



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 06:42 AM UTC

PDB ID : 5VYF / pdb_00005vyf
Title : Structure of single chain Fel d 1 bound to a neutralizing antibody
Authors : Franklin, M.C.
Deposited on : 2017-05-25
Resolution : 2.90 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	:	4-5-2 with Phenix2.0
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

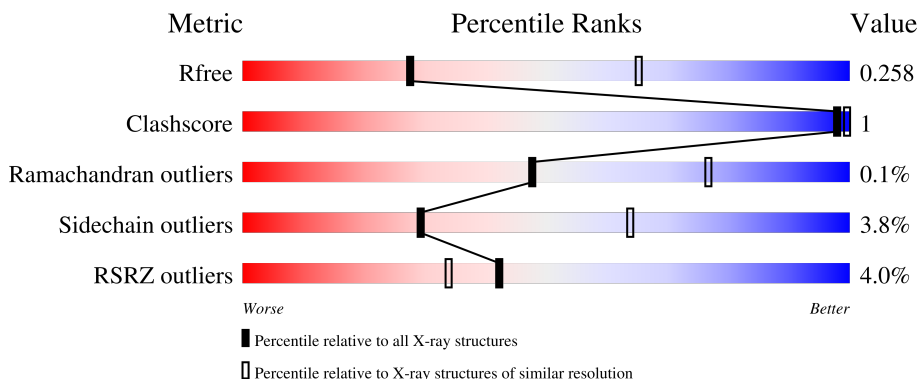
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	214	5% 94% • •
1	L	214	95% 5%
2	B	220	5% 87% 5% 7%
2	H	220	4% 87% 6% • 6%
3	C	199	3% 66% • 32%

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Mol	Chain	Length	Quality of chain
3	F	199	5% 66% . 31%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8563 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 Antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	2	0
			1638	1027	274	332	5			
1	A	211	Total	C	N	O	S	0	2	0
			1625	1020	272	328	5			

- Molecule 2 is a protein called Antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	206	Total	C	N	O	S	0	0	0
			1548	977	258	307	6			
2	B	205	Total	C	N	O	S	0	0	0
			1538	972	257	303	6			

- Molecule 3 is a protein called Chimera of Major allergen I polypeptide chain 2, Major allergen I polypeptide chain 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	137	Total	C	N	O	S	0	0	0
			1059	672	168	210	9			
3	C	136	Total	C	N	O	S	0	0	0
			1052	668	167	208	9			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	33	ALA	ASN	engineered mutation	UNP P30440
F	152	LEU	VAL	variant	UNP P30438
F	163	GLY	-	expression tag	UNP P30438
F	164	PRO	-	expression tag	UNP P30438
F	165	GLY	-	expression tag	UNP P30438
F	166	GLY	-	expression tag	UNP P30438
F	167	GLU	-	expression tag	UNP P30438

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Chain	Residue	Modelled	Actual	Comment	Reference
F	168	GLN	-	expression tag	UNP P30438
F	169	LYS	-	expression tag	UNP P30438
F	170	LEU	-	expression tag	UNP P30438
F	171	ILE	-	expression tag	UNP P30438
F	172	SER	-	expression tag	UNP P30438
F	173	GLU	-	expression tag	UNP P30438
F	174	GLU	-	expression tag	UNP P30438
F	175	ASP	-	expression tag	UNP P30438
F	176	LEU	-	expression tag	UNP P30438
F	177	GLY	-	expression tag	UNP P30438
F	178	GLY	-	expression tag	UNP P30438
F	179	GLU	-	expression tag	UNP P30438
F	180	GLN	-	expression tag	UNP P30438
F	181	LYS	-	expression tag	UNP P30438
F	182	LEU	-	expression tag	UNP P30438
F	183	ILE	-	expression tag	UNP P30438
F	184	SER	-	expression tag	UNP P30438
F	185	GLU	-	expression tag	UNP P30438
F	186	GLU	-	expression tag	UNP P30438
F	187	ASP	-	expression tag	UNP P30438
F	188	LEU	-	expression tag	UNP P30438
F	189	SER	-	expression tag	UNP P30438
F	190	GLY	-	expression tag	UNP P30438
F	191	HIS	-	expression tag	UNP P30438
F	192	HIS	-	expression tag	UNP P30438
F	193	HIS	-	expression tag	UNP P30438
F	194	HIS	-	expression tag	UNP P30438
F	195	HIS	-	expression tag	UNP P30438
F	196	HIS	-	expression tag	UNP P30438
F	197	SER	-	expression tag	UNP P30438
F	198	SER	-	expression tag	UNP P30438
F	199	GLY	-	expression tag	UNP P30438
C	33	ALA	ASN	engineered mutation	UNP P30440
C	152	LEU	VAL	variant	UNP P30438
C	163	GLY	-	expression tag	UNP P30438
C	164	PRO	-	expression tag	UNP P30438
C	165	GLY	-	expression tag	UNP P30438
C	166	GLY	-	expression tag	UNP P30438
C	167	GLU	-	expression tag	UNP P30438
C	168	GLN	-	expression tag	UNP P30438
C	169	LYS	-	expression tag	UNP P30438
C	170	LEU	-	expression tag	UNP P30438

