



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 06:56 am BST

PDB ID : 6OOR  
Title : Structure of 1B1 bound to mouse CD1d  
Authors : Ying, G.; Zajonc, D.M.  
Deposited on : 2019-04-23  
Resolution : 2.45 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

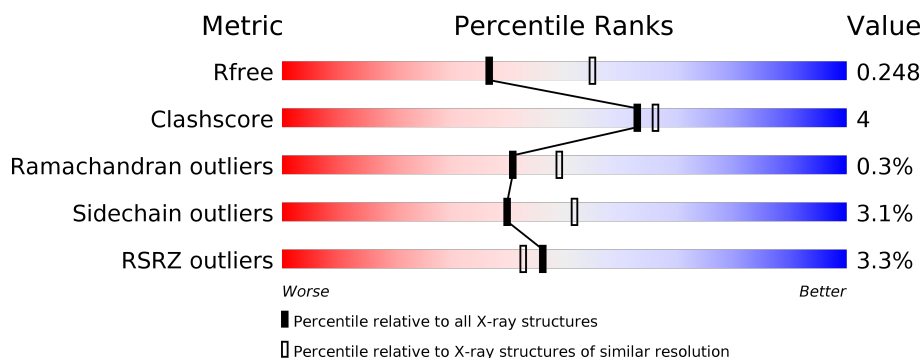
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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 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	285	<div> <div>82%</div> <div>14%</div> <div>•</div> </div>
2	B	99	<div> <div>92%</div> <div>7%</div> <div>•</div> </div>
3	L	219	<div> <div>3%</div> <div>84%</div> <div>16%</div> </div>
4	H	234	<div> <div>7%</div> <div>79%</div> <div>13%</div> <div>8%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6526 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 Antigen-presenting glycoprotein CD1d1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2192	1396	378	406	12			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	SER	CYS	engineered mutation	UNP A0A0R4J090
A	280	HIS	-	expression tag	UNP A0A0R4J090
A	281	HIS	-	expression tag	UNP A0A0R4J090
A	282	HIS	-	expression tag	UNP A0A0R4J090
A	283	HIS	-	expression tag	UNP A0A0R4J090
A	284	HIS	-	expression tag	UNP A0A0R4J090
A	285	HIS	-	expression tag	UNP A0A0R4J090

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			810	518	137	148	7			

- Molecule 3 is a protein called Antibody 1B1 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	219	Total	C	N	O	S	0	0	0
			1684	1057	282	337	8			

- Molecule 4 is a protein called Antibody 1B1 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	216	Total	C	N	O	S	0	0	0
			1648	1052	274	314	8			

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total 2	Na 2	0	0
5	L	2	Total 2	Na 2	0	0

- Molecule 6 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total 48	C 48	0	0

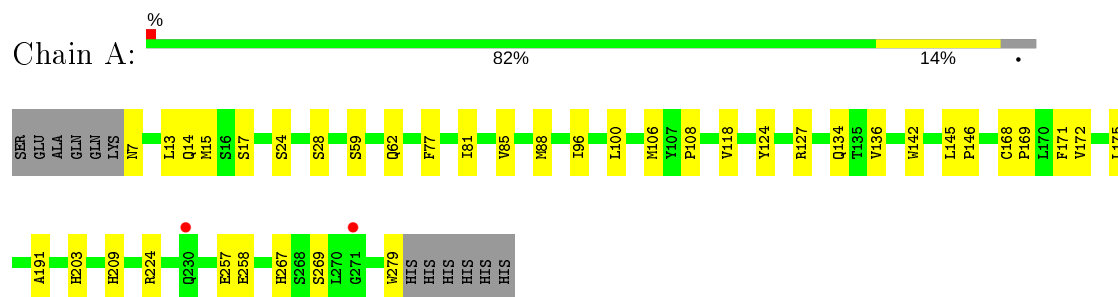
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	64	Total 64	O 64	0	0
7	B	25	Total 25	O 25	0	0
7	L	20	Total 20	O 20	0	0
7	H	31	Total 31	O 31	0	0

