802:HEC:HMC1	2:D:802:HEC:HBC3	1.93	0.49
1:B:660:TRP:CD1	1:B:679:GLY:HA3	2.48	0.49
1:C:239:LEU:HD22	2:C:802:HEC:CHB	2.43	0.49
1:B:317:PRO:HG3	1:B:391:TYR:CE2	2.48	0.49
1:D:565:LYS:O	2:D:806:HEC:HMC3	2.14	0.48
1:C:198:GLN:OE1	1:C:198:GLN:N	2.42	0.48
1:A:304:LYS:NZ	1:A:306:ILE:HD11	2.28	0.48
1:B:442:TYR:CZ	2:B:908:HEC:HBC1	2.49	0.48
2:B:909:HEC:HBB2	2:B:910:HEC:HBC2	1.95	0.48
1:D:73:LEU:HD11	1:D:84:LEU:HD22	1.95	0.48
1:B:577:TYR:CE2	2:B:908:HEC:HBC2	2.49	0.48
1:D:355:PRO:HG3	2:D:805:HEC:C1B	2.44	0.48
1:D:661:LEU:HD11	1:D:671:VAL:HG13	1.95	0.48
1:D:384:HIS:CE1	2:D:803:HEC:HBB3	2.48	0.48
1:A:53:LEU:HD21	1:A:73:LEU:HD22	1.96	0.48
1:B:510:THR:HB	5:B:1143:HOH:O	2.14	0.48
1:D:244:ARG:CZ	2:D:802:HEC:HBC2	2.44	0.48
1:B:577:TYR:CZ	2:B:908:HEC:HBC2	2.49	0.47
1:A:510:THR:HB	5:A:904:HOH:O	2.13	0.47
2:A:807:HEC:HHA	2:A:807:HEC:HBA1	1.97	0.47
1:C:620:LEU:HD13	2:C:801:HEC:HBD1	1.95	0.47
1:A:630:VAL:HG13	2:A:806:HEC:HBC2	1.97	0.47
1:A:557:ARG:HH22	2:A:808:HEC:CGD	2.28	0.47
1:D:442:TYR:CZ	2:D:807:HEC:HBC1	2.50	0.47
1:A:696:HIS:HD2	2:A:810:HEC:NA	2.09	0.47
1:C:630:VAL:HG13	2:C:806:HEC:HBC2	1.97	0.47
1:B:625:VAL:HG22	2:B:902:HEC:CGD	2.45	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:576:HIS:HE1	2:B:908:HEC:C4D	2.27	0.47
1:A:313:TYR:CE1	2:A:801:HEC:HBC2	2.50	0.46
2:A:804:HEC:O1D	5:A:1270:HOH:O	2.21	0.46
2:C:802:HEC:HBC3	2:C:802:HEC:HMC1	1.97	0.46
1:A:313:TYR:CE2	1:A:315:GLN:HB2	2.51	0.46
1:A:498:THR:OG1	5:A:1266:HOH:O	2.21	0.46
1:A:384:HIS:CE1	2:A:803:HEC:HBB3	2.51	0.46
1:B:630:VAL:HG13	2:B:907:HEC:HBC2	1.96	0.46
1:A:693:ALA:O	1:A:697:ILE:HG12	2.16	0.46
1:B:565:LYS:O	2:B:907:HEC:HMC3	2.15	0.46
1:C:80:ALA:HB1	1:C:161:GLY:HA3	1.98	0.46
1:A:404:ILE:HD12	1:A:550:THR:HG21	1.99	0.45
1:A:376:GLY:HA3	1:A:517:TYR:CE2	2.52	0.45
1:B:657:GLU:H	1:B:657:GLU:CD	2.20	0.45
1:C:577:TYR:CE2	2:C:807:HEC:HBC2	2.51	0.45
1:D:240:HIS:O	1:D:243:ARG:HG2	2.17	0.45
1:B:244:ARG:CZ	2:B:903:HEC:HBC2	2.47	0.45
1:D:84:LEU:HB3	1:D:163:TYR:CE2	2.51	0.45
1:B:244:ARG:HG2	2:B:903:HEC:HMC2	1.98	0.45
1:C:118:TYR:CE1	1:C:171:VAL:HG13	2.51	0.45
1:D:711:ASP:OD2	1:D:715:ARG:NH1	2.50	0.45
1:D:733:HIS:CD2	2:D:809:HEC:ND	2.84	0.45
1:A:646:VAL:HG22	5:A:1267:HOH:O	2.17	0.45
1:C:313:TYR:CE1	2:C:801:HEC:HBC2	2.52	0.45
