



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:26 PM UTC

PDB ID : 4ITT / pdb\_00004itt  
Title : Crystal structure of iron soaked (5 min) ferritin from Pseudo-nitzschia multi-series  
Authors : Pfaffen, S.; Murphy, M.E.P.  
Deposited on : 2013-01-18  
Resolution : 2.10 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

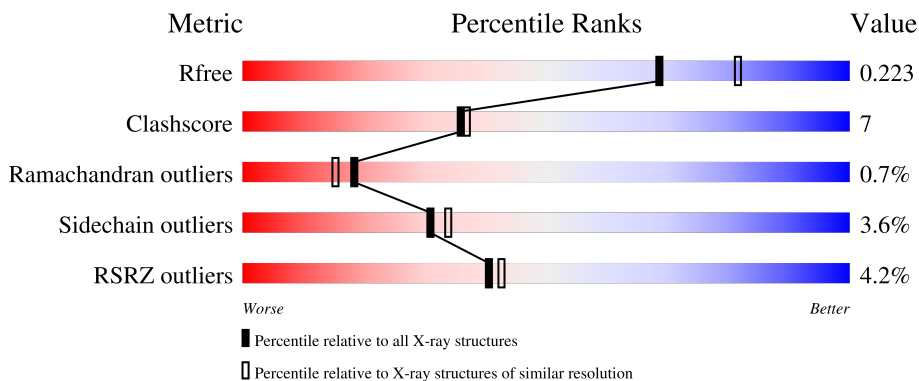
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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.



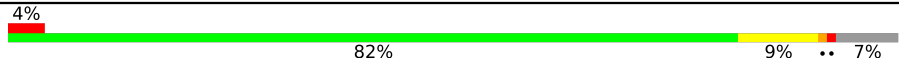


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	168	 5% 83% 10% • 5%
1	B	168	 3% 78% 14% • 5%
1	C	168	 3% 80% 11% •• 6%
1	D	168	 2% 83% 10% •• 6%
1	E	168	 5% 80% 11% • 6%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	168	 <p>4% 82% 9% •• 7%</p>
1	G	168	 <p>5% 74% 14% •• 7%</p>
1	H	168	 <p>5% 81% 12% • 6%</p>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11140 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	159	1298	815	215	262	6	0	5	0
1	D	158	1296	810	217	263	6	0	6	0
1	B	159	1292	811	215	260	6	0	4	0
1	C	158	1281	803	214	258	6	0	4	0
1	E	158	1297	813	215	263	6	0	7	0
1	F	157	1265	794	210	256	5	0	3	0
1	G	156	1285	806	215	258	6	0	7	0
1	H	158	1299	814	216	263	6	0	7	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP B6DMH6
D	0	GLY	-	expression tag	UNP B6DMH6
B	0	GLY	-	expression tag	UNP B6DMH6
C	0	GLY	-	expression tag	UNP B6DMH6
E	0	GLY	-	expression tag	UNP B6DMH6
F	0	GLY	-	expression tag	UNP B6DMH6
G	0	GLY	-	expression tag	UNP B6DMH6
H	0	GLY	-	expression tag	UNP B6DMH6

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	E	1	Total Fe 1 1	0	0
2	G	1	Total Fe 1 1	0	0
2	H	1	Total Fe 1 1	0	0

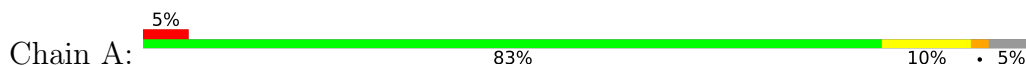
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	97	Total O 97 97	0	0
3	D	106	Total O 106 106	0	0
3	B	99	Total O 99 99	0	0
3	C	106	Total O 106 106	0	0
3	E	106	Total O 106 106	0	0
3	F	94	Total O 94 94	0	0
3	G	113	Total O 113 113	0	0
3	H	100	Total O 100 100	0	0

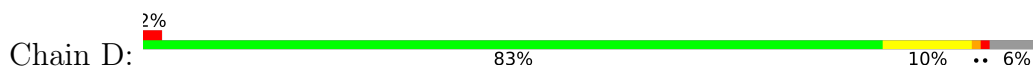
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