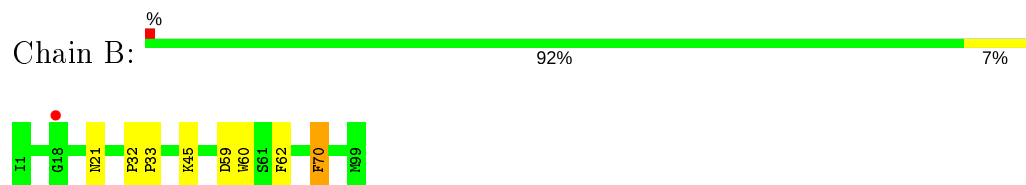
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

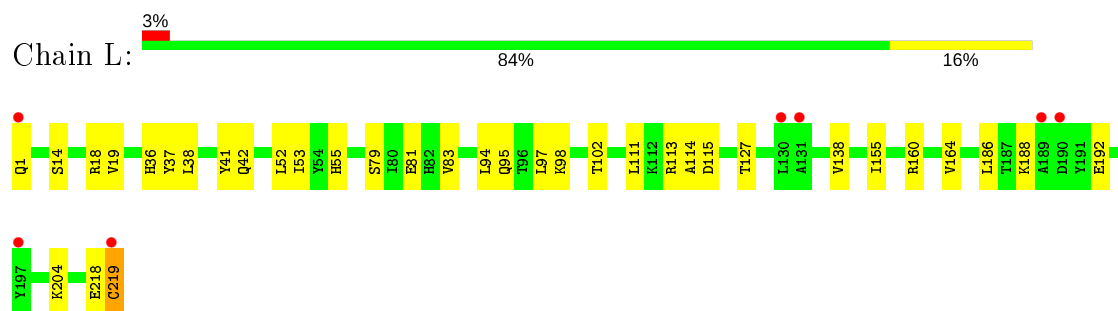
- Molecule 1: Antigen-presenting glycoprotein CD1d1



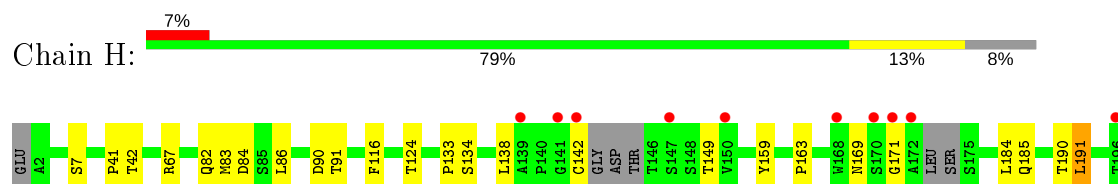
- Molecule 2: Beta-2-microglobulin

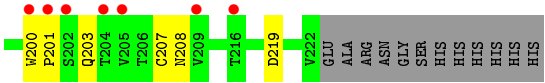


- Molecule 3: Antibody 1B1 Light chain



- Molecule 4: Antibody 1B1 Heavy chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.05Å 160.96Å 165.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.13 – 2.45 39.10 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.13-2.45) 99.3 (39.10-2.44)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.208 , 0.244 0.212 , 0.248	Depositor DCC
$R_{free}$ test set	1215 reflections (2.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	50.0	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 33.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6526	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: NA, UNL

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	0.63	0/2257	0.75	0/3069
2	B	0.60	0/836	0.78	0/1135
3	L	0.66	0/1722	0.79	0/2344
4	H	0.65	0/1693	0.80	0/2317
All	All	0.64	0/6508	0.77	0/8865

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	2192	0	2097	22	0
2	B	810	0	782	4	0
3	L	1684	0	1613	18	0
4	H	1648	0	1596	13	0
5	A	2	0	0	0	0
5	L	2	0	0	0	0
6	A	48	0	0	0	0
7	A	64	0	0	1	0
7	B	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	31	0	0	0	0
7	L	20	0	0	0	0
All	All	6526	0	6088	54	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 4.

