



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:41 am GMT

PDB ID : 2FG8  
Title : Structure of Human Ferritin L Chain  
Authors : Wang, Z.M.; Li, C.; Ellenburg, M.P.; Ruble, J.R.; Ho, J.X.; Carter, D.C.  
Deposited on : 2005-12-21  
Resolution : 2.50 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:

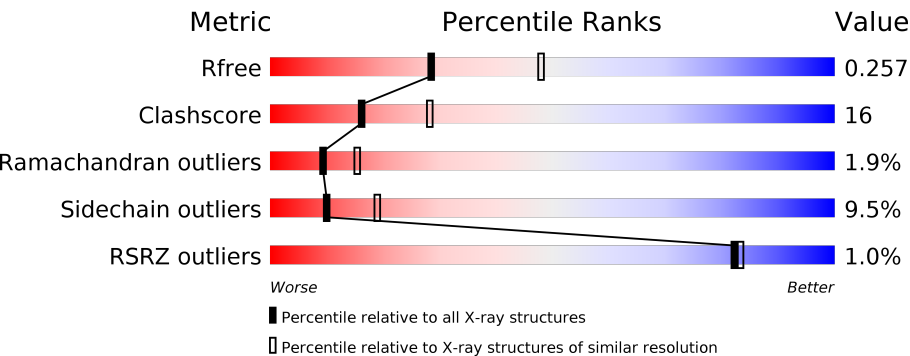
MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	174	<div><div></div><div><div></div><div>67%</div><div>27%</div><div>6%</div></div></div>
1	B	174	<div><div></div><div><div></div><div>%</div><div>64%</div><div>30%</div><div>6%</div></div></div>
1	C	174	<div><div></div><div><div></div><div>2%</div><div>63%</div><div>28%</div><div>9%</div></div></div>
1	D	174	<div><div></div><div><div></div><div>2%</div><div>61%</div><div>32%</div><div>7%</div><div>.</div></div></div>
1	E	174	<div><div></div><div><div></div><div>%</div><div>72%</div><div>21%</div><div>7%</div></div></div>
1	F	174	<div><div></div><div><div></div><div>%</div><div>69%</div><div>26%</div><div>5%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	174	<div><div>%</div><div><div></div><div>64%</div><div>32%</div><div></div></div><div></div></div>
1	H	174	<div><div>2%</div><div><div></div><div>71%</div><div>23%</div><div>6%</div></div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11373 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 Ferritin light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1402	885	244	268	5			
1	B	174	Total	C	N	O	S	0	0	0
			1402	885	244	268	5			
1	C	174	Total	C	N	O	S	0	0	0
			1402	885	244	268	5			
1	D	174	Total	C	N	O	S	0	0	0
			1402	885	244	268	5			
1	E	174	Total	C	N	O	S	0	0	0
			1402	885	244	268	5			
1	F	174	Total	C	N	O	S	0	0	0
			1402	885	244	268	5			
1	G	174	Total	C	N	O	S	0	0	0
			1402	885	244	268	5			
1	H	174	Total	C	N	O	S	0	0	0
			1402	885	244	268	5			

- Molecule 2 is CESIUM ION (three-letter code: CS) (formula: Cs).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Cs	0	0
			1	1		
2	D	1	Total	Cs	0	0
			1	1		
2	E	2	Total	Cs	0	0
			2	2		
2	C	1	Total	Cs	0	0
			1	1		
2	A	2	Total	Cs	0	0
			2	2		
2	F	3	Total	Cs	0	0
			3	3		