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Chain	Residue	Modelled	Actual	Comment	Reference
C	171	ILE	-	expression tag	UNP P30438
C	172	SER	-	expression tag	UNP P30438
C	173	GLU	-	expression tag	UNP P30438
C	174	GLU	-	expression tag	UNP P30438
C	175	ASP	-	expression tag	UNP P30438
C	176	LEU	-	expression tag	UNP P30438
C	177	GLY	-	expression tag	UNP P30438
C	178	GLY	-	expression tag	UNP P30438
C	179	GLU	-	expression tag	UNP P30438
C	180	GLN	-	expression tag	UNP P30438
C	181	LYS	-	expression tag	UNP P30438
C	182	LEU	-	expression tag	UNP P30438
C	183	ILE	-	expression tag	UNP P30438
C	184	SER	-	expression tag	UNP P30438
C	185	GLU	-	expression tag	UNP P30438
C	186	GLU	-	expression tag	UNP P30438
C	187	ASP	-	expression tag	UNP P30438
C	188	LEU	-	expression tag	UNP P30438
C	189	SER	-	expression tag	UNP P30438
C	190	GLY	-	expression tag	UNP P30438
C	191	HIS	-	expression tag	UNP P30438
C	192	HIS	-	expression tag	UNP P30438
C	193	HIS	-	expression tag	UNP P30438
C	194	HIS	-	expression tag	UNP P30438
C	195	HIS	-	expression tag	UNP P30438
C	196	HIS	-	expression tag	UNP P30438
C	197	SER	-	expression tag	UNP P30438
C	198	SER	-	expression tag	UNP P30438
C	199	GLY	-	expression tag	UNP P30438

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total Ca 1 1	0	0
4	C	1	Total Ca 1 1	0	0

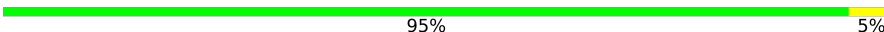
- Molecule 5 is water.

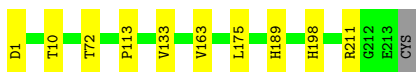
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	30	Total 30	O 30	0	0
5	H	14	Total 14	O 14	0	0
5	F	13	Total 13	O 13	0	0
5	A	22	Total 22	O 22	0	0
5	B	17	Total 17	O 17	0	0
5	C	5	Total 5	O 5	0	0

3 Residue-property plots [i](#)

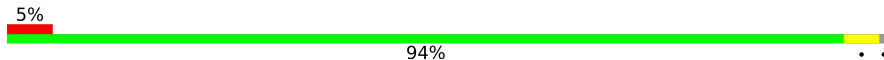
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

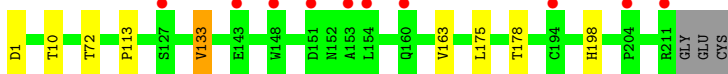
- Molecule 1: Antibody light chain

Chain L: 



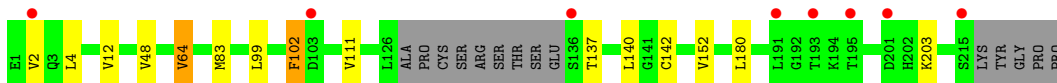
- Molecule 1: Antibody light chain

Chain A: 



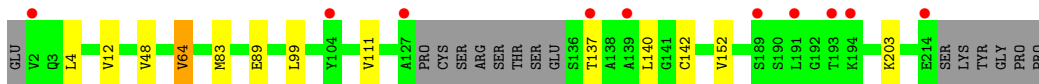
- Molecule 2: Antibody Fab heavy chain

Chain H: 



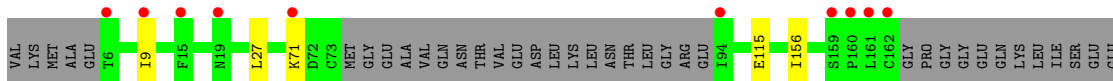
- Molecule 2: Antibody Fab heavy chain

Chain B: 



- Molecule 3: Chimera of Major allergen I polypeptide chain 2, Major allergen I polypeptide chain 1

Chain F: 



ASP
LEU
GLY
GLY
GLU
GLN
LYS
LEU
ILE
SER
GLU
GLU
ASP
LEU
SER
GLY
HIS
HIS
HIS
HIS
HIS
SER
SER
GLY

- Molecule 3: Chimera of Major allergen I polypeptide chain 2, Major allergen I polypeptide chain 1