All (54) 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:A:59:SER:H	1:A:62:GLN:HE21	1.38	0.71
3:L:95:GLN:NE2	3:L:98:LYS:H	1.88	0.70
1:A:168:CYS:HB3	1:A:169:PRO:HD3	1.80	0.63
3:L:1:GLN:HE21	3:L:102:THR:CG2	2.14	0.60
3:L:113:ARG:NH1	3:L:114:ALA:O	2.34	0.60
1:A:15:MET:HG2	2:B:62:PHE:HE2	1.65	0.60
4:H:67:ARG:NH2	4:H:90:ASP:OD2	2.36	0.59
1:A:224:ARG:NH2	1:A:257:GLU:O	2.37	0.56
3:L:42:GLN:HB2	3:L:52:LEU:HD11	1.88	0.56
1:A:258:GLU:HB3	1:A:279:TRP:CD1	2.42	0.55
3:L:95:GLN:HE21	3:L:97:LEU:N	2.04	0.55
4:H:200:TRP:CG	4:H:201:PRO:HA	2.42	0.54
3:L:138:VAL:HG21	4:H:138:LEU:HD21	1.90	0.54
3:L:95:GLN:HE22	3:L:98:LYS:H	1.56	0.54
3:L:115:ASP:OD2	3:L:204:LYS:NZ	2.40	0.53
4:H:191:LEU:C	4:H:191:LEU:HD23	2.29	0.53
1:A:203:HIS:NE2	7:A:403:HOH:O	2.34	0.52
4:H:203:GLN:HE21	4:H:203:GLN:HA	1.75	0.51
4:H:41:PRO:O	4:H:42:THR:HB	2.10	0.51
1:A:267:HIS:HD2	1:A:269:SER:OG	1.94	0.51
1:A:171:PHE:CE2	1:A:175:LEU:HD11	2.45	0.50
1:A:191:ALA:HA	1:A:209:HIS:O	2.12	0.49
1:A:145:LEU:HB3	1:A:146:PRO:HD3	1.94	0.48
4:H:83:MET:HB3	4:H:86:LEU:HD21	1.94	0.48
3:L:95:GLN:HE21	3:L:97:LEU:H	1.60	0.48
3:L:37:TYR:CE2	3:L:55:HIS:HE1	2.32	0.47
4:H:82:GLN:NE2	4:H:84:ASP:OD1	2.45	0.47
1:A:14:GLN:HB3	1:A:100:LEU:HB2	1.96	0.46
1:A:85:VAL:HG22	1:A:96:ILE:CD1	2.45	0.46
2:B:32:PRO:HB2	2:B:33:PRO:HD2	1.97	0.46
1:A:124:TYR:CZ	1:A:136:VAL:HG11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:MET:HG3	1:A:172:VAL:CG1	2.47	0.45
1:A:88:MET:SD	1:A:142:TRP:CE3	3.09	0.45
2:B:59:ASP:O	2:B:60:TRP:HB2	2.17	0.45
4:H:133:PRO:HB3	4:H:159:TYR:HB3	1.99	0.45
3:L:155:ILE:HD12	3:L:160:ARG:HB2	1.99	0.45
3:L:41:TYR:HE1	3:L:94:LEU:HB3	1.81	0.45
4:H:91:THR:HG23	4:H:124:THR:HA	1.98	0.45
3:L:1:GLN:HE21	3:L:102:THR:HG22	1.80	0.45
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.52	0.44
4:H:203:GLN:NE2	4:H:203:GLN:HA	2.34	0.42
3:L:36:HIS:O	3:L:55:HIS:HA	2.20	0.42
3:L:19:VAL:CG2	3:L:83:VAL:CG2	2.98	0.42
3:L:188:LYS:O	3:L:192:GLU:HG2	2.19	0.42
1:A:100:LEU:HG	1:A:118:VAL:HG22	2.02	0.41
1:A:7:ASN:ND2	1:A:108:PRO:HD3	2.35	0.41
3:L:18:ARG:HG3	3:L:81:GLU:O	2.21	0.41
1:A:17:SER:O	1:A:24:SER:HA	2.21	0.41
1:A:77:PHE:O	1:A:81:ILE:HG12	2.20	0.41
3:L:219:CYS:SG	4:H:142:CYS:C	3.00	0.41
4:H:169:ASN:O	4:H:208:ASN:ND2	2.54	0.40
1:A:13:LEU:O	1:A:28:SER:HA	2.21	0.40
1:A:106:MET:HG3	1:A:172:VAL:HG11	2.02	0.40
1:A:127:ARG:NH2	1:A:134:GLN:OE1	2.46	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	A	271/285 (95%)	265 (98%)	6 (2%)	0	100	100
2	B	97/99 (98%)	94 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	217/219 (99%)	205 (94%)	11 (5%)	1 (0%)	29	34
4	H	210/234 (90%)	193 (92%)	16 (8%)	1 (0%)	29	34
All	All	795/837 (95%)	757 (95%)	36 (4%)	2 (0%)	41	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	218	GLU
4	H	171	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	A	238/249 (96%)	238 (100%)	0	100	100
2	B	91/93 (98%)	89 (98%)	2 (2%)	52	64
3	L	188/194 (97%)	179 (95%)	9 (5%)	25	33
4	H	182/199 (92%)	171 (94%)	11 (6%)	19	24
All	All	699/735 (95%)	677 (97%)	22 (3%)	40	52