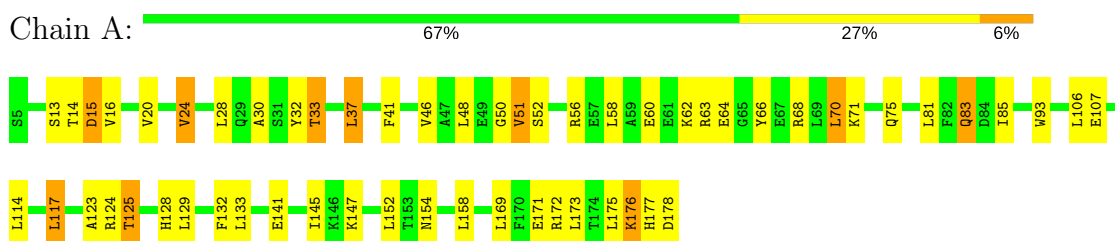
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total 21	O 21	0	0
3	B	15	Total 15	O 15	0	0
3	C	12	Total 12	O 12	0	0
3	D	21	Total 21	O 21	0	0
3	E	18	Total 18	O 18	0	0
3	F	25	Total 25	O 25	0	0
3	G	6	Total 6	O 6	0	0
3	H	29	Total 29	O 29	0	0

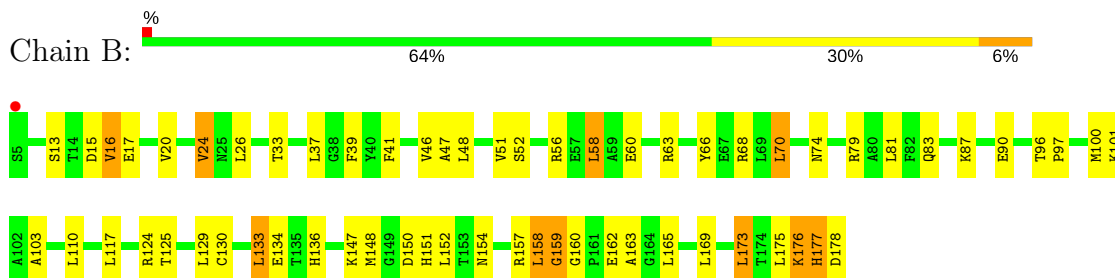
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

