



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 23, 2024 – 08:29 AM EDT

PDB ID : 6DZX
Title : Crystal structure of the *N. meningitidis* methionine-binding protein in its D-methionine bound conformation.
Authors : Nguyen, P.T.; Lai, J.Y.; Kaiser, J.T.; Rees, D.C.
Deposited on : 2018-07-05
Resolution : 1.68 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

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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.20.1
EDS : 2.37.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

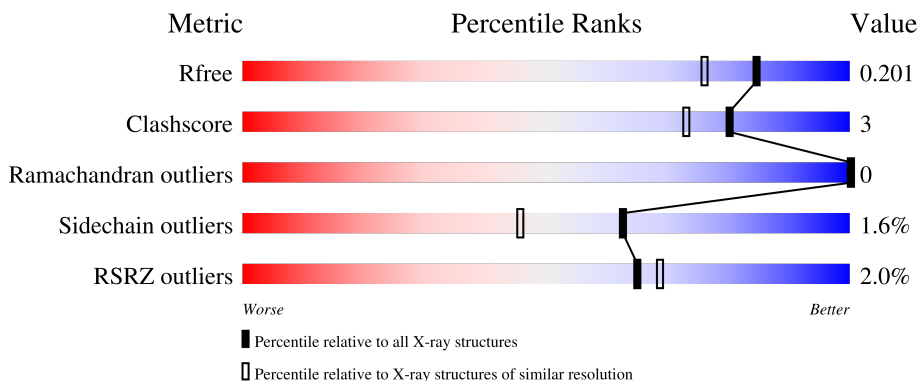
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.68 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}	130704	6780 (1.70-1.66)
Clashscore	141614	7310 (1.70-1.66)
Ramachandran outliers	138981	7173 (1.70-1.66)
Sidechain outliers	138945	7172 (1.70-1.66)
RSRZ outliers	127900	6661 (1.70-1.66)

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 ≥ 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	 91% 5% . .
1	B	247	 93% 5% .
1	C	247	 5% 90% 6% . .
1	D	247	 93% . . .
1	E	247	 3% 94% . .

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Mol	Chain	Length	Quality of chain
1	F	247	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into three segments: a large green segment (87%), a smaller yellow segment (9%), and a very small grey segment (4%). A small red square is at the beginning of the bar. The percentage values are printed below the bar.</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 24101 atoms, of which 11260 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 Lipoprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	240	3754	1215	1860	307	369	3	0	0	0
1	B	241	3775	1221	1872	309	370	3	0	0	0
1	C	241	3760	1218	1861	308	370	3	0	0	0
1	D	241	3775	1221	1872	309	370	3	0	0	0
1	E	242	3782	1223	1875	310	371	3	0	0	0
1	F	240	3754	1215	1860	307	369	3	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

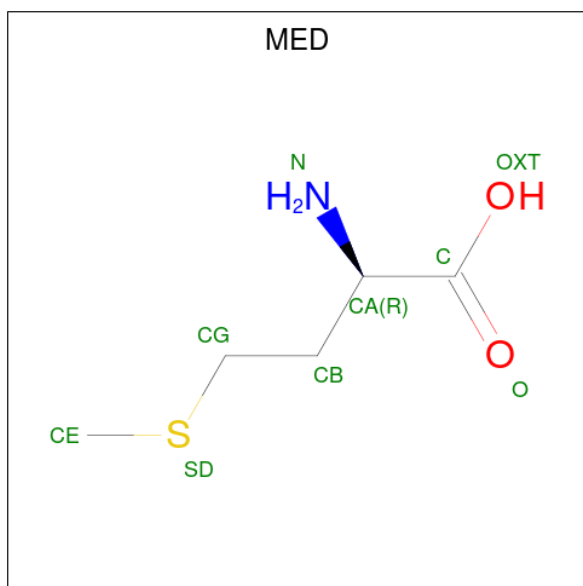
Chain	Residue	Modelled	Actual	Comment	Reference
A	41	LYS	-	expression tag	UNP C6S9R8
A	42	HIS	-	expression tag	UNP C6S9R8
A	64	ALA	PRO	conflict	UNP C6S9R8
B	41	LYS	-	expression tag	UNP C6S9R8
B	42	HIS	-	expression tag	UNP C6S9R8
B	64	ALA	PRO	conflict	UNP C6S9R8
C	41	LYS	-	expression tag	UNP C6S9R8
C	42	HIS	-	expression tag	UNP C6S9R8
C	64	ALA	PRO	conflict	UNP C6S9R8
D	41	LYS	-	expression tag	UNP C6S9R8
D	42	HIS	-	expression tag	UNP C6S9R8
D	64	ALA	PRO	conflict	UNP C6S9R8
E	41	LYS	-	expression tag	UNP C6S9R8
E	42	HIS	-	expression tag	UNP C6S9R8
E	64	ALA	PRO	conflict	UNP C6S9R8
F	41	LYS	-	expression tag	UNP C6S9R8
F	42	HIS	-	expression tag	UNP C6S9R8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	64	ALA	PRO	conflict	UNP C6S9R8

