



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:30 AM GMT

PDB ID : 2HFF  
Title : Crystal structure of CB2 Fab  
Authors : Hymowitz, S.G.  
Deposited on : 2006-06-23  
Resolution : 1.95 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

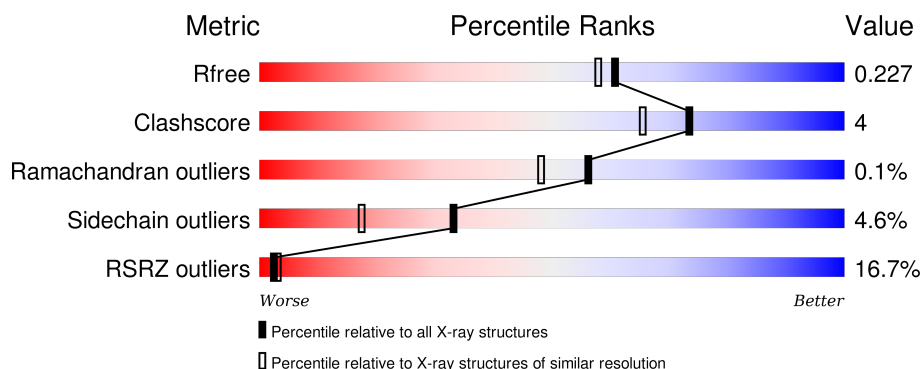
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	214	<div> <div>9%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
1	L	214	<div> <div>30%</div> <div>89%</div> <div>8%</div> <div>..</div> </div>
2	B	232	<div> <div>9%</div> <div>83%</div> <div>8%</div> <div>.</div> <div>8%</div> </div>
2	H	232	<div> <div>16%</div> <div>83%</div> <div>7%</div> <div>.</div> <div>9%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6539 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 CB2 Fab, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1628	1019	273	330	6			
1	L	211	Total	C	N	O	S	0	0	0
			1617	1013	271	328	5			

- Molecule 2 is a protein called CB2 Fab, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1581	994	267	313	7			
2	H	212	Total	C	N	O	S	0	0	0
			1563	982	265	310	6			

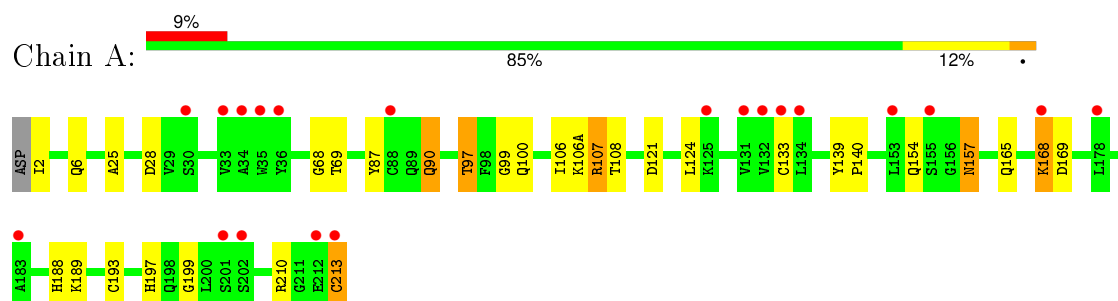
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	37	Total	O	0	0
			37	37		
3	B	56	Total	O	0	0
			56	56		
3	H	41	Total	O	0	0
			41	41		
3	L	16	Total	O	0	0
			16	16		

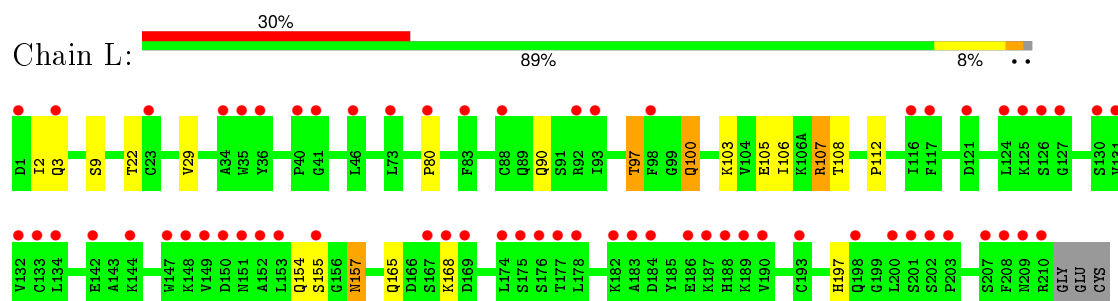
### 3 Residue-property plots [i](#)

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.