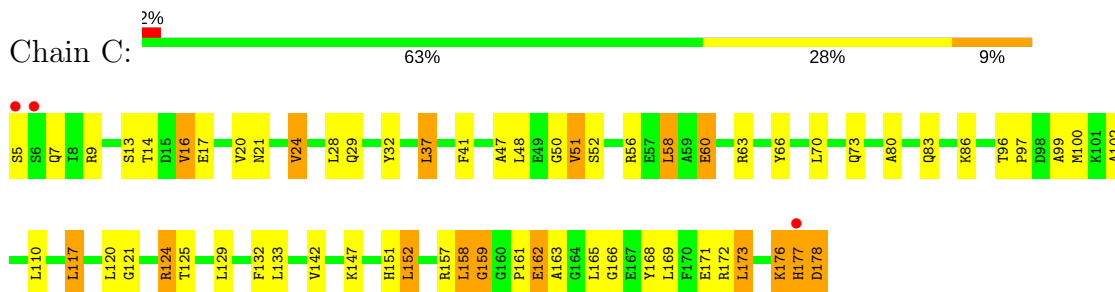
#### • Molecule 1: Ferritin light chain



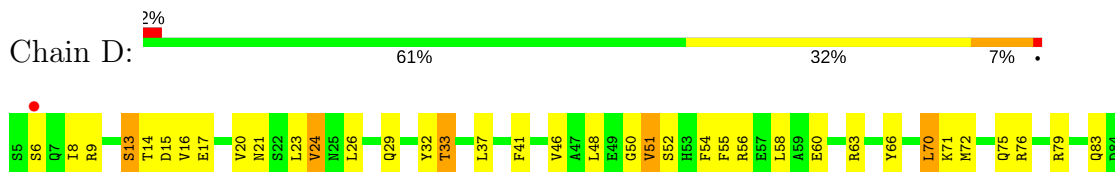
#### • Molecule 1: Ferritin light chain



#### • Molecule 1: Ferritin light chain



#### • Molecule 1: Ferritin light chain

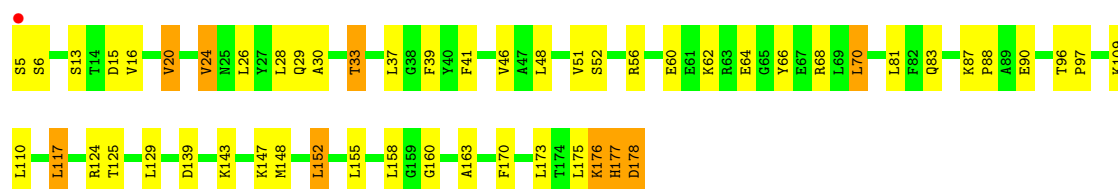




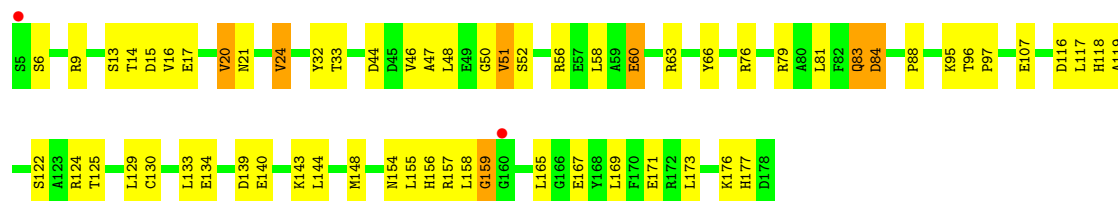
• Molecule 1: Ferritin light chain



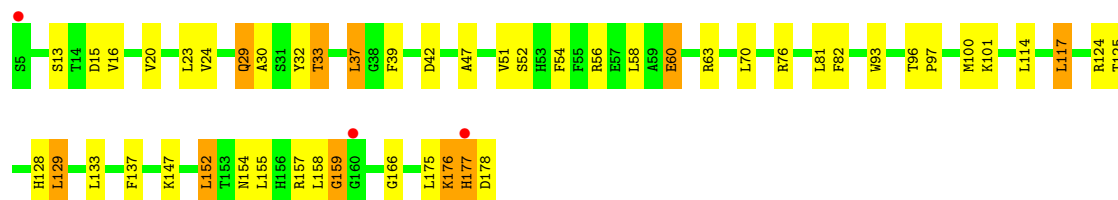
• Molecule 1: Ferritin light chain



• Molecule 1: Ferritin light chain



• Molecule 1: Ferritin light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.79Å 182.79Å 354.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.57 – 2.50 43.57 – 2.50	Depositor EDS
% Data completeness (in resolution range)	85.6 (43.57-2.50) 85.4 (43.57-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.51Å)	Xtriage
Refinement program	CNX 2000.1	Depositor
R, $R_{free}$	0.224 , 0.267 0.217 , 0.257	Depositor DCC
$R_{free}$ test set	3394 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 27.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11373	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CS

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	0.41	0/1429	0.60	0/1921
1	B	0.39	0/1429	0.59	0/1921
1	C	0.37	0/1429	0.55	0/1921
1	D	0.41	0/1429	0.59	0/1921
1	E	0.42	0/1429	0.59	0/1921
1	F	0.41	0/1429	0.60	0/1921
1	G	0.35	0/1429	0.55	0/1921
1	H	0.40	0/1429	0.58	0/1921
All	All	0.40	0/11432	0.58	0/15368

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1402	0	1372	46	0
1	B	1402	0	1372	52	0
1	C	1402	0	1372	57	0
1	D	1402	0	1372	54	0
1	E	1402	0	1372	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1402	0	1372	41	0
1	G	1402	0	1372	48	0
1	H	1402	0	1372	45	0
2	A	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	3	0	0	0	0
2	G	1	0	0	0	0
3	A	21	0	0	2	0
3	B	15	0	0	0	0
3	C	12	0	0	0	0
3	D	21	0	0	0	0
3	E	18	0	0	0	0
3	F	25	0	0	0	0
3	G	6	0	0	0	0
3	H	29	0	0	0	0
All	All	11373	0	10976	358	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 16.

