



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:20 PM GMT

PDB ID : 1F58  
Title : IGG1 FAB FRAGMENT (58.2) COMPLEX WITH 24-RESIDUE PEPTIDE  
(RESIDUES 308-333 OF HIV-1 GP120 (MN ISOLATE) WITH ALA TO AIB  
SUBSTITUTION AT POSITION 323  
Authors : Stanfield, R.L.; Cabezas, E.; Satterthwait, A.C.; Stura, E.A.; Profy, A.T.;  
Wilson, I.A.  
Deposited on : 1998-10-21  
Resolution : 2.00 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

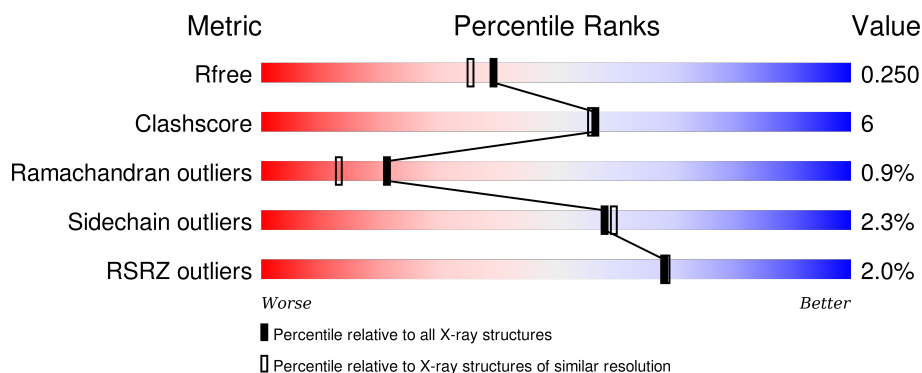
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	L	216	<div> <div>90%</div> <div>9% .</div> </div>
2	H	228	<div> <div>4%</div> <div>86%</div> <div>10% .</div> </div>
3	P	23	<div> <div>43%</div> <div>52%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3617 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 PROTEIN (IGG1 ANTIBODY 58.2 (LIGHT CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1658	1034	280	338	6			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	1	ASP	GLU	CONFLICT	PIR S68241
L	2	ILE	LEU	CONFLICT	PIR S68241
L	24	LYS	ARG	CONFLICT	PIR S68241
L	27	GLN	LYS	CONFLICT	PIR S68241
L	27A	GLY	SER	CONFLICT	PIR S68241
L	27C	ASP	SER	CONFLICT	PIR S68241
L	27D	PHE	ALA	CONFLICT	PIR S68241
L	28	ASP	SER	CONFLICT	PIR S68241
L	30	ALA	TYR	CONFLICT	PIR S68241
L	31	SER	ILE	CONFLICT	PIR S68241
L	32	PHE	TYR	CONFLICT	PIR S68241
L	34	ASN	HIS	CONFLICT	PIR S68241
L	49	PHE	SER	CONFLICT	PIR S68241
L	50	ALA	LEU	CONFLICT	PIR S68241
L	52	SER	THR	CONFLICT	PIR S68241
L	53	THR	ASN	CONFLICT	PIR S68241
L	58	ILE	VAL	CONFLICT	PIR S68241
L	65	ARG	SER	CONFLICT	PIR S68241
L	83	ALA	VAL	CONFLICT	PIR S68241
L	90	GLN	HIS	CONFLICT	PIR S68241
L	92	HIS	ARG	CONFLICT	PIR S68241
L	94	ASP	LEU	CONFLICT	PIR S68241

- Molecule 2 is a protein called PROTEIN (IGG1 ANTIBODY 58.2 (HEAVY CHAIN)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	228	Total	C	N	O	S	0	0	0
			1747	1101	288	348	10			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	6	GLN	GLU	CONFLICT	UNP P01869
H	10	ASP	GLY	CONFLICT	UNP P01869
H	29	ILE	VAL	CONFLICT	UNP P01869
H	32	GLY	GLU	CONFLICT	UNP P01869
H	34	SER	ALA	CONFLICT	UNP P01869
H	35A	HIS	ASN	CONFLICT	UNP P01869
H	48	MET	LEU	CONFLICT	UNP P01869
H	52	HIS	ASN	CONFLICT	UNP P01869
H	55	ALA	GLY	CONFLICT	UNP P01869
H	56	GLY	SER	CONFLICT	UNP P01869
H	58	ASN	SER	CONFLICT	UNP P01869
H	94	ARG	ASP	CONFLICT	UNP P01869
H	95	GLU	ARG	CONFLICT	UNP P01869
H	96	GLU	SER	CONFLICT	UNP P01869
H	97	ALA	TRP	CONFLICT	UNP P01869
H	98	MET	PHE	CONFLICT	UNP P01869
H	99	PRO	ALA	CONFLICT	UNP P01869
H	108	THR	LEU	CONFLICT	UNP P01869
H	113	SER	ALA	CONFLICT	UNP P01869
H	198	PRO	THR	CONFLICT	UNP P01869
H	199	ARG	TRP	CONFLICT	UNP P01869
H	100A	GLY	-	ENGINEERED	UNP P01869
H	100B	ASN	-	ENGINEERED	UNP P01869
H	100C	GLN	-	ENGINEERED	UNP P01869
H	100D	ALA	-	ENGINEERED	UNP P01869
H	100E	TYR	-	ENGINEERED	UNP P01869
H	100F	TYR	-	ENGINEERED	UNP P01869
H	100G	TYR	-	ENGINEERED	UNP P01869
H	100H	ALA	-	ENGINEERED	UNP P01869
H	100I	MET	-	ENGINEERED	UNP P01869
H	101	ASP	-	ENGINEERED	UNP P01869
H	102	CYS	-	ENGINEERED	UNP P01869