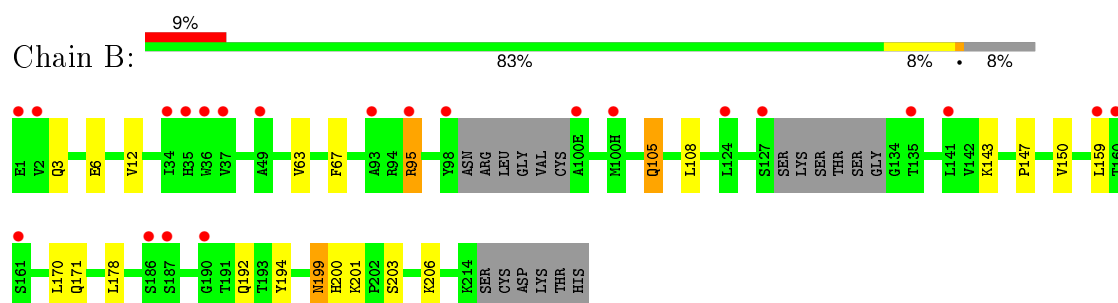
- Molecule 1: CB2 Fab, light chain



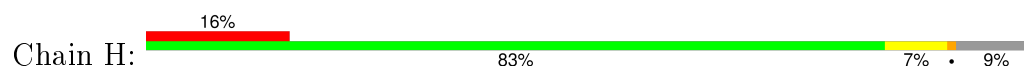
- Molecule 1: CB2 Fab, light chain

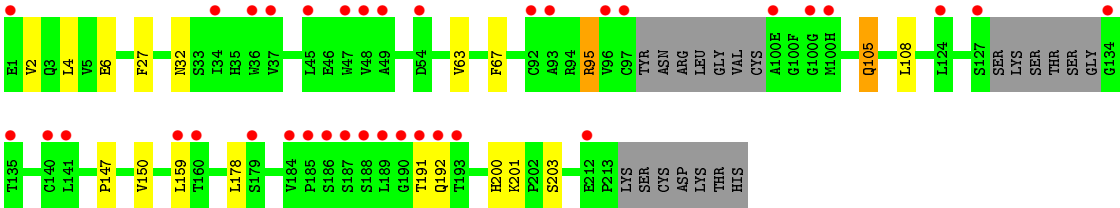


- Molecule 2: CB2 Fab, heavy chain



- Molecule 2: CB2 Fab, heavy chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	38.71Å 72.98Å 89.92Å 109.42° 100.96° 96.10°	Depositor
Resolution (Å)	30.00 – 1.95 29.39 – 1.95	Depositor EDS
% Data completeness (in resolution range)	97.7 (30.00-1.95) 85.9 (29.39-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.189 , 0.221 0.197 , 0.227	Depositor DCC
$R_{free}$ test set	6425 reflections (11.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.5	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 63790 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6539	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.41	0/1663	0.58	0/2259
1	L	0.36	0/1652	0.53	0/2245
2	B	0.46	0/1617	0.66	2/2206 (0.1%)
2	H	0.41	0/1598	0.60	2/2180 (0.1%)
All	All	0.41	0/6530	0.59	4/8890 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	95	ARG	NE-CZ-NH1	6.54	123.57	120.30
2	B	95	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	H	95	ARG	NE-CZ-NH1	5.63	123.12	120.30
2	H	95	ARG	NE-CZ-NH2	-5.59	117.50	120.30

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	1628	0	1590	17	0
1	L	1617	0	1581	10	0
2	B	1581	0	1539	10	0
2	H	1563	0	1525	12	0
3	A	37	0	0	0	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	56	0	0	1	0
3	H	41	0	0	1	0
3	L	16	0	0	1	1
All	All	6539	0	6235	49	1