- Molecule 2 is D-METHIONINE (three-letter code: MED) (formula: C₅H₁₁NO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
2	A	1	Total	C	H	N	O	S	0	0
			19	5	10	1	2	1		
2	B	1	Total	C	H	N	O	S	0	0
			19	5	10	1	2	1		
2	C	1	Total	C	H	N	O	S	0	0
			19	5	10	1	2	1		
2	D	1	Total	C	H	N	O	S	0	0
			19	5	10	1	2	1		
2	E	1	Total	C	H	N	O	S	0	0
			19	5	10	1	2	1		
2	F	1	Total	C	H	N	O	S	0	0
			19	5	10	1	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	251	Total	O	0	0
			251	251		
3	B	244	Total	O	0	0
			244	244		
3	C	207	Total	O	0	0
			207	207		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	246	Total 246	O 246	0	0
3	E	209	Total 209	O 209	0	0
3	F	230	Total 230	O 230	0	0

3 Residue-property plots [i](#)

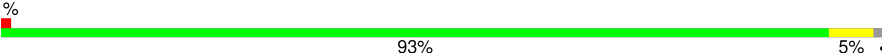
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

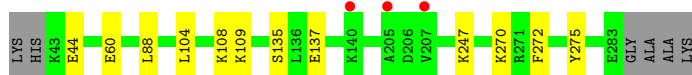
- Molecule 1: Lipoprotein

Chain A:  91% 5% . . .




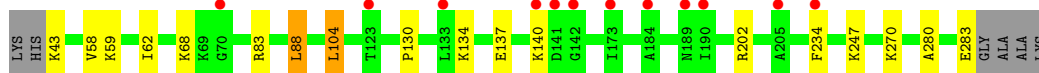
- Molecule 1: Lipoprotein

Chain B:  93% 5% .

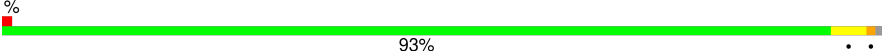


- Molecule 1: Lipoprotein

Chain C:  90% 6% . . .



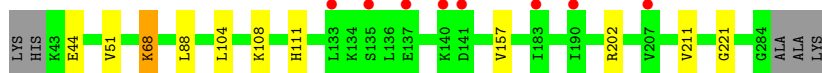
- Molecule 1: Lipoprotein

Chain D:  93% . . .

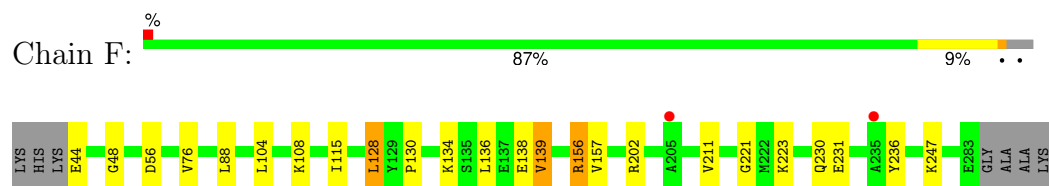


- Molecule 1: Lipoprotein

Chain E:  94% . . .



- Molecule 1: Lipoprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.66Å 87.93Å 91.64Å 114.83° 104.12° 105.39°	Depositor
Resolution (Å)	39.67 – 1.68 39.67 – 1.68	Depositor EDS
% Data completeness (in resolution range)	96.0 (39.67-1.68) 96.4 (39.67-1.68)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.68Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.176 , 0.201 0.177 , 0.201	Depositor DCC
R_{free} test set	11107 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtrriage
Anisotropy	0.507	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	24101	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MED

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	0.50	0/1936	0.65	2/2626 (0.1%)
1	B	0.52	0/1945	0.63	0/2637
1	C	0.50	0/1941	0.64	2/2633 (0.1%)
1	D	0.49	0/1945	0.66	2/2637 (0.1%)
1	E	0.49	0/1949	0.63	0/2642
1	F	0.51	0/1936	0.85	4/2626 (0.2%)
All	All	0.50	0/11652	0.68	10/15801 (0.1%)

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	156	ARG	NE-CZ-NH2	-20.03	110.29	120.30
1	F	156	ARG	NE-CZ-NH1	17.93	129.26	120.30
1	F	128	LEU	CA-CB-CG	7.09	131.62	115.30
1	D	128	LEU	CA-CB-CG	6.80	130.95	115.30
1	D	88	LEU	CA-CB-CG	5.79	128.61	115.30

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	1894	1860	1863	12	0
1	B	1903	1872	1876	8	0
1	C	1899	1861	1865	10	0
1	D	1903	1872	1876	9	0
1	E	1907	1875	1879	10	0
1	F	1894	1860	1863	18	0
2	A	9	10	10	0	0
2	B	9	10	10	0	0
2	C	9	10	10	0	0
2	D	9	10	10	0	0
2	E	9	10	10	0	0
2	F	9	10	10	0	0
3	A	251	0	0	6	1
3	B	244	0	0	2	0
3	C	207	0	0	6	0
3	D	246	0	0	5	0
3	E	209	0	0	4	0
3	F	230	0	0	7	1
All	All	12841	11260	11282	61	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 3.

