



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:35 AM GMT

PDB ID : 2HRC  
Title : 1.7 angstrom structure of human ferrochelatase variant R115L  
Authors : Medlock, A.; Swartz, L.; Dailey, T.A.; Dailey, H.A.; Lanzilotta, W.N.  
Deposited on : 2006-07-20  
Resolution : 1.70 Å(reported)

This is a wwPDB X-ray Structure 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/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

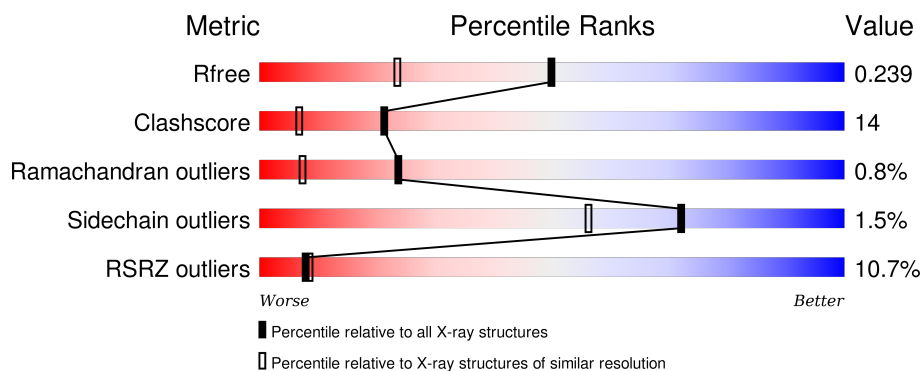
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 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))
$R_{free}$	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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. 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	A	359	<div> <div>11%</div> <div> <div></div> <div>72%</div> <div>27%</div> </div> <div>.</div> </div>
1	B	359	<div> <div>11%</div> <div> <div></div> <div>74%</div> <div>24%</div> </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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	IMD	A	1601	-	-	-	X
4	IMD	B	1602	-	-	-	X
6	GOL	A	707	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6923 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 Ferrochelatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	21	0
			3057	1935	533	569	20			
1	B	359	Total	C	N	O	S	0	20	0
			3062	1939	537	567	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	LEU	ARG	ENGINEERED	UNP P22830
B	615	LEU	ARG	ENGINEERED	UNP P22830

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

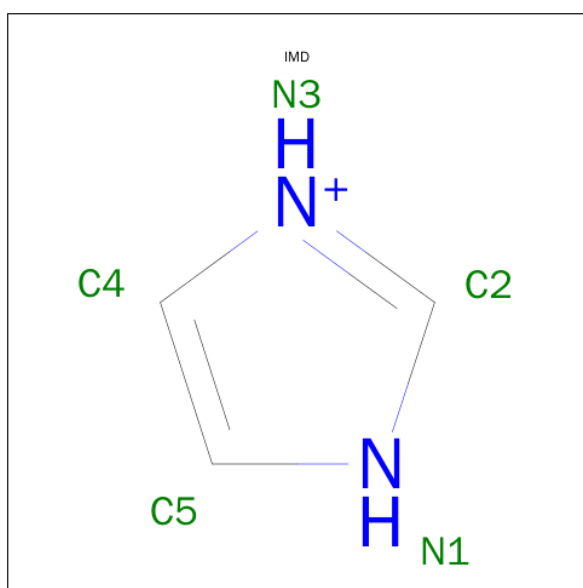
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula:  $C_3H_5N_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			5	3	2		
4	B	1	Total	C	N	0	0
			5	3	2		

- 
- The ORTEP diagram illustrates the molecular structure of compound 1, a complex polycyclic molecule. The structure is shown with thermal ellipsoids at the 50% probability level. Key features include a central fused ring system with multiple stereocenters indicated by wedged and dashed bonds. A prominent carboxylic acid group is attached to the structure, with the carbonyl oxygen (O25) and hydroxyl oxygen (O26) clearly visible. The molecule also contains several other hydroxyl groups (O7, O12, O13) and a methoxy group (O14). The atoms are labeled with their respective element symbols and numbers, and the bonds are color-coded: red for C-H bonds, green for C-C bonds, and blue for C-O bonds. The overall structure is highly symmetrical, with the central ring system forming the core of the molecule.

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $\text{C}_3\text{H}_8\text{O}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