VAL
LYS
MET
ALA
THR
C7
P8
I9
L27
T66
K71
D72
C73
MET
GLY
GLU
ALA
VAL
GLN
ASN
THR
VAL
GLU
ASP
LEU
LYS
LEU
ASN
THR
LEU
GLY
ARG
GLU
I94
E115
I156
P160
L161
C162
GLY
PRO
GLY
GLY
GLU
GLN
LYS
LEU
ILE
SER
GLU
ASP
LEU

GLY
GLY
GLU
GLN
LYS
LEU
ILE
SER
GLU
GLU
ASP
LEU
SER
GLY
HIS
HIS
HIS
HIS
SER
SER
GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.98Å 131.48Å 148.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.40 – 2.90 98.40 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (98.40-2.90) 98.1 (98.40-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.225 , 0.259 0.228 , 0.258	Depositor DCC
R_{free} test set	1652 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8563	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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 22.90 % 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 5.1931e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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:
CA

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	0.54	0/1661	0.69	0/2255
1	L	0.53	0/1674	0.69	0/2272
2	B	0.54	0/1573	0.75	1/2140 (0.0%)
2	H	0.53	0/1583	0.77	2/2153 (0.1%)
3	C	0.57	0/1065	0.86	0/1444
3	F	0.57	0/1072	0.86	0/1454
All	All	0.54	0/8628	0.76	3/11718 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	102	PHE	N-CA-C	8.49	122.94	112.58
2	H	64	VAL	N-CA-CB	-5.44	106.23	112.21
2	B	64	VAL	N-CA-CB	-5.37	106.31	112.21

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	1625	0	1581	3	0
1	L	1638	0	1590	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1538	0	1498	1	0
2	H	1548	0	1507	2	0
3	C	1052	0	1064	1	0
3	F	1059	0	1071	1	0
4	C	1	0	0	0	0
4	F	1	0	0	0	0
5	A	22	0	0	0	0
5	B	17	0	0	0	0
5	C	5	0	0	0	0
5	F	13	0	0	0	0
5	H	14	0	0	0	0
5	L	30	0	0	0	0
All	All	8563	0	8311	11	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 1.

The worst 5 of 11 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)
3:F:9:ILE:HG23	3:F:156:ILE:HG23	1.94	0.49
3:C:9:ILE:HG23	3:C:156:ILE:HG23	1.94	0.48
1:L:163:VAL:HG22	1:L:175:LEU:HD12	1.97	0.46
1:A:163:VAL:HG22	1:A:175:LEU:HD12	1.97	0.46
1:L:189:HIS:O	1:L:211:ARG:NH1	2.49	0.46

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	209/214 (98%)	200 (96%)	9 (4%)	0	100	100
1	L	211/214 (99%)	203 (96%)	8 (4%)	0	100	100
2	B	201/220 (91%)	197 (98%)	4 (2%)	0	100	100
2	H	202/220 (92%)	197 (98%)	4 (2%)	1 (0%)	24	54
3	C	132/199 (66%)	131 (99%)	1 (1%)	0	100	100
3	F	133/199 (67%)	132 (99%)	1 (1%)	0	100	100
All	All	1088/1266 (86%)	1060 (97%)	27 (2%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	2	VAL

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	186/188 (99%)	182 (98%)	4 (2%)	45	77
1	L	187/188 (100%)	183 (98%)	4 (2%)	47	77
2	B	170/184 (92%)	159 (94%)	11 (6%)	15	44
2	H	172/184 (94%)	161 (94%)	11 (6%)	16	44
3	C	121/173 (70%)	118 (98%)	3 (2%)	42	74
3	F	122/173 (70%)	119 (98%)	3 (2%)	42	74
All	All	958/1090 (88%)	922 (96%)	36 (4%)	29	64

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	137	THR
3	C	115	GLU
2	B	140	LEU
2	B	203	LYS

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Mol	Chain	Res	Type
2	H	142	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	57	ASN
2	B	166	HIS
2	H	166	HIS
1	A	137	ASN
1	A	155	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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, 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	211/214 (98%)	0.57	10 (4%) 36 28	34, 63, 125, 147	1 (0%)
1	L	213/214 (99%)	0.20	0 100 100	33, 51, 72, 82	1 (0%)
2	B	205/220 (93%)	0.44	10 (4%) 35 27	33, 54, 112, 151	0
2	H	206/220 (93%)	0.27	8 (3%) 43 35	31, 47, 85, 105	0
3	C	136/199 (68%)	0.55	6 (4%) 39 30	41, 62, 109, 127	0
3	F	137/199 (68%)	0.43	10 (7%) 21 17	37, 52, 90, 107	0
All	All	1108/1266 (87%)	0.40	44 (3%) 42 34	31, 54, 108, 151	2 (0%)

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	161	LEU	3.9
3	F	94	ILE	3.6
1	A	211	ARG	3.5
2	H	103	ASP	3.4
2	B	127	ALA	3.1

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, 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(Å ²)	Q<0.9
4	CA	F	201	1/1	0.94	0.07	35,35,35,35	0
4	CA	C	201	1/1	0.96	0.07	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.