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 (49) 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:L:22:THR:HG23	3:L:214:HOH:O	1.85	0.76
1:A:133:CYS:HG	1:A:193:CYS:HG	0.93	0.74
2:B:95:ARG:NH2	3:B:252:HOH:O	2.20	0.73
2:H:95:ARG:NH2	3:H:239:HOH:O	2.26	0.69
2:B:105:GLN:HE21	2:B:105:GLN:H	1.40	0.66
2:B:6:GLU:H	2:B:105:GLN:HE22	1.43	0.65
1:A:188:HIS:O	1:A:210:ARG:NH1	2.29	0.65
1:L:80:PRO:HA	1:L:106:ILE:HD13	1.78	0.64
1:A:6:GLN:HE21	1:A:99:GLY:HA3	1.64	0.62
2:H:6:GLU:H	2:H:105:GLN:HE22	1.48	0.62
2:H:147:PRO:O	2:H:200:HIS:HE1	1.84	0.60
2:B:147:PRO:O	2:B:200:HIS:HE1	1.84	0.60
1:A:90:GLN:HG3	1:A:97:THR:HG23	1.86	0.58
2:H:63:VAL:HG13	2:H:67:PHE:HB2	1.85	0.57
1:L:2:ILE:O	1:L:97:THR:HG21	2.07	0.54
2:B:199:ASN:HD21	2:B:206:LYS:HE3	1.72	0.54
2:B:63:VAL:HG13	2:B:67:PHE:HB2	1.89	0.54
1:A:106:ILE:H	1:A:165:GLN:HE22	1.54	0.54
1:A:2:ILE:O	1:A:97:THR:HG21	2.08	0.53
2:B:200:HIS:HD2	2:B:203:SER:OG	1.92	0.53
1:L:154:GLN:HB3	1:L:157:ASN:HD21	1.74	0.53
1:A:168:LYS:HG2	1:A:169:ASP:N	2.24	0.52
2:H:4:LEU:HD21	2:H:27:PHE:HZ	1.75	0.52
1:A:197:HIS:CD2	1:A:199:GLY:H	2.28	0.52
1:A:140:PRO:O	1:A:197:HIS:HE1	1.94	0.51
1:A:25:ALA:O	1:A:69:THR:HG23	2.12	0.50
2:H:105:GLN:HE21	2:H:105:GLN:H	1.60	0.49
1:L:29:VAL:CG1	1:L:29:VAL:O	2.61	0.49
2:H:191:THR:OG1	2:H:192:GLN:N	2.45	0.49
2:H:105:GLN:NE2	2:H:105:GLN:H	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:2:VAL:HG13	2:H:27:PHE:HD1	1.79	0.48
1:L:106:ILE:H	1:L:165:GLN:HE22	1.61	0.47
1:A:154:GLN:HB3	1:A:157:ASN:HD21	1.80	0.47
2:B:143:LYS:NZ	2:B:171:GLN:HE22	2.12	0.47
2:H:200:HIS:HD2	2:H:203:SER:OG	1.99	0.45
1:A:90:GLN:CG	1:A:97:THR:HG23	2.46	0.45
2:H:2:VAL:HG13	2:H:27:PHE:CD1	2.51	0.45
1:A:28:ASP:OD1	1:A:68:GLY:HA2	2.17	0.45
1:L:107:ARG:HD3	1:L:108:THR:O	2.18	0.44
2:B:192:GLN:HG2	2:B:194:TYR:CZ	2.53	0.44
1:L:105:GLU:HG2	1:L:165:GLN:HE22	1.84	0.42
1:A:107:ARG:HD3	1:A:108:THR:O	2.19	0.42
1:A:189:LYS:NZ	1:A:213:CYS:SG	2.80	0.42
1:L:112:PRO:HD3	1:L:197:HIS:CD2	2.55	0.42
2:H:178:LEU:HD12	2:H:178:LEU:C	2.39	0.42
1:L:9:SER:HB3	1:L:100:GLN:HE22	1.85	0.42
1:A:139:TYR:CG	1:A:140:PRO:HA	2.55	0.41
2:B:178:LEU:HD12	2:B:178:LEU:C	2.41	0.41
1:A:6:GLN:HE22	1:A:87:TYR:HA	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:232:HOH:O	3:L:221:HOH:O[1_554]	1.85	0.35