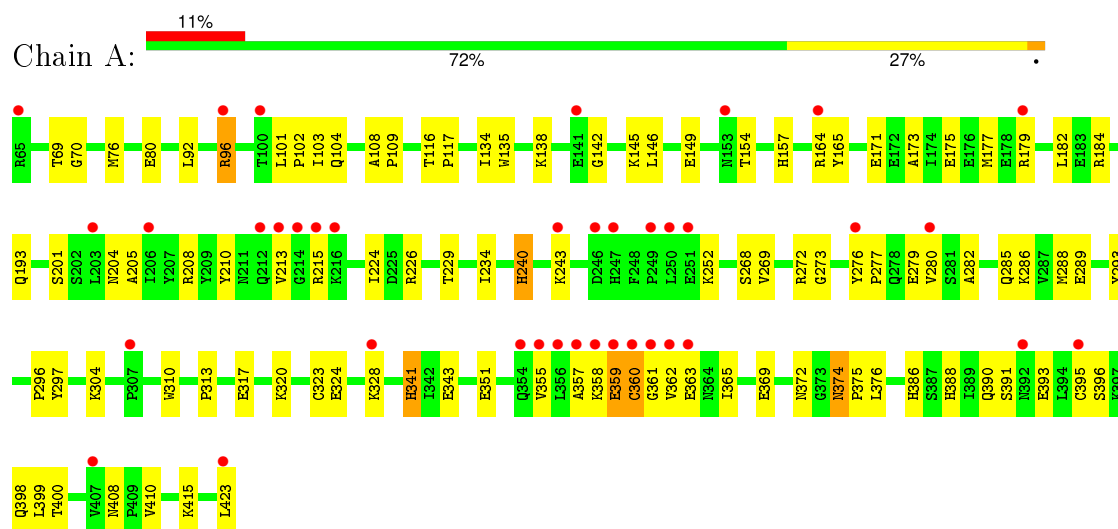
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	306	Total	O	0	0
			306	306		
7	B	298	Total	O	0	0
			298	298		

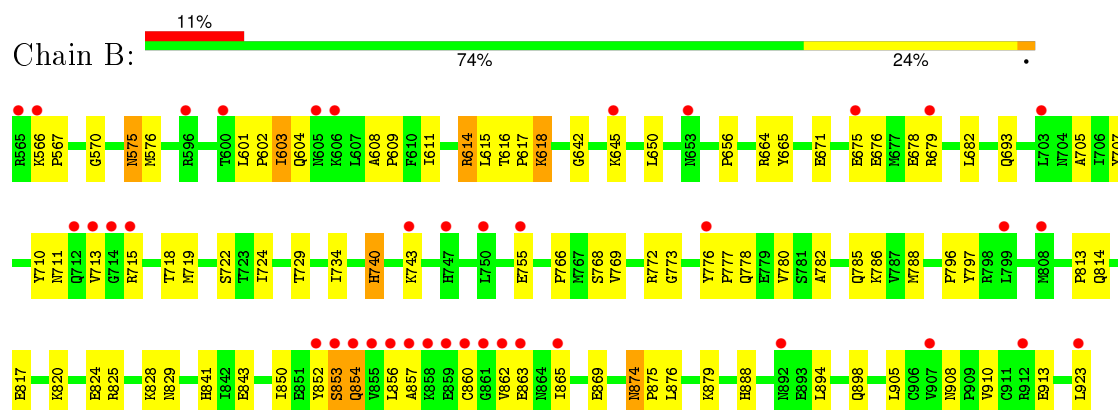
### 3 Residue-property plots

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: Ferrochelatase



#### • Molecule 1: Ferrochelatase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	88.53Å 92.98Å 110.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.84 – 1.70 41.84 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.84-1.70) 99.7 (41.84-1.50)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 1.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.221 , 0.242 0.221 , 0.239	Depositor DCC
$R_{free}$ test set	4998 reflections (5.24%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.9	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.43 , 54.7	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 145522 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6923	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	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 54.37 % 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 3.6882e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: GOL, CHD, IMD, FES, CL

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	0.28	0/3127	0.56	1/4230 (0.0%)
1	B	0.28	0/3132	0.57	1/4234 (0.0%)
All	All	0.28	0/6259	0.56	2/8464 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	724	ILE	N-CA-C	-5.66	95.72	111.00
1	A	224	ILE	N-CA-C	-5.52	96.11	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	A	3057	0	3025	87	0
1	B	3062	0	3047	105	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	5	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	5	0	5	1	0
5	A	87	0	117	1	0
5	B	87	0	117	3	0
6	A	6	0	8	3	0
7	A	306	0	0	5	0
7	B	298	0	0	9	0
All	All	6923	0	6324	181	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 14.

The worst 5 of 181 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)
1:B:664[A]:ARG:NH1	1:B:705:ALA:HB2	1.68	1.07
1:B:664[A]:ARG:HH11	1:B:705:ALA:HB2	1.26	1.00
1:A:164[A]:ARG:NH1	1:A:205:ALA:HB2	1.76	0.99
1:A:164[A]:ARG:HH11	1:A:205:ALA:HB2	1.29	0.96
1:A:398:GLN:HE22	1:B:797:TYR:H	1.17	0.93

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	A	378/359 (105%)	365 (97%)	9 (2%)	4 (1%)	17	4
1	B	377/359 (105%)	365 (97%)	10 (3%)	2 (0%)	34	15
All	All	755/718 (105%)	730 (97%)	19 (2%)	6 (1%)	24	7

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	853	SER
1	B	854	GLN
1	A	357	ALA
1	A	358	LYS
1	A	360	CYS

### 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	343/324 (106%)	339 (99%)	4 (1%)	78	65
1	B	344/324 (106%)	338 (98%)	6 (2%)	68	51
All	All	687/648 (106%)	677 (98%)	10 (2%)	72	56