1:D:193:GLU:OE1	1:D:243:ARG:NH2	2.49	0.45
1:A:497:LEU:O	1:A:545:TRP:HB3	2.17	0.44
1:A:576:HIS:HE1	2:A:807:HEC:C4D	2.30	0.44
2:B:904:HEC:HBB3	2:B:904:HEC:HMB1	1.98	0.44
1:A:355:PRO:HG3	2:A:805:HEC:C1B	2.47	0.44
1:B:298:ILE:HG21	2:B:903:HEC:HAA1	1.99	0.44
1:C:396:GLY:HA3	1:C:420:ASN:HB3	1.99	0.44
1:B:179:LYS:NZ	1:B:181:THR:OG1	2.49	0.44
1:B:314:PRO:HB3	2:B:907:HEC:C2D	2.47	0.44
1:C:430:ILE:HG21	1:C:467:LEU:HD12	1.99	0.44
1:B:315:GLN:HG2	1:B:569:CYS:O	2.17	0.44
2:D:810:HEC:CHA	2:D:810:HEC:HBD2	2.47	0.44
1:A:398:LYS:HD2	1:A:418:LEU:HB2	1.99	0.44
1:A:565:LYS:O	2:A:806:HEC:HMC3	2.16	0.44
1:B:53:LEU:HD11	1:B:73:LEU:HB3	2.00	0.44
1:C:338:PHE:CZ	1:C:339:LYS:HE3	2.53	0.44
1:A:674:VAL:HG13	1:A:704:LEU:HD23	2.00	0.44
1:C:279:GLY:HA2	1:C:308:TYR:O	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:416:GLN:NE2	1:A:479:THR:O	2.51	0.43
1:D:99:PRO:HG3	1:D:113:TYR:CE1	2.53	0.43
1:D:420:ASN:OD1	1:D:420:ASN:N	2.51	0.43
1:A:463:ARG:NH1	5:A:1213:HOH:O	2.50	0.43
1:D:560:ILE:HG21	2:D:808:HEC:HBD2	1.99	0.43
1:B:389:LYS:HE2	1:B:393:ASP:OD2	2.19	0.43
1:D:619:TYR:CD1	1:D:632:LYS:HG2	2.54	0.43
1:A:403:ASN:ND2	1:A:414:ASP:OD2	2.42	0.43
1:A:84:LEU:HB3	1:A:163:TYR:CE2	2.52	0.43
1:C:728:GLN:HB2	1:C:728:GLN:HE21	1.66	0.43
1:B:141:PHE:O	1:B:258:SER:HA	2.18	0.43
1:A:312:HIS:HB2	4:A:814:DMS:H22	2.00	0.43
1:C:442:TYR:CZ	2:C:807:HEC:HBC1	2.54	0.43
1:B:118:TYR:CE1	1:B:171:VAL:HG13	2.54	0.42
1:B:244:ARG:HD3	2:B:903:HEC:C2C	2.48	0.42
1:D:577:TYR:CZ	2:D:807:HEC:HBC2	2.54	0.42
1:A:75:ASN:OD1	1:A:79:VAL:N	2.52	0.42
1:C:535:TYR:CE2	1:C:577:TYR:HA	2.54	0.42
1:C:591:LYS:NZ	2:C:807:HEC:O2D	2.44	0.42
1:D:314:PRO:HB3	2:D:806:HEC:C2D	2.49	0.42
2:A:803:HEC:HBB2	2:A:804:HEC:C3C	2.49	0.42
1:A:88:HIS:O	1:A:90:LEU:N	2.52	0.42
1:C:440:SER:HB2	1:C:442:TYR:CE1	2.53	0.42
1:D:576:HIS:HE1	2:D:807:HEC:C4D	2.33	0.42
1:B:355:PRO:HG3	2:B:906:HEC:C1B	2.49	0.42
1:C:420:ASN:OD1	1:C:420:ASN:N	2.47	0.42
1:C:575:VAL:HG13	1:C:576:HIS:HD2	1.84	0.42
2:B:903:HEC:HBC3	2:B:903:HEC:HMC1	2.01	0.42
1:C:220:ARG:HH22	2:C:803:HEC:CGA	2.33	0.42
1:C:660:TRP:CD1	1:C:679:GLY:HA3	2.55	0.42
1:B:398:LYS:HB3	1:B:538:ASP:HB3	2.02	0.42
1:B:84:LEU:HB3	1:B:163:TYR:CE2	2.53	0.42
1:D:273:ILE:HG13	2:D:803:HEC:HMD2	2.02	0.42
1:D:509:ALA:HA	1:D:535:TYR:HA	2.01	0.42