## 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	211/214 (99%)	204 (97%)	7 (3%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	209/214 (98%)	201 (96%)	7 (3%)	1 (0%)	34	21
2	B	208/232 (90%)	206 (99%)	2 (1%)	0	100	100
2	H	206/232 (89%)	202 (98%)	4 (2%)	0	100	100
All	All	834/892 (94%)	813 (98%)	20 (2%)	1 (0%)	56	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	155	SER

### 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	187/188 (100%)	177 (95%)	10 (5%)	28	13
1	L	186/188 (99%)	178 (96%)	8 (4%)	35	20
2	B	175/192 (91%)	166 (95%)	9 (5%)	29	13
2	H	173/192 (90%)	167 (96%)	6 (4%)	43	29
All	All	721/760 (95%)	688 (95%)	33 (5%)	33	17

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	97	THR
1	A	100	GLN
1	A	106(A)	LYS
1	A	107	ARG
1	A	121	ASP
1	A	124	LEU
1	A	157	ASN
1	A	168	LYS
1	A	213	CYS

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Mol	Chain	Res	Type
2	B	3	GLN
2	B	12	VAL
2	B	105	GLN
2	B	108	LEU
2	B	150	VAL
2	B	159	LEU
2	B	170	LEU
2	B	199	ASN
2	B	201	LYS
1	L	3	GLN
1	L	90	GLN
1	L	97	THR
1	L	100	GLN
1	L	103	LYS
1	L	107	ARG
1	L	157	ASN
1	L	168	LYS
2	H	32	ASN
2	H	105	GLN
2	H	108	LEU
2	H	150	VAL
2	H	159	LEU
2	H	201	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	27	GLN
1	A	37	GLN
1	A	38	GLN
1	A	157	ASN
1	A	165	GLN
1	A	197	HIS
1	A	198	GLN
1	A	209	ASN
2	B	13	GLN
2	B	39	GLN
2	B	105	GLN
2	B	171	GLN
2	B	200	HIS
1	L	6	GLN

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Mol	Chain	Res	Type
1	L	27	GLN
1	L	37	GLN
1	L	38	GLN
1	L	100	GLN
1	L	157	ASN
1	L	165	GLN
1	L	197	HIS
1	L	198	GLN
1	L	209	ASN
2	H	13	GLN
2	H	39	GLN
2	H	82(A)	ASN
2	H	105	GLN
2	H	171	GLN
2	H	199	ASN
2	H	200	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 ⓘ

There are no ligands in this entry.

