Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 03:36 AM EDT

PDB ID	:	5VYF
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 Full wwPDB X-ray Structure Validation 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 (i) 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 (1)) were used in the production of this report:

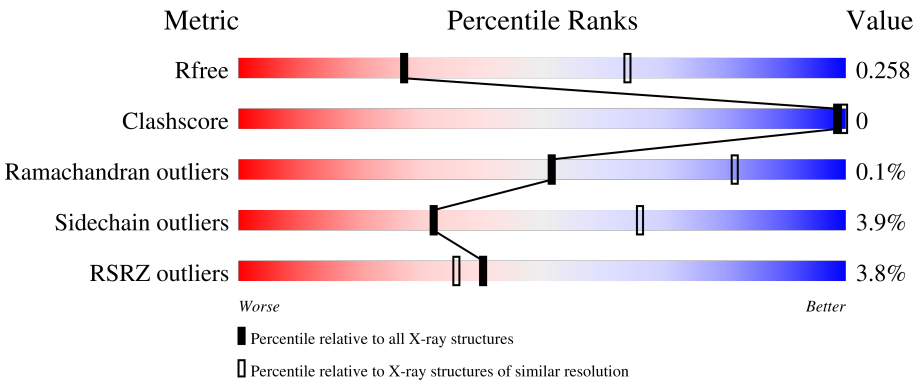
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 <=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	9% 94%
1	L	214	95% 5%
2	B	220	7% 89% 5% 7%
2	H	220	% 89% 5% 6%
3	C	199	% 65% 32%

Continued on next page...

Continued from previous page...

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

2 Entry composition (i)

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
			Total	C	N	O	S			
1	L	213	1638	1027	274	332	5	0	2	0
1	A	211	1625	1020	272	328	5	0	2	0

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

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

- 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
			Total	C	N	O	S			
3	F	137	1059	672	168	210	9	0	0	0
3	C	136	1052	668	167	208	9	0	0	0

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is water.

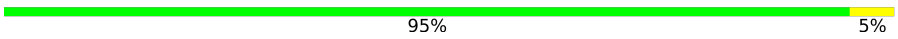
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	L	30	30	30	0	0
			Total	O		
5	H	14	14	14	0	0
			Total	O		
5	F	13	13	13	0	0
			Total	O		
5	A	22	22	22	0	0
			Total	O		
5	B	17	17	17	0	0
			Total	O		
5	C	5	5	5	0	0

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.

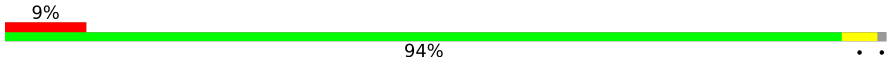
• Molecule 1: Antibody light chain

Chain L:



• Molecule 1: Antibody light chain

Chain A:

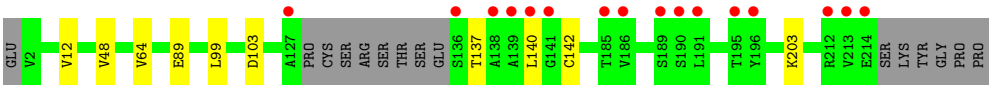


• Molecule 2: Antibody Fab heavy chain

Chain H:

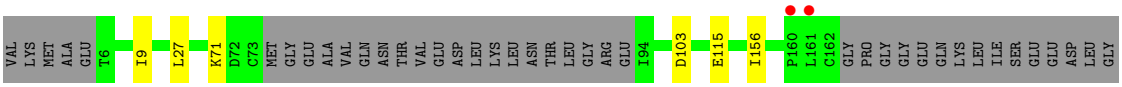
• Molecule 2: Antibody Fab heavy chain

Chain B:



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

Chain F:



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

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

Chain C:

VAL LYS MET ALA GLU THR C7 P8 I9 L27 S28 S69 S70 K71 D72 C73 MET GLY GLU ALA VAL GLN ASN THR VAL GLU ASP LEU LYS LEU ASN THR LEU GLY ARG GLU I94 D103 E115 I156 C162 GLY PRO GLY GLY GLU GLN LYS LEU ILE SER GLU GLU ASP

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

4 Data and refinement statistics (i)

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 49.43 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (98.40-2.90) 98.2 (49.43-2.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	1643 reflections (5.05%)	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 , 36.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.37	0/1661	0.59	0/2255
1	L	0.37	0/1674	0.59	0/2272
2	B	0.39	0/1573	0.63	0/2140
2	H	0.38	0/1583	0.64	0/2153
3	C	0.39	0/1065	0.53	0/1444
3	F	0.39	0/1072	0.54	0/1454
All	All	0.38	0/8628	0.59	0/11718

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 (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
2	B	1538	0	1498	0	0
2	H	1548	0	1507	0	0
3	C	1052	0	1064	1	0
3	F	1059	0	1071	1	0
4	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	8	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 0.

