



# wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 10:55 AM GMT

PDB ID : 3WCP  
Title : Deoxyhemoglobin SH-drug complex  
Authors : Safo, M.K.; Ko, T.P.  
Deposited on : 2013-05-30  
Resolution : 1.94 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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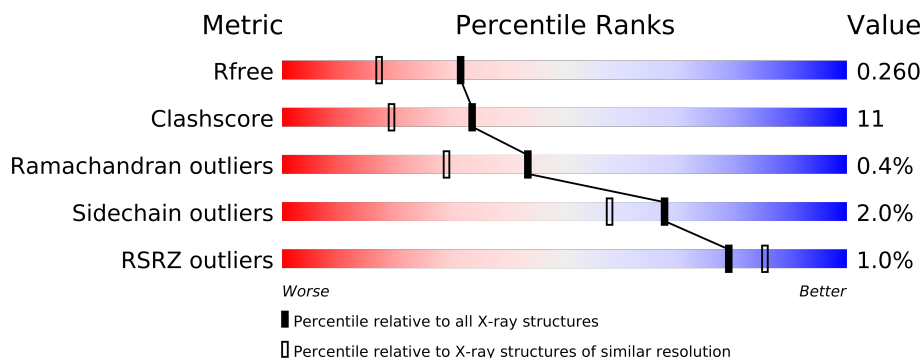
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.94 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	2024 (1.96-1.92)
Clashscore	79885	2281 (1.96-1.92)
Ramachandran outliers	78287	2255 (1.96-1.92)
Sidechain outliers	78261	2255 (1.96-1.92)
RSRZ outliers	66119	2024 (1.96-1.92)

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	141	
1	C	141	
2	B	146	
2	D	146	

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 5262 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 Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	C	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			

- Molecule 2 is a protein called Hemoglobin subunit beta.

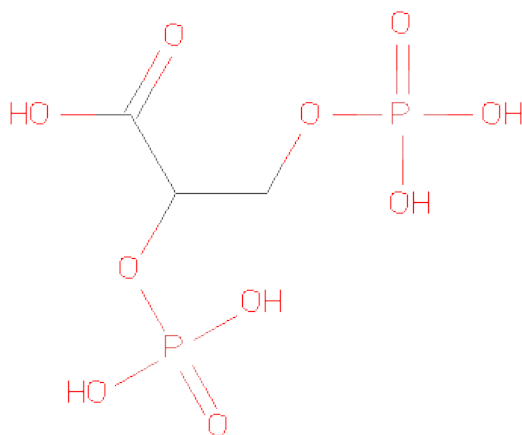
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	0	0	0
			1117	719	194	200	4			
2	D	145	Total	C	N	O	S	0	0	0
			1117	719	194	200	4			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 4 is 2,3-DIPHOSPHOGLYCERICACID (three-letter code: DG2) (formula:  $C_3H_8O_{10}P_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	P	0	1
			15	3	10	2		
4	B	1	Total	C	O	P	0	1
			15	3	10	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	155	Total	O	0	0
			155	155		
5	B	146	Total	O	0	0
			146	146		
5	C	195	Total	O	0	0
			195	195		

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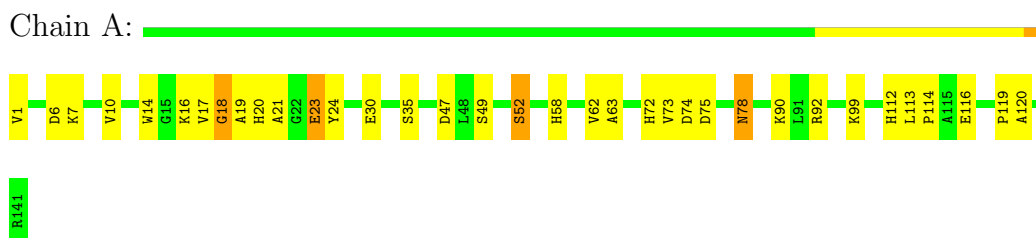
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	192	Total 192	O 192	0	0

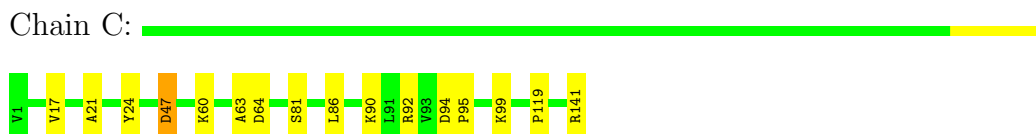
### 3 Residue-property plots

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.

