



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 03:25 PM UTC

PDB ID : 1NMO / pdb\_00001nmo  
Title : Structural genomics, protein ybgI, unknown function  
Authors : Ladner, J.E.; Obmolova, G.; Teplyakov, A.; Khil, P.P.; Camerini-Otero, R.D.;  
Gilliland, G.L.; Structure 2 Function Project (S2F)  
Deposited on : 2003-01-10  
Resolution : 2.20 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

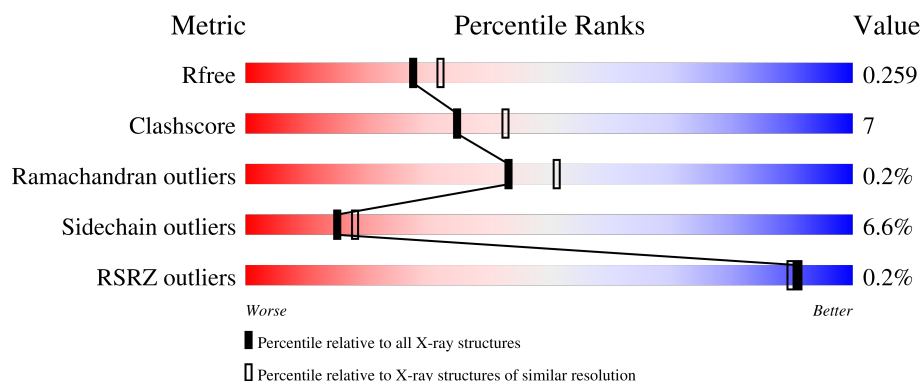
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	247	<div> <div>72%</div> <div>24%</div> <div>..</div> </div>
1	B	247	<div> <div>74%</div> <div>23%</div> <div>.</div> </div>
1	C	247	<div> <div>72%</div> <div>25%</div> <div>.</div> </div>
1	D	247	<div> <div>76%</div> <div>20%</div> <div>.</div> </div>
1	E	247	<div> <div>72%</div> <div>24%</div> <div>..</div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	247	<div><div></div><div>75%</div><div>20%</div><div>.</div><div>.</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12031 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 Hypothetical protein ybgI.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	Se	0	0	0
			1897	1200	332	359	2	4			
1	B	247	Total	C	N	O	S	Se	0	0	0
			1897	1200	332	359	2	4			
1	C	247	Total	C	N	O	S	Se	0	0	0
			1897	1200	332	359	2	4			
1	D	247	Total	C	N	O	S	Se	0	0	0
			1897	1200	332	359	2	4			
1	E	247	Total	C	N	O	S	Se	0	0	0
			1897	1200	332	359	2	4			
1	F	247	Total	C	N	O	S	Se	0	0	0
			1897	1200	332	359	2	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P75743
A	78	MSE	MET	modified residue	UNP P75743
A	121	MSE	MET	modified residue	UNP P75743
A	135	MSE	MET	modified residue	UNP P75743
B	1	MSE	MET	modified residue	UNP P75743
B	78	MSE	MET	modified residue	UNP P75743
B	121	MSE	MET	modified residue	UNP P75743
B	135	MSE	MET	modified residue	UNP P75743
C	1	MSE	MET	modified residue	UNP P75743
C	78	MSE	MET	modified residue	UNP P75743
C	121	MSE	MET	modified residue	UNP P75743
C	135	MSE	MET	modified residue	UNP P75743
D	1	MSE	MET	modified residue	UNP P75743
D	78	MSE	MET	modified residue	UNP P75743
D	121	MSE	MET	modified residue	UNP P75743
D	135	MSE	MET	modified residue	UNP P75743
E	1	MSE	MET	modified residue	UNP P75743

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
E	78	MSE	MET	modified residue	UNP P75743
E	121	MSE	MET	modified residue	UNP P75743
E	135	MSE	MET	modified residue	UNP P75743
F	1	MSE	MET	modified residue	UNP P75743
F	78	MSE	MET	modified residue	UNP P75743
F	121	MSE	MET	modified residue	UNP P75743
F	135	MSE	MET	modified residue	UNP P75743

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Fe 2 2	0	0
2	B	2	Total Fe 2 2	0	0
2	C	2	Total Fe 2 2	0	0
2	D	2	Total Fe 2 2	0	0
2	E	2	Total Fe 2 2	0	0
2	F	2	Total Fe 2 2	0	0