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	45	LYS
2	B	70	PHE
3	L	14	SER
3	L	38	LEU
3	L	53	ILE
3	L	79	SER
3	L	111	LEU
3	L	127	THR
3	L	164	VAL
3	L	186	LEU

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Mol	Chain	Res	Type
3	L	219	CYS
4	H	7	SER
4	H	116	PHE
4	H	134	SER
4	H	149	THR
4	H	163	PRO
4	H	184	LEU
4	H	185	GLN
4	H	190	THR
4	H	191	LEU
4	H	207	CYS
4	H	219	ASP

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

Mol	Chain	Res	Type
1	A	7	ASN
1	A	62	GLN
1	A	267	HIS
3	L	1	GLN
3	L	55	HIS
3	L	95	GLN
3	L	129	GLN
3	L	217	ASN
4	H	203	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 7 ligands modelled in this entry, 3 are unknown and 4 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

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 ⓘ

### 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	A	273/285 (95%)	-0.07	2 (0%) 87 88	30, 47, 81, 106	0
2	B	99/99 (100%)	-0.04	1 (1%) 82 83	33, 54, 79, 91	0
3	L	219/219 (100%)	0.06	7 (3%) 47 44	36, 62, 98, 136	0
4	H	216/234 (92%)	0.33	17 (7%) 12 9	36, 62, 120, 133	0
All	All	807/837 (96%)	0.07	27 (3%) 46 43	30, 57, 101, 136	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	172	ALA	5.4
4	H	142	CYS	4.5
4	H	170	SER	3.9
4	H	171	GLY	3.8
3	L	197	TYR	3.7
4	H	200	TRP	3.6
4	H	204	THR	3.3
4	H	147	SER	3.2
3	L	190	ASP	3.2
4	H	205	VAL	3.1
4	H	216	THR	2.7
4	H	139	ALA	2.7
3	L	131	ALA	2.6
4	H	202	SER	2.6
1	A	271	GLY	2.6
4	H	141	GLY	2.5
4	H	168	TRP	2.5
4	H	209	VAL	2.5
3	L	219	CYS	2.4
3	L	130	LEU	2.4
1	A	230	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	18	GLY	2.2
3	L	189	ALA	2.2
4	H	150	VAL	2.2
4	H	196	THR	2.1
3	L	1	GLN	2.0
4	H	201	PRO	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 carbohydrates 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( $\text{\AA}^2$ )	Q<0.9
6	UNL	A	305	16/-	0.84	0.31	46,54,80,82	0
6	UNL	A	304	16/-	0.89	0.28	47,50,55,60	0
6	UNL	A	303	16/-	0.90	0.29	40,49,52,54	0
5	NA	L	301	1/1	0.90	0.19	50,50,50,50	0
5	NA	A	302	1/1	0.94	0.16	58,58,58,58	0
5	NA	A	301	1/1	0.97	0.14	50,50,50,50	0
5	NA	L	302	1/1	0.99	0.17	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.