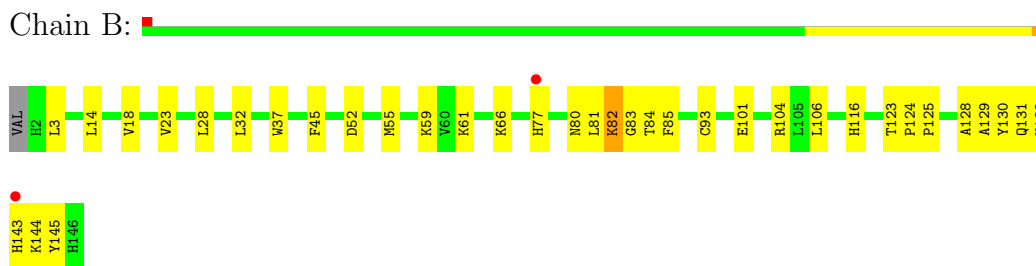
- Molecule 1: Hemoglobin subunit alpha



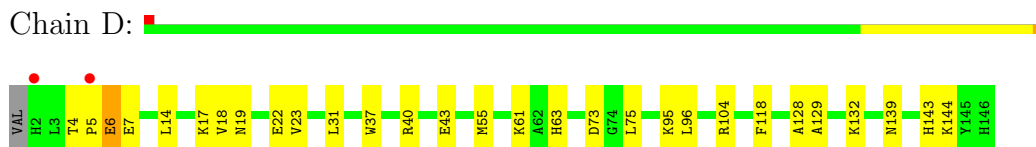
- Molecule 1: Hemoglobin subunit alpha



- Molecule 2: Hemoglobin subunit beta



- Molecule 2: Hemoglobin subunit beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.72Å 96.92Å 65.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.94 29.33 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-1.94) 99.2 (29.33-1.94)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.13 (at 1.93Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.212 , 0.263 0.209 , 0.260	Depositor DCC
$R_{free}$ test set	2242 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.9	EDS
Estimated twinning fraction	0.029 for k,h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	1 of 44716 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5262	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.27% 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: DG2, HEM, CSS

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	0.78	0/1097	0.86	1/1491 (0.1%)
1	C	0.89	0/1097	0.87	1/1491 (0.1%)
2	B	0.81	0/1139	0.80	0/1545
2	D	0.86	0/1139	0.87	1/1545 (0.1%)
All	All	0.83	0/4472	0.85	3/6072 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	47	ASP	N-CA-C	-6.60	93.19	111.00
1	A	47	ASP	N-CA-C	-6.33	93.90	111.00
2	D	40	ARG	NE-CZ-NH1	5.33	122.97	120.30

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	1069	0	1073	30	0
1	C	1069	0	1073	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1117	0	1106	42	0
2	D	1117	0	1106	21	0
3	A	43	0	30	1	0
3	B	43	0	30	5	0
3	C	43	0	30	0	0
3	D	43	0	30	3	0
4	B	30	0	8	3	0
5	A	155	0	0	6	1
5	B	146	0	0	5	0
5	C	195	0	0	2	1
5	D	192	0	0	4	2
All	All	5262	0	4486	100	2

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 11.

The worst 5 of 100 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:73:ASP:HB2	5:D:373:HOH:O	1.68	0.93
2:B:3:LEU:HD13	2:B:132:LYS:HD2	1.57	0.84
2:D:61:LYS:HE2	5:D:371:HOH:O	1.78	0.84
1:A:21:ALA:HB1	1:A:63:ALA:HB1	1.61	0.82
2:D:18:VAL:HG13	2:D:23:VAL:HG21	1.66	0.78

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:A:420:HOH:O	5:D:453:HOH:O[4_556]	2.13	0.07
5:C:489:HOH:O	5:D:381:HOH:O[4_556]	2.18	0.02

## 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	139/141 (99%)	135 (97%)	2 (1%)	2 (1%)	16	5
1	C	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
2	B	142/146 (97%)	138 (97%)	4 (3%)	0	100	100
2	D	142/146 (97%)	140 (99%)	2 (1%)	0	100	100
All	All	562/574 (98%)	548 (98%)	12 (2%)	2 (0%)	43	29