All (8) 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
1:A:113:PRO:HD3	1:A:198:HIS:CD2	2.53	0.44
1:L:113:PRO:HD3	1:L:198:HIS:CD2	2.55	0.42
1:A:133:VAL:HG12	1:A:178:THR:HG23	2.03	0.41

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	201/220 (91%)	197 (98%)	4 (2%)	0	100	100
2	H	202/220 (92%)	197 (98%)	4 (2%)	1 (0%)	29	61
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%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	2	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	186/188 (99%)	182 (98%)	4 (2%)	52	81
1	L	187/188 (100%)	183 (98%)	4 (2%)	53	81
2	B	170/184 (92%)	160 (94%)	10 (6%)	19	49
2	H	172/184 (94%)	162 (94%)	10 (6%)	20	50
3	C	121/173 (70%)	116 (96%)	5 (4%)	30	64
3	F	122/173 (70%)	118 (97%)	4 (3%)	38	72
All	All	958/1090 (88%)	921 (96%)	37 (4%)	32	66

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	10	THR
1	L	72	THR
1	L	133	VAL
2	H	12	VAL
2	H	48	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	64	VAL
2	H	99	LEU
2	H	102	PHE
2	H	103	ASP
2	H	137	THR
2	H	140	LEU
2	H	142	CYS
2	H	203	LYS
3	F	27	LEU
3	F	71	LYS
3	F	103	ASP
3	F	115	GLU
1	A	1	ASP
1	A	10	THR
1	A	72	THR
1	A	133	VAL
2	B	12	VAL
2	B	48	VAL
2	B	64	VAL
2	B	89	GLU
2	B	99	LEU
2	B	103	ASP
2	B	137	THR
2	B	140	LEU
2	B	142	CYS
2	B	203	LYS
3	C	27	LEU
3	C	28	SER
3	C	71	LYS
3	C	103	ASP
3	C	115	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	198	HIS
1	A	198	HIS
2	B	57	ASN

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)

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	20 (9%)	8	6	34, 64, 125, 147	1 (0%)
1	L	213/214 (99%)	0.11	0	100	100	33, 51, 72, 82	1 (0%)
2	B	205/220 (93%)	0.43	16 (7%)	13	10	33, 54, 112, 151	0
2	H	206/220 (93%)	0.16	3 (1%)	73	73	31, 47, 85, 105	0
3	C	136/199 (68%)	0.40	1 (0%)	87	87	41, 62, 109, 127	0
3	F	137/199 (68%)	0.27	2 (1%)	73	73	37, 52, 90, 107	0
All	All	1108/1266 (87%)	0.32	42 (3%)	40	36	31, 54, 108, 151	2 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	136	SER	5.4
1	A	181	LEU	5.1
2	B	140	LEU	4.9
2	B	189	SER	4.7
2	B	191	LEU	3.9
2	B	214	GLU	3.8
2	B	213	VAL	3.5
2	B	139	ALA	3.4
2	B	195	THR	3.4
2	H	195	THR	3.4
1	A	183	LYS	3.2
2	B	190	SER	3.0
2	B	186	VAL	3.0
1	A	153	ALA	3.0
2	B	196	TYR	3.0
2	B	185	THR	2.9
2	H	215	SER	2.8
1	A	191	VAL	2.7
2	B	141	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	179	LEU	2.7
1	A	121	SER	2.7
1	A	152	ASN	2.7
1	A	149	LYS	2.6
1	A	123	GLU	2.6
1	A	130	ALA	2.5
2	H	189	SER	2.5
1	A	184	ALA	2.5
1	A	148	TRP	2.5
3	F	160	PRO	2.3
1	A	187	GLU	2.3
1	A	204	PRO	2.3
1	A	125	LEU	2.3
1	A	209	PHE	2.3
1	A	154	LEU	2.3
2	B	127	ALA	2.2
1	A	114	SER	2.2
2	B	138	ALA	2.2
3	C	69	SER	2.1
1	A	197	THR	2.1
2	B	212	ARG	2.1
3	F	161	LEU	2.0
1	A	188	LYS	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 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.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CA	F	201	1/1	0.94	0.15	35,35,35,35	0
4	CA	C	201	1/1	0.94	0.17	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.