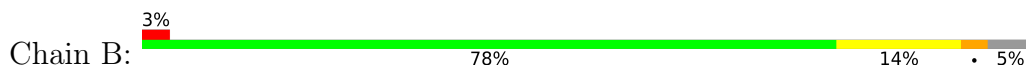
- Molecule 1: Ferritin



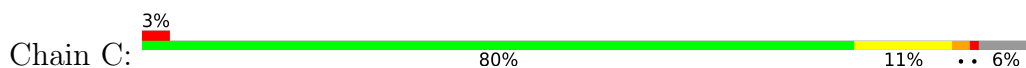
- Molecule 1: Ferritin



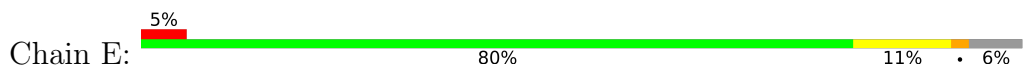
- Molecule 1: Ferritin



- Molecule 1: Ferritin



- Molecule 1: Ferritin



- Molecule 1: Ferritin

Chain F: 4% 82% 9% 7%



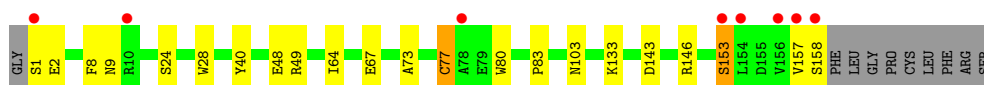
• Molecule 1: Ferritin

Chain G: 5% 74% 14% 7%



• Molecule 1: Ferritin

Chain H: 5% 81% 12% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	175.28Å 175.28Å 175.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.55 – 2.10 42.55 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.55-2.10) 99.6 (42.55-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.60 (at 2.10Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.176 , 0.225 0.174 , 0.223	Depositor DCC
$R_{free}$ test set	5180 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 37.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	0.032 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11140	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.06% 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 i

### 5.1 Standard geometry i

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

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	1.27	1/1307 (0.1%)	1.20	1/1778 (0.1%)
1	B	1.30	3/1298 (0.2%)	1.23	4/1765 (0.2%)
1	C	1.34	2/1289 (0.2%)	1.25	4/1753 (0.2%)
1	D	1.33	2/1301 (0.2%)	1.27	6/1769 (0.3%)
1	E	1.30	2/1308 (0.2%)	1.20	4/1779 (0.2%)
1	F	1.27	0/1280	1.20	7/1741 (0.4%)
1	G	1.32	2/1293 (0.2%)	1.17	3/1759 (0.2%)
1	H	1.27	0/1310	1.19	6/1782 (0.3%)
All	All	1.30	12/10386 (0.1%)	1.22	35/14126 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	65	PRO	CA-C	6.17	1.59	1.52
1	E	86	VAL	N-CA	6.09	1.53	1.46
1	G	3	GLU	N-CA	5.90	1.57	1.46
1	C	64	ILE	CA-C	5.80	1.57	1.53
1	E	75	VAL	N-CA	5.79	1.51	1.46

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	103	ASN	CB-CA-C	-6.84	100.14	110.88
1	E	64	ILE	N-CA-C	-6.83	101.35	107.56
1	H	8	PHE	N-CA-C	-6.50	104.12	111.14
1	D	46	ALA	N-CA-C	-6.29	104.50	111.36
1	F	70	ALA	CA-C-N	-6.23	116.54	123.02

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	3	GLU	Peptide

## 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	1298	0	1226	23	0
1	B	1292	0	1220	21	0
1	C	1281	0	1215	18	0
1	D	1296	0	1222	7	0
1	E	1297	0	1230	18	1
1	F	1265	0	1194	14	0
1	G	1285	0	1217	39	0
1	H	1299	0	1231	9	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	97	0	0	11	0
3	B	99	0	0	5	0
3	C	106	0	0	2	0
3	D	106	0	0	1	0
3	E	106	0	0	3	0
3	F	94	0	0	4	0
3	G	113	0	0	9	0
3	H	100	0	0	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	11140	0	9755	146	1

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 7.

The worst 5 of 146 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:F:77:YCM:HB2	3:F:278:HOH:O	1.17	1.34
1:G:5[A]:LEU:HD22	1:G:5[A]:LEU:H	1.38	0.89
1:C:40:TYR:OH	1:C:133:LYS:HE3	1.72	0.89
1:G:94:GLU:HG3	1:G:134:ILE:HD13	1.55	0.88
1:E:4[B]:LEU:C	1:E:4[B]:LEU:HD23	2.00	0.86

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:ARG:NH1	1:E:10:ARG:NH1[4_565]	2.17	0.03