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ALA
1	A	18	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	A	113/113 (100%)	110 (97%)	3 (3%)	57	44
1	C	113/113 (100%)	111 (98%)	2 (2%)	71	63
2	B	116/117 (99%)	115 (99%)	1 (1%)	87	86
2	D	116/117 (99%)	113 (97%)	3 (3%)	59	45
All	All	458/460 (100%)	449 (98%)	9 (2%)	68	58

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	47	ASP
2	D	75	LEU
2	D	5	PRO
1	A	78	ASN
1	C	81	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

2 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	CSS	B	93	2	5,6,7	7.64	2 (40%)	4,6,8	0.35	0
2	CSS	D	93	2	5,6,7	8.00	2 (40%)	4,6,8	0.55	0

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	CSS	B	93	2	-	0/2/5/7	0/0/0/0
2	CSS	D	93	2	-	0/2/5/7	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	93	CSS	O-C	17.49	1.23	1.11
2	B	93	CSS	O-C	16.68	1.22	1.11
2	D	93	CSS	CA-C	3.74	1.55	1.48
2	B	93	CSS	CA-C	3.55	1.55	1.48

There are no bond angle outliers.

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 ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	HEM	A	201	1	49,50,50	8.08	24 (48%)	46,82,82	1.91	13 (28%)
3	HEM	B	201	2	49,50,50	4.61	21 (42%)	46,82,82	1.96	5 (10%)
4	DG2	B	202[A]	-	14,14,14	1.92	5 (35%)	21,21,21	1.39	2 (9%)
4	DG2	B	203[B]	-	14,14,14	1.46	2 (14%)	21,21,21	1.23	2 (9%)
3	HEM	C	201	1	49,50,50	4.70	21 (42%)	46,82,82	1.87	12 (26%)
3	HEM	D	201	2	49,50,50	4.38	25 (51%)	46,82,82	2.61	16 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	201	1	-	0/14/114/114	0/0/8/8
3	HEM	B	201	2	-	0/14/114/114	0/0/8/8
4	DG2	B	202[A]	-	-	0/15/15/15	0/0/0/0
4	DG2	B	203[B]	-	-	0/15/15/15	0/0/0/0
3	HEM	C	201	1	-	0/14/114/114	0/0/8/8
3	HEM	D	201	2	-	0/14/114/114	0/0/8/8

The worst 5 of 98 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	HEM	C2B-C1B	32.49	1.52	1.44
3	A	201	HEM	C2D-C1D	29.84	1.52	1.44
3	A	201	HEM	C3D-C4D	28.61	1.51	1.44
3	C	201	HEM	C3D-C4D	20.34	1.49	1.44
3	C	201	HEM	C2B-C1B	-18.13	1.40	1.44

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	201	HEM	C4A-C3A-C2A	-9.95	100.07	107.00
3	B	201	HEM	C3B-C4B-NB	-8.43	107.97	114.00
3	D	201	HEM	C3A-C4A-NA	7.03	114.72	109.41
3	B	201	HEM	CBA-CAA-C2A	-6.57	101.11	112.69
3	C	201	HEM	CBA-CAA-C2A	-4.93	104.01	112.69

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	141/141 (100%)	-0.08	0 100 100	21, 33, 48, 55	0
1	C	141/141 (100%)	-0.30	0 100 100	21, 28, 36, 43	0
2	B	145/146 (99%)	0.16	2 (1%) 72 79	24, 36, 52, 61	0
2	D	145/146 (99%)	-0.11	2 (1%) 72 79	18, 28, 42, 68	0
All	All	572/574 (99%)	-0.08	4 (0%) 79 90	18, 31, 48, 68	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	77	HIS	4.3
2	D	2	HIS	3.4
2	B	143	HIS	3.3
2	D	5	PRO	2.3

### 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	CSS	B	93	7/8	0.07	-1.34	33,37,40,45	0
2	CSS	D	93	7/8	0.06	-1.52	25,27,28,42	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
3	HEM	C	201	43/43	0.09	0.04	20,26,32,39	0
4	DG2	B	203[B]	15/15	0.17	0.03	96,97,98,98	15
4	DG2	B	202[A]	15/15	0.16	-0.03	97,97,98,98	15
3	HEM	A	201	43/43	0.09	-0.04	25,29,34,38	0
3	HEM	B	201	43/43	0.10	-0.44	26,35,44,46	0
3	HEM	D	201	43/43	0.08	-0.54	18,22,28,31	0

### 6.5 Other polymers ⓘ

There are no such residues in this entry.