The worst 5 of 358 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:100:MET:HB3	1:B:152:LEU:HD11	1.35	1.06
1:A:13:SER:HB3	1:A:16:VAL:HG12	1.48	0.95
1:D:154:ASN:O	1:D:158:LEU:HD23	1.70	0.90
1:A:60:GLU:HG3	1:A:63:ARG:NH2	1.88	0.87
1:F:176:LYS:O	1:F:178:ASP:N	2.06	0.87

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	172/174 (99%)	161 (94%)	9 (5%)	2 (1%)	15	27
1	B	172/174 (99%)	164 (95%)	4 (2%)	4 (2%)	7	11
1	C	172/174 (99%)	162 (94%)	6 (4%)	4 (2%)	7	11
1	D	172/174 (99%)	163 (95%)	6 (4%)	3 (2%)	11	18
1	E	172/174 (99%)	162 (94%)	7 (4%)	3 (2%)	11	18
1	F	172/174 (99%)	161 (94%)	9 (5%)	2 (1%)	15	27
1	G	172/174 (99%)	158 (92%)	9 (5%)	5 (3%)	5	7
1	H	172/174 (99%)	162 (94%)	7 (4%)	3 (2%)	11	18
All	All	1376/1392 (99%)	1293 (94%)	57 (4%)	26 (2%)	9	15

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	LYS
1	B	159	GLY
1	B	176	LYS
1	C	159	GLY
1	C	176	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	147/147 (100%)	133 (90%)	14 (10%)	10	19
1	B	147/147 (100%)	134 (91%)	13 (9%)	12	22
1	C	147/147 (100%)	128 (87%)	19 (13%)	5	9
1	D	147/147 (100%)	132 (90%)	15 (10%)	8	16
1	E	147/147 (100%)	132 (90%)	15 (10%)	8	16
1	F	147/147 (100%)	134 (91%)	13 (9%)	12	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	147/147 (100%)	135 (92%)	12 (8%)	13	25
1	H	147/147 (100%)	136 (92%)	11 (8%)	16	29
All	All	1176/1176 (100%)	1064 (90%)	112 (10%)	10	19

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	33	THR
1	E	16	VAL
1	H	33	THR
1	D	60	GLU
1	D	124	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	29	GLN
1	D	111	ASN
1	F	29	GLN
1	C	83	GLN
1	E	151	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	174/174 (100%)	-0.44	0 100 100	29, 41, 57, 82	0
1	B	174/174 (100%)	-0.36	1 (0%) 89 89	30, 43, 66, 90	0
1	C	174/174 (100%)	-0.22	3 (1%) 70 72	38, 50, 67, 95	0
1	D	174/174 (100%)	-0.45	3 (1%) 70 72	29, 40, 65, 89	0
1	E	174/174 (100%)	-0.45	1 (0%) 89 89	27, 36, 53, 93	0
1	F	174/174 (100%)	-0.49	1 (0%) 89 89	26, 36, 51, 82	0
1	G	174/174 (100%)	-0.26	2 (1%) 80 81	40, 55, 69, 93	0
1	H	174/174 (100%)	-0.47	3 (1%) 70 72	26, 38, 57, 87	0
All	All	1392/1392 (100%)	-0.39	14 (1%) 82 83	26, 42, 65, 95	0

The worst 5 of 14 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	5	SER	5.3
1	B	5	SER	4.9
1	H	5	SER	3.2
1	F	5	SER	2.7
1	H	160	GLY	2.4

### 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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CS	E	201	1/1	0.86	0.14	-0.26	167,167,167,167	0
2	CS	A	202	1/1	0.75	0.06	-3.99	179,179,179,179	0
2	CS	A	204	1/1	0.89	0.15	-	200,200,200,200	0
2	CS	E	206	1/1	0.85	0.35	-	200,200,200,200	0
2	CS	F	209	1/1	0.52	0.20	-	194,194,194,194	1
2	CS	C	205	1/1	0.93	0.14	-	200,200,200,200	0
2	CS	F	208	1/1	0.79	0.14	-	178,178,178,178	1
2	CS	D	203	1/1	0.82	0.13	-	200,200,200,200	0
2	CS	G	210	1/1	0.85	0.10	-	187,187,187,187	1
2	CS	F	207	1/1	0.47	0.10	-	151,151,151,151	1

## 6.5 Other polymers

There are no such residues in this entry.