### 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	213/214 (99%)	0.63	20 (9%) <b>11</b> <b>17</b>	29, 37, 49, 67	0
1	L	211/214 (98%)	1.43	64 (30%) <b>1</b> <b>0</b>	30, 39, 47, 51	0
2	B	214/232 (92%)	0.43	22 (10%) <b>9</b> <b>14</b>	30, 37, 49, 70	0
2	H	212/232 (91%)	0.79	36 (16%) <b>2</b> <b>3</b>	30, 38, 49, 68	0
All	All	850/892 (95%)	0.82	142 (16%) <b>2</b> <b>3</b>	29, 38, 48, 70	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	153	LEU	9.6
1	L	132	VAL	9.0
2	H	97	CYS	8.5
1	L	183	ALA	8.0
1	A	213	CYS	6.9
1	L	189	LYS	6.6
1	L	149	VAL	6.3
2	H	189	LEU	5.7
2	H	141	LEU	5.5
1	L	187	LYS	5.3
2	B	1	GLU	5.3
1	A	155	SER	5.2
1	L	152	ALA	5.2
2	H	187	SER	5.2
1	L	190	VAL	4.9
2	H	188	SER	4.9
1	L	155	SER	4.9
1	L	124	LEU	4.8
1	L	150	ASP	4.8
1	L	131	VAL	4.8
2	H	190	GLY	4.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	L	1	ASP	4.6
1	A	132	VAL	4.4
1	L	147	TRP	4.4
2	H	1	GLU	4.3
1	L	184	ASP	4.3
1	L	133	CYS	4.3
2	B	127	SER	4.2
2	B	98	TYR	4.2
1	L	151	ASN	4.1
1	L	186	GLU	4.1
2	H	191	THR	4.0
1	L	121	ASP	4.0
1	L	201	SER	3.9
2	H	134	GLY	3.9
1	L	175	SER	3.9
2	H	127	SER	3.9
1	L	177	THR	3.8
1	L	176	SER	3.7
2	H	186	SER	3.7
2	H	93	ALA	3.7
2	H	135	THR	3.6
1	L	88	CYS	3.6
1	L	168	LYS	3.5
2	H	100(H)	MET	3.5
2	H	124	LEU	3.5
1	L	127	GLY	3.5
2	H	192	GLN	3.4
2	B	160	THR	3.4
2	H	193	THR	3.3
1	A	168	LYS	3.3
1	L	200	LEU	3.3
2	H	100(E)	ALA	3.3
1	A	131	VAL	3.2
2	H	37	VAL	3.2
1	L	209	ASN	3.2
1	L	80	PRO	3.1
1	L	126	SER	3.1
2	H	185	PRO	3.1
1	L	134	LEU	3.0
1	L	202	SER	3.0
1	L	40	PRO	3.0
1	A	30	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	L	130	SER	3.0
1	L	83	PHE	3.0
1	L	167	SER	3.0
1	L	125	LYS	2.9
2	H	184	VAL	2.9
2	H	36	TRP	2.9
1	L	178	LEU	2.9
2	B	135	THR	2.9
2	B	34	ILE	2.8
2	B	161	SER	2.8
1	A	134	LEU	2.8
2	H	48	VAL	2.8
1	A	153	LEU	2.8
2	B	100(H)	MET	2.7
2	H	34	ILE	2.7
1	L	182	LYS	2.7
2	H	140	CYS	2.7
2	B	37	VAL	2.7
1	L	36	TYR	2.7
1	A	212	GLU	2.7
2	H	160	THR	2.7
2	H	212	GLU	2.7
1	L	117	PHE	2.7
1	L	193	CYS	2.6
2	B	35	HIS	2.6
1	A	133	CYS	2.6
1	L	34	ALA	2.6
1	L	144	LYS	2.6
1	L	203	PRO	2.5
2	B	36	TRP	2.5
2	B	2	VAL	2.5
1	L	41	GLY	2.5
1	L	207	SER	2.5
2	H	179	SER	2.5
1	A	36	TYR	2.5
2	H	159	LEU	2.5
1	A	33	VAL	2.5
2	H	96	VAL	2.5
2	B	95	ARG	2.5
1	L	142	GLU	2.5
1	L	3	GLN	2.5
1	L	174	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	210	ARG	2.4
1	A	88	CYS	2.4
1	L	73	LEU	2.4
1	L	169	ASP	2.4
1	A	183	ALA	2.4
1	L	198	GLN	2.3
2	B	141	LEU	2.3
1	L	98	PHE	2.3
1	L	188	HIS	2.3
1	L	92	ARG	2.3
1	A	35	TRP	2.2
2	H	92	CYS	2.2
2	H	100(G)	GLY	2.2
2	B	190	GLY	2.2
2	B	49	ALA	2.2
1	L	23	CYS	2.2
2	B	93	ALA	2.2
1	L	148	LYS	2.2
2	B	124	LEU	2.2
1	L	35	TRP	2.2
1	A	125	LYS	2.2
2	B	100(E)	ALA	2.1
2	H	47	TRP	2.1
2	B	187	SER	2.1
1	L	93	ILE	2.1
2	H	54	ASP	2.1
1	L	208	PHE	2.1
1	L	46	LEU	2.1
2	B	159	LEU	2.1
2	H	49	ALA	2.1
1	A	34	ALA	2.0
1	A	178	LEU	2.0
2	B	186	SER	2.0
2	H	45	LEU	2.0
1	A	201	SER	2.0
1	A	202	SER	2.0
1	L	116	ILE	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](#)

There are no ligands in this entry.

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

There are no such residues in this entry.