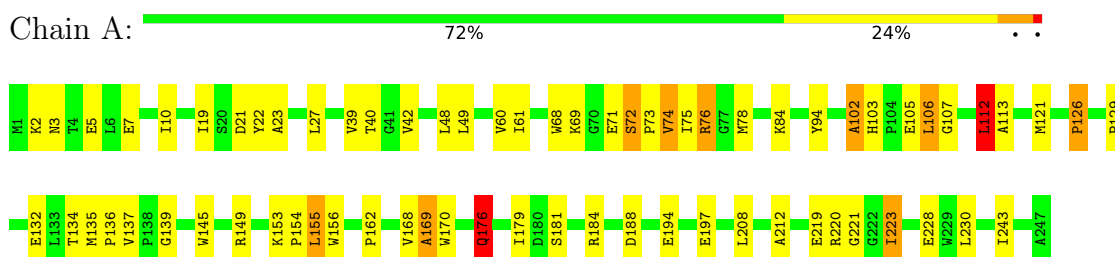
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	95	Total O 95 95	0	0
3	B	89	Total O 89 89	0	0
3	C	94	Total O 94 94	0	0
3	D	114	Total O 114 114	0	0
3	E	113	Total O 113 113	0	0
3	F	132	Total O 132 132	0	0

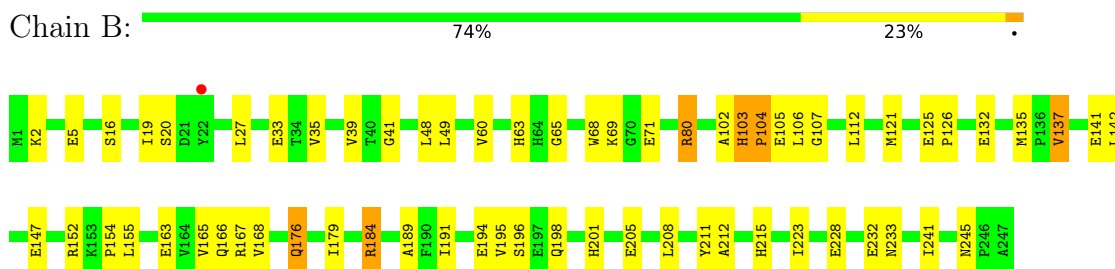
### 3 Residue-property plots

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.

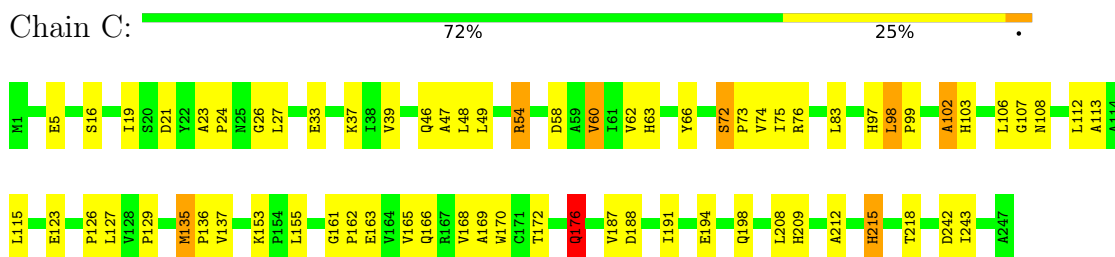
- Molecule 1: Hypothetical protein ybgI



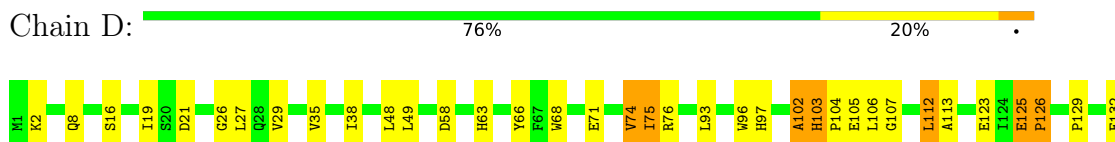
- Molecule 1: Hypothetical protein ybgI



- Molecule 1: Hypothetical protein ybgI



- Molecule 1: Hypothetical protein ybgI





- Molecule 1: Hypothetical protein ybgI

Chain E: 72% 24% ..



- Molecule 1: Hypothetical protein ybgI

Chain F: 75% 20% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	154.66Å 154.66Å 57.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.60 – 2.20 19.60 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.2 (19.60-2.20) 95.0 (19.60-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.211 , 0.259 0.210 , 0.259	Depositor DCC
$R_{free}$ test set	6082 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.8	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l 0.021 for h,-h-k,-l 0.014 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	12031	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% 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

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	1.35	2/1937 (0.1%)	1.54	32/2632 (1.2%)
1	B	1.35	3/1937 (0.2%)	1.48	20/2632 (0.8%)
1	C	1.39	6/1937 (0.3%)	1.48	29/2632 (1.1%)
1	D	1.36	2/1937 (0.1%)	1.48	26/2632 (1.0%)
1	E	1.41	3/1937 (0.2%)	1.49	20/2632 (0.8%)
1	F	1.41	6/1937 (0.3%)	1.55	27/2632 (1.0%)
All	All	1.38	22/11622 (0.2%)	1.50	154/15792 (1.0%)

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	B	0	1
1	D	0	1
All	All	0	2

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	ILE	CA-CB	-8.77	1.44	1.53
1	C	62	VAL	CA-C	-5.96	1.46	1.52
1	B	154	PRO	CA-C	-5.93	1.46	1.52
1	C	126	PRO	CA-C	5.89	1.60	1.52
1	F	126	PRO	C-O	5.83	1.31	1.24

