



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2016 – 06:14 AM EDT

PDB ID : 5IUS  
Title : Crystal structure of human PD-L1 in complex with high affinity PD-1 mutant  
Authors : Pascolutti, R.; Sun, X.; Kao, J.; Maute, R.; Ring, A.M.; Bowman, G.R.; Kruse, A.C.  
Deposited on : 2016-03-18  
Resolution : 2.89 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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
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) : rb-20027939

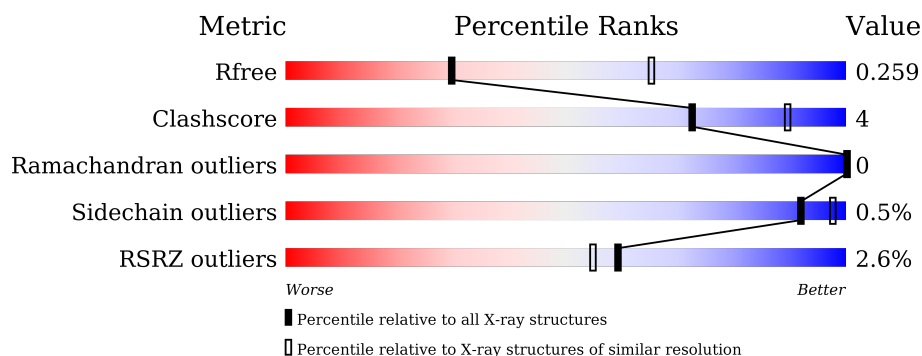
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 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	1945 (2.90-2.86)
Clashscore	102246	2202 (2.90-2.86)
Ramachandran outliers	100387	2149 (2.90-2.86)
Sidechain outliers	100360	2152 (2.90-2.86)
RSRZ outliers	91569	1950 (2.90-2.86)

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	A	129	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	129	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>8%</div> <div>11%</div> </div> </div>
2	C	225	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>5%</div> </div> </div>
2	D	225	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>9%</div> <div>6%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5114 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 Programmed cell death protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	S	0	0	0
			900	560	165	172	3			
1	B	115	Total	C	N	O	S	0	0	0
			890	554	163	170	3			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	GLY	-	expression tag	UNP Q15116
A	23	PRO	-	expression tag	UNP Q15116
A	24	GLY	-	expression tag	UNP Q15116
A	25	SER	-	expression tag	UNP Q15116
A	64	HIS	VAL	engineered mutation	UNP Q15116
A	65	VAL	LEU	engineered mutation	UNP Q15116
A	66	VAL	ASN	engineered mutation	UNP Q15116
A	68	HIS	TYR	engineered mutation	UNP Q15116
A	70	GLU	MET	engineered mutation	UNP Q15116
A	74	GLY	ASN	engineered mutation	UNP Q15116
A	78	THR	LYS	engineered mutation	UNP Q15116
A	93	ALA	CYS	engineered mutation	UNP Q15116
A	122	VAL	LEU	engineered mutation	UNP Q15116
A	125	VAL	ALA	engineered mutation	UNP Q15116
A	132	ILE	ALA	engineered mutation	UNP Q15116
A	147	ARG	-	expression tag	UNP Q15116
A	148	ALA	-	expression tag	UNP Q15116
A	149	ALA	-	expression tag	UNP Q15116
A	150	ALA	-	expression tag	UNP Q15116
B	22	GLY	-	expression tag	UNP Q15116
B	23	PRO	-	expression tag	UNP Q15116
B	24	GLY	-	expression tag	UNP Q15116
B	25	SER	-	expression tag	UNP Q15116
B	64	HIS	VAL	engineered mutation	UNP Q15116
B	65	VAL	LEU	engineered mutation	UNP Q15116