## 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	160/168 (95%)	156 (98%)	3 (2%)	1 (1%)	21 18
1	B	159/168 (95%)	154 (97%)	4 (2%)	1 (1%)	21 18
1	C	158/168 (94%)	154 (98%)	3 (2%)	1 (1%)	21 18
1	D	160/168 (95%)	156 (98%)	3 (2%)	1 (1%)	21 18
1	E	161/168 (96%)	158 (98%)	2 (1%)	1 (1%)	21 18

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	157/168 (94%)	153 (98%)	2 (1%)	2 (1%)	9	6
1	G	159/168 (95%)	157 (99%)	1 (1%)	1 (1%)	21	18
1	H	161/168 (96%)	157 (98%)	3 (2%)	1 (1%)	21	18
All	All	1275/1344 (95%)	1245 (98%)	21 (2%)	9 (1%)	18	15

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	VAL
1	B	157	VAL
1	C	157	VAL
1	E	157	VAL
1	F	157	VAL

### 5.3.2 Protein sidechains [i](#)

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	140/143 (98%)	137 (98%)	3 (2%)	47	54
1	B	139/143 (97%)	133 (96%)	6 (4%)	26	27
1	C	138/143 (96%)	132 (96%)	6 (4%)	26	27
1	D	140/143 (98%)	136 (97%)	4 (3%)	37	42
1	E	141/143 (99%)	137 (97%)	4 (3%)	38	43
1	F	137/143 (96%)	133 (97%)	4 (3%)	37	42
1	G	139/143 (97%)	131 (94%)	8 (6%)	18	16
1	H	141/143 (99%)	135 (96%)	6 (4%)	26	27
All	All	1115/1144 (98%)	1074 (96%)	41 (4%)	31	33

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	5[A]	LEU

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	1	SER
1	G	5[B]	LEU
1	G	93	LEU
1	H	67	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	121	ASN
1	G	9	ASN
1	C	51	HIS
1	F	145	ASN
1	B	124	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](#)

15 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
1	YCM	A	77[A]	1	7,9,10	2.27	2 (28%)	5,10,12	0.68	0
1	YCM	A	77[B]	1	7,9,10	1.08	1 (14%)	5,10,12	1.25	1 (20%)
1	YCM	B	77[A]	1	7,9,10	0.96	0	5,10,12	0.70	0
1	YCM	H	77[A]	-	7,9,10	1.00	1 (14%)	5,10,12	0.69	0
1	YCM	B	77[B]	1	7,9,10	1.01	0	5,10,12	0.57	0
1	YCM	G	77[A]	-	7,9,10	0.82	0	5,10,12	0.62	0
1	YCM	H	77[B]	-	7,9,10	1.45	2 (28%)	5,10,12	0.47	0
1	YCM	C	77[A]	1	7,9,10	0.68	0	5,10,12	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	YCM	F	77	1	7,9,10	2.52	2 (28%)	5,10,12	0.38	0
1	YCM	G	77[B]	-	7,9,10	1.90	1 (14%)	5,10,12	0.54	0
1	YCM	D	77[A]	1	7,9,10	1.16	1 (14%)	5,10,12	1.00	1 (20%)
1	YCM	C	77[B]	1	7,9,10	1.30	1 (14%)	5,10,12	0.43	0
1	YCM	E	77[A]	-	7,9,10	0.92	0	5,10,12	0.66	0
1	YCM	D	77[B]	1	7,9,10	1.46	1 (14%)	5,10,12	0.71	0
1	YCM	E	77[B]	-	7,9,10	1.69	2 (28%)	5,10,12	0.88	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
1	YCM	A	77[A]	1	-	0/6/8/10	-
1	YCM	A	77[B]	1	-	2/6/8/10	-
1	YCM	B	77[A]	1	-	3/6/8/10	-
1	YCM	H	77[A]	-	-	1/6/8/10	-
1	YCM	B	77[B]	1	-	1/6/8/10	-
1	YCM	G	77[A]	-	-	3/6/8/10	-
1	YCM	H	77[B]	-	-	1/6/8/10	-
1	YCM	C	77[A]	1	-	2/6/8/10	-
1	YCM	F	77	1	-	0/6/8/10	-
1	YCM	G	77[B]	-	-	1/6/8/10	-
1	YCM	D	77[A]	1	-	1/6/8/10	-
1	YCM	C	77[B]	1	-	1/6/8/10	-
1	YCM	E	77[A]	-	-	3/6/8/10	-
1	YCM	D	77[B]	1	-	1/6/8/10	-
1	YCM	E	77[B]	-	-	1/6/8/10	-