The worst 5 of 154 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	135	MSE	CA-C-N	10.63	132.31	119.98
1	F	135	MSE	C-N-CA	10.63	132.31	119.98
1	D	16	SER	N-CA-C	9.55	122.89	111.33
1	A	220	ARG	N-CA-C	-9.21	102.17	113.41
1	B	102	ALA	N-CA-C	9.19	124.62	113.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	211	TYR	Sidechain
1	D	66	TYR	Sidechain

## 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	1897	0	1866	32	0
1	B	1897	0	1866	28	0
1	C	1897	0	1866	24	0
1	D	1897	0	1866	22	0
1	E	1897	0	1866	38	0
1	F	1897	0	1866	29	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	95	0	0	0	0
3	B	89	0	0	3	0
3	C	94	0	0	4	0
3	D	114	0	0	1	0
3	E	113	0	0	5	0
3	F	132	0	0	2	0
All	All	12031	0	11196	169	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 7.

The worst 5 of 169 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:135:MSE:CG	1:F:136:PRO:HD2	1.85	1.06
1:A:40:THR:HB	1:A:223:ILE:HD11	1.38	1.05
1:F:135:MSE:HG3	1:F:136:PRO:CD	1.91	1.00
1:E:75:ILE:HD12	1:E:80:ARG:HA	1.45	0.98
1:F:135:MSE:HG3	1:F:136:PRO:HD2	0.94	0.92

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	245/247 (99%)	237 (97%)	7 (3%)	1 (0%)	30	34
1	B	245/247 (99%)	234 (96%)	11 (4%)	0	100	100
1	C	245/247 (99%)	236 (96%)	9 (4%)	0	100	100
1	D	245/247 (99%)	235 (96%)	8 (3%)	2 (1%)	16	16
1	E	245/247 (99%)	233 (95%)	12 (5%)	0	100	100
1	F	245/247 (99%)	234 (96%)	11 (4%)	0	100	100
All	All	1470/1482 (99%)	1409 (96%)	58 (4%)	3 (0%)	43	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	74	VAL
1	D	126	PRO
1	A	162	PRO

### 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	197/193 (102%)	182 (92%)	15 (8%)	12	14
1	B	197/193 (102%)	184 (93%)	13 (7%)	15	18
1	C	197/193 (102%)	187 (95%)	10 (5%)	21	27
1	D	197/193 (102%)	184 (93%)	13 (7%)	15	18
1	E	197/193 (102%)	183 (93%)	14 (7%)	13	16
1	F	197/193 (102%)	184 (93%)	13 (7%)	15	18
All	All	1182/1158 (102%)	1104 (93%)	78 (7%)	15	18

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	75	ILE
1	F	112	LEU
1	E	112	LEU
1	F	27	LEU
1	F	165	VAL

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	F	46	GLN
1	F	36	GLN
1	C	206	GLN
1	E	46	GLN
1	C	166	GLN

### 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 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	243/247 (98%)	-0.35	0 <b>100</b> <b>100</b>	9, 16, 26, 31	0
1	B	243/247 (98%)	-0.32	1 (0%) <b>88</b> <b>87</b>	8, 17, 28, 30	0
1	C	243/247 (98%)	-0.40	0 <b>100</b> <b>100</b>	8, 15, 25, 30	0
1	D	243/247 (98%)	-0.38	1 (0%) <b>88</b> <b>87</b>	9, 15, 27, 31	0
1	E	243/247 (98%)	-0.41	1 (0%) <b>88</b> <b>87</b>	6, 15, 25, 32	0
1	F	243/247 (98%)	-0.46	0 <b>100</b> <b>100</b>	5, 14, 22, 29	0
All	All	1458/1482 (98%)	-0.39	3 (0%) <b>91</b> <b>90</b>	5, 15, 26, 32	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	22	TYR	2.3
1	D	232	GLU	2.0
1	E	22	TYR	2.0

### 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 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	F	301	1/1	0.94	0.13	30,30,30,30	0
2	FE	B	301	1/1	0.96	0.19	27,27,27,27	0
2	FE	C	302	1/1	0.96	0.11	26,26,26,26	0
2	FE	D	302	1/1	0.96	0.14	18,18,18,18	0
2	FE	A	301	1/1	0.96	0.17	30,30,30,30	0
2	FE	C	301	1/1	0.97	0.13	27,27,27,27	0
2	FE	E	301	1/1	0.97	0.14	22,22,22,22	0
2	FE	E	302	1/1	0.97	0.16	17,17,17,17	0
2	FE	B	302	1/1	0.97	0.12	22,22,22,22	0
2	FE	F	302	1/1	0.98	0.14	21,21,21,21	0
2	FE	D	301	1/1	0.99	0.17	27,27,27,27	0
2	FE	A	302	1/1	0.99	0.09	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.