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Chain	Residue	Modelled	Actual	Comment	Reference
B	66	VAL	ASN	engineered mutation	UNP Q15116
B	68	HIS	TYR	engineered mutation	UNP Q15116
B	70	GLU	MET	engineered mutation	UNP Q15116
B	74	GLY	ASN	engineered mutation	UNP Q15116
B	78	THR	LYS	engineered mutation	UNP Q15116
B	93	ALA	CYS	engineered mutation	UNP Q15116
B	122	VAL	LEU	engineered mutation	UNP Q15116
B	125	VAL	ALA	engineered mutation	UNP Q15116
B	132	ILE	ALA	engineered mutation	UNP Q15116
B	147	ARG	-	expression tag	UNP Q15116
B	148	ALA	-	expression tag	UNP Q15116
B	149	ALA	-	expression tag	UNP Q15116
B	150	ALA	-	expression tag	UNP Q15116

- Molecule 2 is a protein called Programmed cell death 1 ligand 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	214	Total	C	N	O	S	0	0	0
			1648	1045	274	322	7			
2	D	211	Total	C	N	O	S	0	0	0
			1642	1038	276	321	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	17	MET	-	initiating methionine	UNP Q9NZQ7
C	240	LEU	-	expression tag	UNP Q9NZQ7
C	241	GLU	-	expression tag	UNP Q9NZQ7
D	17	MET	-	initiating methionine	UNP Q9NZQ7
D	240	LEU	-	expression tag	UNP Q9NZQ7
D	241	GLU	-	expression tag	UNP Q9NZQ7

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

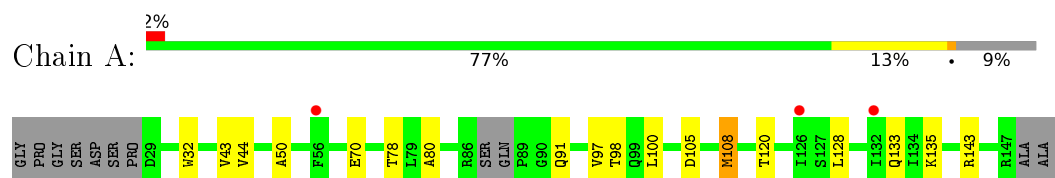
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total 6	O 6	0	0
4	B	6	Total 6	O 6	0	0
4	C	13	Total 13	O 13	0	0
4	D	8	Total 8	O 8	0	0

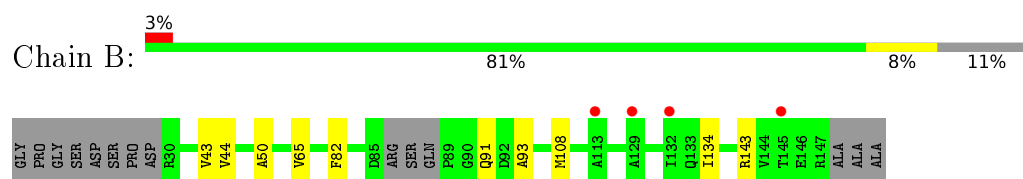
### 3 Residue-property plots [i](#)

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

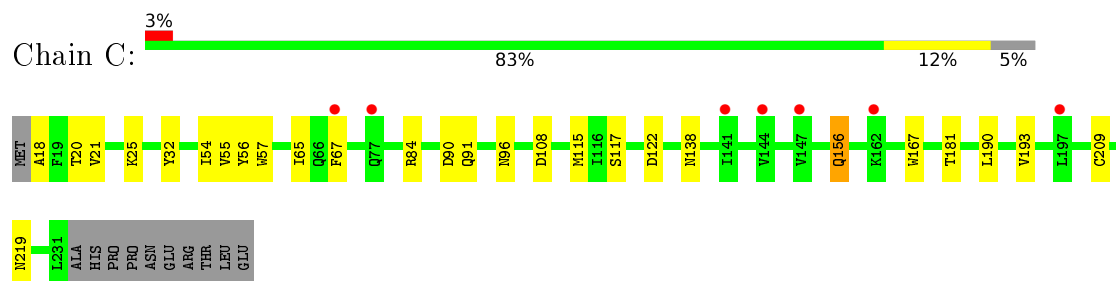
- Molecule 1: Programmed cell death protein 1