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	77	YCM	CD-SG	5.61	1.95	1.81
1	A	77[A]	YCM	CD-SG	5.38	1.95	1.81
1	G	77[B]	YCM	CD-SG	3.98	1.91	1.81
1	D	77[A]	YCM	CD-SG	-2.86	1.74	1.81
1	E	77[B]	YCM	CD-SG	2.85	1.88	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	77[B]	YCM	CE-CD-SG	-2.17	106.95	113.81
1	D	77[A]	YCM	CE-CD-SG	-2.03	107.41	113.81

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	77[B]	YCM	C-CA-CB-SG
1	D	77[B]	YCM	SG-CD-CE-NZ2
1	B	77[A]	YCM	N-CA-CB-SG
1	B	77[A]	YCM	C-CA-CB-SG
1	C	77[A]	YCM	N-CA-CB-SG

There are no ring outliers.

13 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	77[A]	YCM	5	0
1	A	77[B]	YCM	2	0
1	B	77[A]	YCM	2	0
1	H	77[A]	YCM	1	0
1	B	77[B]	YCM	3	0
1	G	77[A]	YCM	4	0
1	H	77[B]	YCM	2	0
1	F	77	YCM	3	0
1	G	77[B]	YCM	3	0
1	C	77[B]	YCM	3	0
1	E	77[A]	YCM	1	0
1	D	77[B]	YCM	3	0
1	E	77[B]	YCM	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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

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 [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	158/168 (94%)	-0.22	8 (5%) 33 35	10, 25, 54, 77	5 (3%)
1	B	158/168 (94%)	-0.27	5 (3%) 50 53	9, 25, 49, 78	4 (2%)
1	C	157/168 (93%)	-0.21	5 (3%) 50 53	9, 25, 46, 77	4 (2%)
1	D	157/168 (93%)	-0.35	4 (2%) 58 61	7, 22, 45, 75	5 (3%)
1	E	157/168 (93%)	-0.19	8 (5%) 33 35	9, 25, 53, 76	6 (3%)
1	F	156/168 (92%)	-0.24	7 (4%) 38 40	9, 26, 47, 75	3 (1%)
1	G	155/168 (92%)	-0.28	8 (5%) 33 35	8, 22, 40, 71	7 (4%)
1	H	157/168 (93%)	-0.29	8 (5%) 33 35	8, 24, 52, 70	6 (3%)
All	All	1255/1344 (93%)	-0.25	53 (4%) 40 42	7, 24, 49, 78	40 (3%)

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	157	VAL	6.0
1	F	157	VAL	5.9
1	A	157	VAL	5.8
1	C	157	VAL	5.6
1	G	158	SER	5.3

### 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	YCM	A	77[A]	10/11	0.72	0.18	23,27,30,30	10

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	YCM	A	77[B]	10/11	0.72	0.18	22,25,29,29	10
1	YCM	B	77[A]	10/11	0.81	0.19	25,31,35,40	10
1	YCM	B	77[B]	10/11	0.81	0.19	17,21,25,26	10
1	YCM	C	77[A]	10/11	0.81	0.17	28,31,33,35	10
1	YCM	C	77[B]	10/11	0.81	0.17	19,24,29,30	10
1	YCM	F	77	10/11	0.85	0.17	29,39,55,56	0
1	YCM	G	77[A]	10/11	0.86	0.16	30,33,37,38	7
1	YCM	G	77[B]	10/11	0.86	0.16	24,31,35,38	7
1	YCM	E	77[B]	10/11	0.87	0.16	30,33,36,38	7
1	YCM	E	77[A]	10/11	0.87	0.16	32,36,39,40	7
1	YCM	H	77[A]	10/11	0.89	0.16	28,33,37,38	7
1	YCM	H	77[B]	10/11	0.89	0.16	23,31,36,37	7
1	YCM	D	77[B]	10/11	0.90	0.12	20,24,28,28	10
1	YCM	D	77[A]	10/11	0.90	0.12	19,23,29,29	10

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	FE	H	201	1/1	0.92	0.10	46,46,46,46	1
2	FE	D	201	1/1	0.94	0.07	34,34,34,34	1
2	FE	G	201	1/1	0.95	0.07	36,36,36,36	1
2	FE	C	201	1/1	0.95	0.06	39,39,39,39	1
2	FE	B	201	1/1	0.97	0.05	37,37,37,37	1
2	FE	E	201	1/1	0.97	0.05	41,41,41,41	1

### 6.5 Other polymers [i](#)

There are no such residues in this entry.