- Molecule 3 is a protein called PROTEIN (EXTERIOR MEMBRANE GLYCOPROTEIN(GP120)).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	11	Total	C	N	O	0	0	0
			92	61	19	12			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	323	AIB	ALA	ENGINEERED	UNP P05877

- Molecule 4 is water.

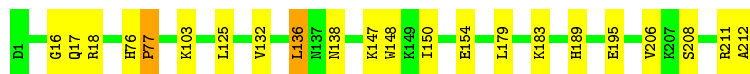
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	50	Total	O	0	0
			50	50		
4	L	67	Total	O	0	0
			67	67		
4	P	3	Total	O	0	0
			3	3		

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


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: PROTEIN (IGG1 ANTIBODY 58.2 (LIGHT CHAIN))

Chain L:  90% 9% .



- Molecule 2: PROTEIN (IGG1 ANTIBODY 58.2 (HEAVY CHAIN))

Chain H:  4% 86% 10% .



- Molecule 3: PROTEIN (EXTERIOR MEMBRANE GLYCOPROTEIN(GP120))

Chain P:  43% 52% .



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.89Å 71.91Å 88.25Å 90.00° 98.31° 90.00°	Depositor
Resolution (Å)	44.00 – 2.00 43.66 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.00-2.00) 99.6 (43.66-2.00)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.69 (at 2.00Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.196 , 0.256 0.194 , 0.250	Depositor DCC
$R_{free}$ test set	3024 reflections (9.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.9	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 45.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 30461 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3617	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	L	0.49	0/1696	0.80	2/2303 (0.1%)
2	H	0.51	0/1796	0.84	5/2460 (0.2%)
3	P	0.40	0/89	0.75	0/118
All	All	0.50	0/3581	0.82	7/4881 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	149	PRO	N-CA-CB	-6.74	95.19	102.60
2	H	151	PRO	N-CA-CB	-6.08	95.91	102.60
1	L	136	LEU	CA-CB-CG	6.06	129.24	115.30
2	H	130	ALA	N-CA-C	-5.76	95.46	111.00
1	L	77	PRO	N-CA-CB	-5.42	96.64	102.60
2	H	136	SER	N-CA-C	5.29	125.29	111.00
2	H	200	PRO	N-CA-C	5.08	125.30	112.10

There are no chirality outliers.

There are no planarity outliers.

### 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	L	1658	0	1587	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1747	0	1683	25	0
3	P	92	0	92	1	0
4	H	50	0	0	0	0
4	L	67	0	0	4	0
4	P	3	0	0	0	0
All	All	3617	0	3362	42	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 6.