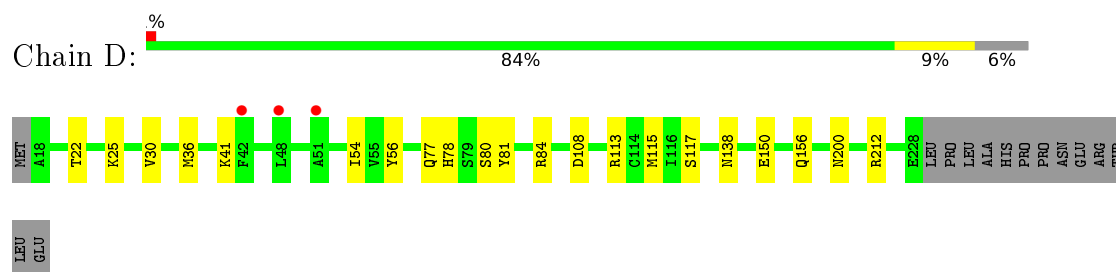
- Molecule 1: Programmed cell death protein 1



- Molecule 2: Programmed cell death 1 ligand 1



- Molecule 2: Programmed cell death 1 ligand 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.85Å 86.85Å 111.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.02 – 2.89 47.02 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.02-2.89) 87.0 (47.02-2.89)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.17	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.207 , 0.260 0.209 , 0.259	Depositor DCC
$R_{free}$ test set	1615 reflections (9.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	77.9	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 70.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5114	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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

### 5.1 Standard geometry

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

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	0.21	0/921	0.41	0/1255
1	B	0.21	0/911	0.38	0/1241
2	C	0.22	0/1680	0.39	0/2294
2	D	0.21	0/1672	0.39	0/2280
All	All	0.22	0/5184	0.39	0/7070

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

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	900	0	844	12	0
1	B	890	0	840	5	0
2	C	1648	0	1574	17	0
2	D	1642	0	1577	14	0
3	A	1	0	0	0	0
4	A	6	0	0	1	0
4	B	6	0	0	0	0
4	C	13	0	0	0	0
4	D	8	0	0	0	0
All	All	5114	0	4835	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 4.