1:A:94:ILE:HG23	1:A:118:TYR:HB2	2.01	0.42
1:B:314:PRO:HD3	2:B:902:HEC:HMD2	2.02	0.42
2:B:905:HEC:HMA3	2:B:906:HEC:C2A	2.50	0.42
1:C:448:ASP:OD1	1:C:501:ASN:ND2	2.51	0.42
1:A:560:ILE:HG21	2:A:808:HEC:HBD2	2.00	0.42
1:D:389:LYS:NZ	1:D:393:ASP:OD2	2.49	0.42
1:B:697:ILE:HG12	2:B:911:HEC:HMB2	2.02	0.42
1:B:197:PRO:HB2	1:C:422:ASP:O	2.20	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:619:TYR:CD1	1:C:632:LYS:HG2	2.55	0.42
1:C:617:GLY:HA2	4:C:815:DMS:H11	2.01	0.41
1:D:50:THR:OG1	1:D:52:THR:O	2.31	0.41
1:D:313:TYR:CE1	2:D:801:HEC:HBC2	2.54	0.41
1:B:111:ARG:HD3	1:B:342:LEU:O	2.20	0.41
1:C:416:GLN:NE2	1:C:479:THR:O	2.50	0.41
1:C:697:ILE:HG12	2:C:810:HEC:HMB2	2.03	0.41
1:C:84:LEU:HB3	1:C:163:TYR:CE2	2.55	0.41
1:B:509:ALA:HA	1:B:535:TYR:HA	2.02	0.41
2:B:904:HEC:HBB2	2:B:905:HEC:C3C	2.50	0.41
1:A:459:ARG:O	1:A:463:ARG:HG3	2.21	0.41
1:B:377:THR:HB	2:B:906:HEC:HBD2	2.02	0.41
1:D:457:GLY:HA2	1:D:490:ASN:O	2.20	0.41
1:B:398:LYS:HD2	1:B:418:LEU:HB2	2.02	0.41
1:D:338:PHE:CZ	1:D:339:LYS:HE3	2.56	0.41
1:C:118:TYR:CZ	1:C:171:VAL:HG13	2.55	0.41
1:C:703:ILE:HD11	1:C:715:ARG:O	2.21	0.41
1:B:619:TYR:CD1	1:B:632:LYS:HG2	2.56	0.41
1:B:91:ARG:HG2	1:B:147:SER:HA	2.01	0.41
1:B:54:LYS:HE3	1:B:56:LYS:HG2	2.03	0.41
1:A:239:LEU:HD22	2:A:802:HEC:CHB	2.51	0.40
2:D:805:HEC:CHD	4:D:813:DMS:H22	2.51	0.40
1:C:312:HIS:HB2	4:C:815:DMS:H12	2.03	0.40
1:A:657:GLU:OE1	1:A:657:GLU:N	2.41	0.40
1:A:682:LEU:HD11	1:A:704:LEU:HD22	2.04	0.40
2:A:806:HEC:HAD2	4:A:814:DMS:H22	2.04	0.40
4:A:816:DMS:O	2:B:906:HEC:HBC2	2.20	0.40
1:D:285:PHE:O	1:D:354:LYS:HD3	2.21	0.40
1:B:299:ILE:HD12	1:B:305:VAL:HG22	2.03	0.40
1:B:376:GLY:HA3	1:B:517:TYR:CE2	2.56	0.40
1:D:377:THR:HB	2:D:805:HEC:HBD2	2.03	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	A	691/760 (91%)	656 (95%)	34 (5%)	1 (0%)	59	89
1	B	692/760 (91%)	669 (97%)	22 (3%)	1 (0%)	59	89
1	C	690/760 (91%)	664 (96%)	24 (4%)	2 (0%)	50	82
1	D	693/760 (91%)	670 (97%)	22 (3%)	1 (0%)	59	89
All	All	2766/3040 (91%)	2659 (96%)	102 (4%)	5 (0%)	56	86

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	575	VAL
1	A	575	VAL
1	C	676	SER
1	D	575	VAL
1	C	575	VAL

### 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	558/609 (92%)	547 (98%)	11 (2%)	68	92
1	B	559/609 (92%)	550 (98%)	9 (2%)	75	94