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	575	ASN
1	B	603	ILE
1	B	618	LYS
1	A	374	ASN
1	B	614	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	814	GLN
1	B	829	ASN
1	B	888	HIS
1	B	575	ASN
1	B	740	HIS

### 5.3.3 RNA ⓘ

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 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 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	$\# Z  > 2$
3	FES	A	1501	1	0,4,4	0.00	-	0,4,4	0.00	-
4	IMD	A	1601	-	3,5,5	0.35	0	4,5,5	0.58	0
5	CHD	A	701	-	29,32,32	1.96	11 (37%)	48,51,51	1.74	13 (27%)
5	CHD	A	702	-	29,32,32	1.92	9 (31%)	48,51,51	1.66	13 (27%)
5	CHD	A	703	-	29,32,32	1.94	11 (37%)	48,51,51	1.72	15 (31%)
6	GOL	A	707	-	5,5,5	0.14	0	5,5,5	0.21	0
3	FES	B	1502	1	0,4,4	0.00	-	0,4,4	0.00	-
4	IMD	B	1602	-	3,5,5	0.35	0	4,5,5	0.58	0
5	CHD	B	1603	-	29,32,32	1.90	10 (34%)	48,51,51	1.69	14 (29%)
5	CHD	B	1604	-	29,32,32	1.96	11 (37%)	48,51,51	1.72	14 (29%)
5	CHD	B	1605	-	29,32,32	1.95	13 (44%)	48,51,51	1.78	14 (29%)

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	FES	A	1501	1	-	0/0/4/4	0/1/1/1
4	IMD	A	1601	-	-	0/0/0/0	0/1/1/1
5	CHD	A	701	-	-	0/7/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CHD	A	702	-	-	0/7/74/74	0/4/4/4
5	CHD	A	703	-	-	0/7/74/74	0/4/4/4
6	GOL	A	707	-	-	0/4/4/4	0/0/0/0
3	FES	B	1502	1	-	0/0/4/4	0/1/1/1
4	IMD	B	1602	-	-	0/0/0/0	0/1/1/1
5	CHD	B	1603	-	-	0/7/74/74	0/4/4/4
5	CHD	B	1604	-	-	0/7/74/74	0/4/4/4
5	CHD	B	1605	-	-	0/7/74/74	0/4/4/4

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	703	CHD	C8-C9	2.01	1.57	1.53
5	B	1605	CHD	C20-C17	2.01	1.58	1.54
5	B	1603	CHD	O7-C7	2.02	1.47	1.43
5	B	1605	CHD	O7-C7	2.02	1.47	1.43
5	B	1605	CHD	C4-C3	2.03	1.55	1.51

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1605	CHD	C18-C13-C12	-4.47	104.73	109.09
5	A	701	CHD	C18-C13-C12	-4.47	104.73	109.09
5	A	703	CHD	C18-C13-C12	-4.05	105.14	109.09
5	B	1604	CHD	C18-C13-C12	-4.01	105.18	109.09
5	A	702	CHD	C18-C13-C12	-3.85	105.33	109.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	701	CHD	1	0
6	A	707	GOL	3	0
4	B	1602	IMD	1	0
5	B	1603	CHD	2	0
5	B	1605	CHD	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	359/359 (100%)	0.84	38 (10%) 8 9	10, 19, 33, 44	1 (0%)
1	B	359/359 (100%)	0.81	39 (10%) 7 8	10, 19, 34, 43	0
All	All	718/718 (100%)	0.82	77 (10%) 8 8	10, 19, 34, 44	1 (0%)

The worst 5 of 77 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	360	CYS	16.6
1	A	359	GLU	10.9
1	B	857	ALA	10.7
1	B	860	CYS	9.5
1	B	854	GLN	8.8

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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( $\text{\AA}^2$ )	Q<0.9
6	GOL	A	707	6/6	0.81	0.25	6.61	29,29,29,29	0
4	IMD	A	1601	5/5	0.52	0.27	4.57	37,37,37,37	0
4	IMD	B	1602	5/5	0.62	0.23	4.35	36,36,36,36	0
5	CHD	A	701	29/29	0.89	0.14	1.39	20,21,24,25	0
5	CHD	B	1605	29/29	0.89	0.14	1.18	20,21,25,26	0
5	CHD	B	1603	29/29	0.56	0.17	1.05	33,33,36,36	0
5	CHD	A	703	29/29	0.68	0.18	0.82	35,35,36,37	0
5	CHD	B	1604	29/29	0.71	0.17	0.52	41,41,43,43	0
5	CHD	A	702	29/29	0.77	0.13	0.42	31,31,33,33	0
2	CL	A	802	1/1	0.99	0.09	-0.96	17,17,17,17	0
3	FES	A	1501	4/4	0.99	0.06	-1.63	15,16,16,17	0
3	FES	B	1502	4/4	0.99	0.05	-1.96	16,16,16,17	0
2	CL	B	924	1/1	0.99	0.07	-2.56	18,18,18,18	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.