All (42) 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)
2:H:194:PRO:O	2:H:198:PRO:HD2	1.87	0.75
2:H:6:GLN:H	2:H:6:GLN:HE21	1.35	0.75
2:H:6:GLN:H	2:H:6:GLN:NE2	1.93	0.65
1:L:132:VAL:HG22	1:L:179:LEU:HB3	1.81	0.63
2:H:194:PRO:HB2	2:H:198:PRO:CD	2.29	0.63
1:L:103:LYS:HG3	4:L:274:HOH:O	2.01	0.61
1:L:189:HIS:O	1:L:211:ARG:HD3	2.01	0.61
2:H:194:PRO:HB2	2:H:198:PRO:HD2	1.83	0.61
2:H:196:SER:OG	2:H:198:PRO:HD3	2.01	0.60
1:L:132:VAL:CG2	1:L:179:LEU:HB3	2.33	0.58
2:H:47:TRP:HZ2	2:H:50:TYR:CD2	2.24	0.56
2:H:6:GLN:NE2	2:H:106:GLY:H	2.04	0.56
2:H:128:SER:O	2:H:129:ALA:HB2	2.07	0.54
2:H:136:SER:O	2:H:195:SER:N	2.39	0.54
2:H:135:ASN:ND2	2:H:136:SER:H	2.06	0.53
2:H:198:PRO:O	2:H:203:GLU:HB2	2.08	0.53
2:H:47:TRP:HZ2	2:H:50:TYR:HD2	1.55	0.53
2:H:94:ARG:O	2:H:100(I):MET:HA	2.10	0.52
4:L:231:HOH:O	3:P:315:HIS:HD2	1.92	0.52
1:L:147:LYS:HE2	1:L:154:GLU:OE1	2.11	0.51
2:H:149:PRO:HD2	2:H:214:ALA:CB	2.41	0.51
1:L:18:ARG:HB2	1:L:76:HIS:CD2	2.46	0.50
2:H:119:PRO:HB3	2:H:147:TYR:HB3	1.95	0.49
2:H:194:PRO:C	2:H:198:PRO:HD2	2.33	0.49
2:H:130:ALA:O	2:H:133:GLN:HB2	2.13	0.49
1:L:132:VAL:HG23	1:L:148:TRP:CH2	2.48	0.49
1:L:18:ARG:HB2	1:L:76:HIS:HD2	1.79	0.47
1:L:17:GLN:HG2	1:L:18:ARG:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:195:GLU:HG3	1:L:206:VAL:HG22	1.96	0.47
2:H:133:GLN:HG2	2:H:134:THR:H	1.80	0.47
4:L:234:HOH:O	2:H:127:GLY:HA3	2.13	0.47
1:L:138:ASN:OD1	2:H:172:HIS:HE1	1.99	0.46
1:L:150:ILE:HD11	1:L:179:LEU:HD21	1.98	0.46
2:H:135:ASN:HD22	2:H:136:SER:H	1.65	0.45
1:L:211:ARG:O	1:L:212:ALA:HB2	2.17	0.45
2:H:35:TRP:HB3	2:H:78:PHE:CZ	2.52	0.44
1:L:125:LEU:O	1:L:183:LYS:HD3	2.18	0.43
2:H:54:SER:O	2:H:55:ALA:HB3	2.19	0.42
2:H:6:GLN:HE22	2:H:106:GLY:H	1.68	0.41
1:L:103:LYS:HE2	4:L:264:HOH:O	2.21	0.41
1:L:76:HIS:HA	1:L:77:PRO:HA	1.84	0.41
1:L:16:GLY:HA2	1:L:77:PRO:HB2	2.04	0.40

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	L	214/216 (99%)	208 (97%)	6 (3%)	0	100	100
2	H	226/228 (99%)	212 (94%)	10 (4%)	4 (2%)	11	4
3	P	8/23 (35%)	7 (88%)	1 (12%)	0	100	100
All	All	448/467 (96%)	427 (95%)	17 (4%)	4 (1%)	21	13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	129	ALA
2	H	128	SER
2	H	136	SER

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Mol	Chain	Res	Type
2	H	127	GLY

### 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	L	185/185 (100%)	183 (99%)	2 (1%)	80	83
2	H	201/201 (100%)	194 (96%)	7 (4%)	43	40
3	P	8/19 (42%)	8 (100%)	0	100	100
All	All	394/405 (97%)	385 (98%)	9 (2%)	58	60

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	136	LEU
1	L	208	SER
2	H	6	GLN
2	H	81	GLN
2	H	135	ASN
2	H	136	SER
2	H	187	LEU
2	H	198	PRO
2	H	203	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	76	HIS
1	L	145	ASN
2	H	6	GLN
2	H	43	ASN
2	H	82(A)	ASN
2	H	105	GLN
2	H	135	ASN

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Mol	Chain	Res	Type
2	H	172	HIS
3	P	315	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
3	AIB	P	323	3	1,5,6	1.09	0	1,7,9	1.23	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
3	AIB	P	323	3	-	0/2/3/6	0/0/0/0

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.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	L	216/216 (100%)	-0.33	0 100 100	11, 20, 35, 48	0
2	H	228/228 (100%)	-0.06	9 (3%) 43 45	9, 21, 45, 85	0
3	P	10/23 (43%)	-0.13	0 100 100	14, 22, 35, 42	0
All	All	454/467 (97%)	-0.19	9 (1%) 68 69	9, 21, 39, 85	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	130	ALA	15.1
2	H	129	ALA	7.9
2	H	134	THR	5.7
2	H	135	ASN	5.5
2	H	136	SER	4.4
2	H	230	CYS	3.5
2	H	133	GLN	3.4
2	H	128	SER	2.5
2	H	229	ASP	2.4

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	AIB	P	323	6/7	0.95	0.10	-	16,18,19,21	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.