The worst 5 of 61 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:C:43:LYS:N	3:C:1101:HOH:O	2.03	0.90
1:F:156:ARG:HD2	1:F:231:GLU:OE2	1.71	0.90
1:F:44:GLU:N	3:F:1101:HOH:O	2.07	0.88
1:B:247:LYS:NZ	3:B:1102:HOH:O	2.06	0.87
1:B:44:GLU:OE2	3:B:1101:HOH:O	1.92	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)
3:A:1264:HOH:O	3:F:1288:HOH:O[1_545]	2.09	0.11

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	238/247 (96%)	233 (98%)	5 (2%)	0	100	100
1	B	239/247 (97%)	234 (98%)	5 (2%)	0	100	100
1	C	239/247 (97%)	234 (98%)	5 (2%)	0	100	100
1	D	239/247 (97%)	234 (98%)	5 (2%)	0	100	100
1	E	240/247 (97%)	235 (98%)	5 (2%)	0	100	100
1	F	238/247 (96%)	233 (98%)	5 (2%)	0	100	100
All	All	1433/1482 (97%)	1403 (98%)	30 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	203/207 (98%)	201 (99%)	2 (1%)	76	65
1	B	204/207 (99%)	202 (99%)	2 (1%)	76	65
1	C	203/207 (98%)	198 (98%)	5 (2%)	47	26
1	D	204/207 (99%)	200 (98%)	4 (2%)	55	36
1	E	204/207 (99%)	201 (98%)	3 (2%)	65	48
1	F	203/207 (98%)	199 (98%)	4 (2%)	55	36
All	All	1221/1242 (98%)	1201 (98%)	20 (2%)	62	46

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	88	LEU
1	F	104	LEU
1	F	139	VAL
1	F	128	LEU
1	C	104	LEU

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

Mol	Chain	Res	Type
1	E	111	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	MED	C	1001	-	7,8,8	0.83	0	5,9,9	1.04	1 (20%)
2	MED	D	1001	-	7,8,8	0.91	0	5,9,9	0.92	0
2	MED	E	1001	-	7,8,8	0.84	0	5,9,9	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MED	B	1001	-	7,8,8	1.06	1 (14%)	5,9,9	1.91	2 (40%)
2	MED	F	1001	-	7,8,8	1.18	1 (14%)	5,9,9	1.43	1 (20%)
2	MED	A	1001	-	7,8,8	0.95	0	5,9,9	0.92	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	MED	C	1001	-	-	4/8/8/8	-
2	MED	D	1001	-	-	4/8/8/8	-
2	MED	E	1001	-	-	4/8/8/8	-
2	MED	B	1001	-	-	5/8/8/8	-
2	MED	F	1001	-	-	5/8/8/8	-
2	MED	A	1001	-	-	4/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1001	MED	OXT-C	-2.31	1.23	1.30
2	B	1001	MED	OXT-C	-2.09	1.24	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	MED	CB-CA-N	-3.13	101.97	110.12
2	F	1001	MED	CB-CA-C	2.93	118.22	110.45
2	B	1001	MED	CB-CA-C	2.81	117.88	110.45
2	C	1001	MED	CB-CA-C	2.01	115.78	110.45

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	MED	O-C-CA-N
2	B	1001	MED	O-C-CA-N
2	C	1001	MED	O-C-CA-N
2	D	1001	MED	O-C-CA-N
2	F	1001	MED	O-C-CA-N

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, 95th 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 ²)	Q<0.9
1	A	240/247 (97%)	-0.12	1 (0%) 92 93	22, 31, 51, 73	0
1	B	241/247 (97%)	-0.08	3 (1%) 79 82	22, 31, 51, 74	0
1	C	241/247 (97%)	0.14	12 (4%) 28 30	22, 32, 50, 84	0
1	D	241/247 (97%)	0.09	3 (1%) 79 82	23, 30, 48, 76	0
1	E	242/247 (97%)	0.04	8 (3%) 46 49	24, 33, 52, 90	0
1	F	240/247 (97%)	0.01	2 (0%) 86 88	23, 31, 51, 83	0
All	All	1445/1482 (97%)	0.01	29 (2%) 65 69	22, 31, 51, 90	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	190	ILE	3.8
1	E	140	LYS	3.0
1	E	190	ILE	2.8
1	E	133	LEU	2.7
1	F	205	ALA	2.7

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 monosaccharides 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, 95th 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(\AA^2)	Q<0.9
2	MED	C	1001	9/9	0.86	0.20	26,32,38,47	0
2	MED	D	1001	9/9	0.98	0.17	24,29,35,35	0
2	MED	F	1001	9/9	0.98	0.13	24,30,37,37	0
2	MED	B	1001	9/9	0.99	0.11	23,27,39,39	0
2	MED	E	1001	9/9	0.99	0.10	22,29,37,37	0
2	MED	A	1001	9/9	0.99	0.10	20,32,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.