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:C:54:ILE:HB	2:C:117:SER:HB3	1.68	0.73
1:A:32:TRP:O	1:A:135:LYS:NZ	2.24	0.71
2:D:54:ILE:HB	2:D:117:SER:HB3	1.78	0.65
2:C:56:TYR:HB3	2:C:115:MET:HB3	1.82	0.62
2:C:55:VAL:HB	2:C:67:PHE:HB3	1.82	0.60
2:D:56:TYR:HB3	2:D:115:MET:HB3	1.86	0.57
2:C:84:ARG:NH1	2:C:108:ASP:OD2	2.35	0.57
2:C:57:TRP:HB2	2:C:65:ILE:HB	1.86	0.56
2:D:30:VAL:HG11	2:D:36:MET:HB2	1.87	0.56
2:D:78:HIS:CD2	2:D:80:SER:H	2.25	0.54
1:A:98:THR:OG1	4:A:301:HOH:O	2.19	0.53
2:D:84:ARG:NH1	2:D:108:ASP:OD2	2.36	0.53
2:D:77:GLN:NE2	2:D:81:TYR:O	2.43	0.52
1:B:44:VAL:HG21	1:B:50:ALA:HB2	1.91	0.51
1:B:134:ILE:HD13	2:D:113:ARG:HD3	1.93	0.50
1:B:91:GLN:HG3	1:B:93:ALA:H	1.76	0.50
2:D:138:ASN:HB2	2:D:156:GLN:HG3	1.94	0.50
2:D:78:HIS:HD2	2:D:80:SER:H	1.60	0.49
1:A:43:VAL:HG22	1:A:143:ARG:HB2	1.93	0.49
2:D:22:THR:HG23	2:D:41:LYS:HB2	1.95	0.48
2:D:78:HIS:HB3	2:D:81:TYR:HD2	1.78	0.48
2:C:219:ASN:HD22	2:D:212:ARG:HA	1.78	0.48
1:B:43:VAL:HG22	1:B:143:ARG:HB2	1.96	0.47
1:A:44:VAL:HG21	1:A:50:ALA:HB2	1.96	0.46
1:A:80:ALA:HB3	1:A:97:VAL:HG23	1.98	0.46
1:A:32:TRP:HE1	1:A:133:GLN:NE2	2.14	0.46
2:C:138:ASN:HB2	2:C:156:GLN:HG3	1.98	0.46
2:D:150:GLU:HA	2:D:200:ASN:HA	1.98	0.45
1:A:91:GLN:HB3	2:C:18:ALA:N	2.32	0.44
1:A:70:GLU:O	1:A:120:THR:OG1	2.36	0.44
1:A:78:THR:HB	2:C:20:THR:HG22	2.00	0.44
2:C:25:LYS:HG2	2:D:25:LYS:HG2	1.99	0.44
1:A:128:LEU:HD23	2:C:54:ILE:HD12	1.99	0.44
2:C:90:ASP:OD1	2:C:90:ASP:N	2.49	0.43
1:B:65:VAL:HG13	1:B:82:PHE:HB3	2.01	0.43
2:C:32:TYR:CZ	2:C:190:LEU:HD11	2.54	0.42
2:C:167:TRP:CZ3	2:C:209:CYS:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:HD12	1:A:105:ASP:HB2	2.01	0.41
2:C:21:VAL:HG23	2:C:122:ASP:HB3	2.03	0.41
2:C:91:GLN:HB3	2:C:96:ASN:HB3	2.02	0.41
2:C:181:THR:HG23	2:C:193:VAL:HG22	2.02	0.40
1:A:97:VAL:HG22	1:A:108:MET:HG3	2.03	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	113/129 (88%)	108 (96%)	5 (4%)	0	100	100
1	B	111/129 (86%)	105 (95%)	6 (5%)	0	100	100
2	C	212/225 (94%)	207 (98%)	5 (2%)	0	100	100
2	D	209/225 (93%)	204 (98%)	5 (2%)	0	100	100
All	All	645/708 (91%)	624 (97%)	21 (3%)	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	97/110 (88%)	96 (99%)	1 (1%)	82	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	97/110 (88%)	96 (99%)	1 (1%)	82	95
2	C	177/204 (87%)	176 (99%)	1 (1%)	90	97
2	D	177/204 (87%)	177 (100%)	0	100	100
All	All	548/628 (87%)	545 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	MET
1	B	108	MET
2	C	156	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	133	GLN
1	B	75	GLN
2	C	69	HIS
2	C	138	ASN
2	C	156	GLN
2	C	192	ASN
2	C	219	ASN
2	D	77	GLN
2	D	78	HIS

### 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 1 ligands modelled in this entry, 1 is 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	117/129 (90%)	0.21	3 (2%) 59 55	71, 103, 167, 186	0
1	B	115/129 (89%)	0.26	4 (3%) 48 41	75, 118, 171, 215	0
2	C	214/225 (95%)	0.25	7 (3%) 50 43	71, 117, 178, 234	0
2	D	211/225 (93%)	0.07	3 (1%) 78 76	71, 110, 177, 216	0
All	All	657/708 (92%)	0.19	17 (2%) 59 55	71, 113, 175, 234	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	48	LEU	3.8
2	C	147	VAL	3.7
1	A	132	ILE	2.9
1	B	145	THR	2.9
1	B	129	ALA	2.8
1	B	113	ALA	2.4
2	C	144	VAL	2.3
2	C	141	ILE	2.3
1	B	132	ILE	2.3
1	A	56	PHE	2.3
2	D	42	PHE	2.2
2	C	197	LEU	2.1
1	A	126	ILE	2.1
2	D	51	ALA	2.1
2	C	162	LYS	2.1
2	C	77	GLN	2.1
2	C	67	PHE	2.0

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

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. 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( $\text{\AA}^2$ )	Q<0.9
3	CL	A	201	1/1	0.70	0.40	-	151,151,151,151	0

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

There are no such residues in this entry.