1	C	557/609 (92%)	552 (99%)	5 (1%)	87	97
1	D	559/609 (92%)	553 (99%)	6 (1%)	84	96
All	All	2233/2436 (92%)	2202 (99%)	31 (1%)	78	95

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	LEU
1	A	398	LYS
1	A	576	HIS
1	A	598	THR
1	A	643	LYS
1	A	688	TYR
1	A	699	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	707	THR
1	A	720	CYS
1	A	722	THR
1	A	728	GLN
1	B	63	ASP
1	B	82	LEU
1	B	107	THR
1	B	191	THR
1	B	321	CYS
1	B	398	LYS
1	B	420	ASN
1	B	576	HIS
1	B	594	LYS
1	C	288	THR
1	C	398	LYS
1	C	474	THR
1	C	576	HIS
1	C	728	GLN
1	D	85	THR
1	D	192	MET
1	D	288	THR
1	D	398	LYS
1	D	576	HIS
1	D	728	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	713	GLN
1	C	59	ASN
1	C	70	ASN
1	C	735	ASN
1	D	735	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

Mogul failed to run properly - this section will therefore be empty.

## 5.5 Carbohydrates ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.6 Ligand geometry ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 5.7 Other polymers ⓘ

Mogul failed to run properly - this section will therefore be empty.

## 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	693/760 (91%)	-0.37	3 (0%) 90 93	18, 36, 70, 148	0
1	B	694/760 (91%)	-0.37	2 (0%) 91 95	18, 35, 63, 113	0
1	C	692/760 (91%)	-0.35	2 (0%) 91 95	17, 37, 74, 110	0
1	D	695/760 (91%)	-0.50	0 100 100	15, 31, 55, 111	0
All	All	2774/3040 (91%)	-0.40	7 (0%) 91 95	15, 34, 67, 148	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	688	TYR	3.2
1	B	321	CYS	2.7
1	C	666	LYS	2.4
1	A	697	ILE	2.3
1	A	667	ASN	2.2
1	B	104	VAL	2.0
1	C	106	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
4	DMS	D	815	4/4	0.49	16.07	115,115,115,115	0
4	DMS	B	914	4/4	0.27	5.17	46,49,57,59	0
4	DMS	B	915	4/4	0.31	4.74	92,92,92,92	0
4	DMS	A	814	4/4	0.26	4.73	61,67,77,91	0
4	DMS	C	816	4/4	0.21	3.90	56,67,67,88	0
4	DMS	C	815	4/4	0.27	3.56	84,84,84,84	0
4	DMS	C	814	4/4	0.23	3.50	59,59,59,59	0
3	CA	A	812	1/1	0.24	3.35	69,69,69,69	0
4	DMS	A	813	4/4	0.20	3.11	46,50,53,58	0
4	DMS	A	815	4/4	0.19	3.04	57,58,61,80	0
4	DMS	D	816	4/4	0.19	2.92	66,66,66,66	0
4	DMS	D	814	4/4	0.17	2.55	23,35,38,42	0
2	HEC	B	907	43/43	0.15	1.77	18,24,35,42	0
2	HEC	C	804	43/43	0.15	1.73	20,27,37,43	0
2	HEC	B	908	43/43	0.15	1.48	19,26,35,54	0
2	HEC	A	804	43/43	0.14	1.46	20,27,33,51	0
4	DMS	B	901	4/4	0.19	1.33	31,36,37,45	0
4	DMS	D	813	4/4	0.19	1.21	36,43,45,52	0
4	DMS	C	813	4/4	0.20	1.14	41,42,46,47	0
2	HEC	B	911	43/43	0.16	1.03	26,32,52,58	0
2	HEC	D	807	43/43	0.15	1.02	18,25,36,62	0
2	HEC	B	905	43/43	0.15	0.96	26,33,42,50	0
2	HEC	C	802	43/43	0.16	0.90	16,23,30,36	0
2	HEC	D	809	43/43	0.14	0.88	21,29,59,69	0
2	HEC	D	804	43/43	0.14	0.71	24,31,36,51	0
2	HEC	D	810	43/43	0.14	0.68	22,27,44,48	0
2	HEC	D	806	43/43	0.14	0.65	17,22,36,43	0
2	HEC	D	802	43/43	0.15	0.60	21,27,36,44	0
2	HEC	B	910	43/43	0.14	0.59	24,31,67,73	0
2	HEC	C	809	43/43	0.17	0.58	46,60,71,75	0
3	CA	C	811	1/1	0.13	0.54	39,39,39,39	0
2	HEC	A	803	43/43	0.13	0.53	16,20,24,32	0
2	HEC	A	802	43/43	0.15	0.49	15,22,29,35	0
3	CA	A	811	1/1	0.14	0.49	30,30,30,30	0
2	HEC	A	805	43/43	0.14	0.47	25,30,35,37	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEC	C	808	43/43	0.15	0.47	29,37,43,48	0
2	HEC	C	801	43/43	0.14	0.45	20,23,28,30	0
2	HEC	C	806	43/43	0.14	0.43	27,31,43,52	0
2	HEC	B	903	43/43	0.15	0.34	24,31,43,46	0
4	DMS	B	916	4/4	0.16	0.28	46,48,50,71	0
2	HEC	C	810	43/43	0.20	0.24	62,71,76,83	0
2	HEC	B	904	43/43	0.15	0.19	25,32,37,40	0
2	HEC	A	806	43/43	0.13	0.19	23,29,41,45	0
2	HEC	A	801	43/43	0.13	0.12	18,22,29,34	0
4	DMS	A	816	4/4	0.15	0.08	28,31,36,41	0
2	HEC	B	906	43/43	0.14	0.07	27,34,37,39	0
2	HEC	A	809	43/43	0.16	0.01	40,53,71,81	0
2	HEC	C	807	43/43	0.14	0.01	28,34,46,63	0
2	HEC	D	808	43/43	0.12	0.01	16,23,27,30	0
2	HEC	A	810	43/43	0.19	-0.02	58,67,75,80	0
2	HEC	B	902	43/43	0.14	-0.03	19,24,27,30	0
3	CA	C	812	1/1	0.14	-0.05	57,57,57,57	0
2	HEC	D	803	43/43	0.13	-0.07	19,26,30,33	0
2	HEC	A	807	43/43	0.14	-0.08	27,33,41,49	0
2	HEC	B	909	43/43	0.12	-0.08	17,24,28,32	0
2	HEC	D	801	43/43	0.13	-0.18	16,20,26,28	0
2	HEC	D	805	43/43	0.13	-0.27	23,32,39,46	0
2	HEC	C	803	43/43	0.12	-0.39	18,23,27,32	0
2	HEC	C	805	43/43	0.12	-0.39	23,28,34,46	0
3	CA	D	812	1/1	0.14	-0.43	60,60,60,60	0
2	HEC	A	808	43/43	0.12	-0.53	28,38,43,44	0
3	CA	B	913	1/1	0.15	-1.06	58,58,58,58	0
3	CA	D	811	1/1	0.06	-3.70	38,38,38,38	0
3	CA	B	912	1/1	0.09	-6.36	51,51,51,51	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.