



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:56 PM GMT

PDB ID : 5C0S  
Title : Crystal structure of a generation 4 influenza hemagglutinin stabilized stem in complex with the broadly neutralizing antibody CR6261  
Authors : Boyington, J.C.; Kwong, P.D.; Nabel, G.J.; Mascola, J.R.  
Deposited on : 2015-06-12  
Resolution : 4.30 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.

---

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-20026982  
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-20026982

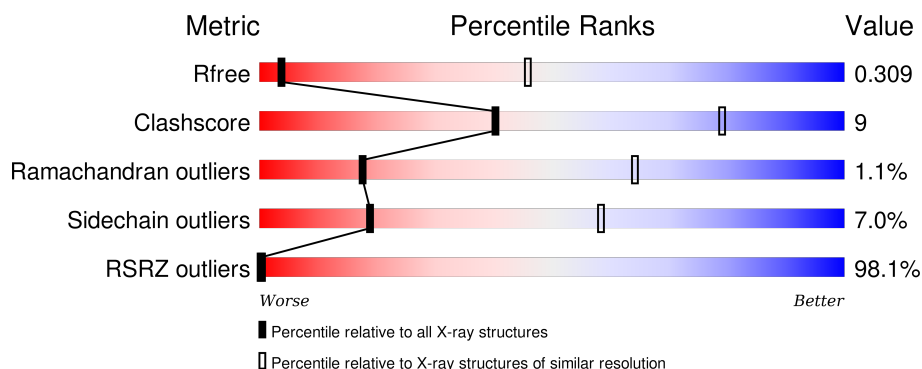
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.30 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	1059 (5.00-3.60)
Clashscore	102246	1166 (5.00-3.60)
Ramachandran outliers	100387	1106 (5.00-3.60)
Sidechain outliers	100360	1089 (5.00-3.60)
RSRZ outliers	91569	1062 (5.00-3.60)

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	305	<div> <div>78%</div> <div>56% 21% • 21%</div> </div>
2	H	226	<div> <div>95%</div> <div>78% 17% • •</div> </div>
3	L	221	<div> <div>95%</div> <div>77% 16% • •</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5158 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 Hemagglutinin, Envelope glycoprotein, Fibrin fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1930	1198	336	388	8			

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLY	-	linker	UNP Q6WG00
A	34	SER	-	linker	UNP Q6WG00
A	35	GLY	-	linker	UNP Q6WG00
A	47	GLN	SER	conflict	UNP Q6WG00
A	47A	ARG	ILE	conflict	UNP Q6WG00
A	47B	GLU	GLN	conflict	UNP Q6WG00
A	47C	THR	SER	conflict	UNP Q6WG00
A	108	GLY	-	linker	UNP Q6WG00
A	109	GLY	-	linker	UNP Q6WG00
A	110	ASP	TRP	conflict	UNP P04578
A	111	PRO	MET	conflict	UNP P04578
A	123	ILE	LEU	conflict	UNP P04578
A	125	TYR	HIS	conflict	UNP P04578
A	137	ASN	-	linker	UNP P04578
A	138	GLY	-	linker	UNP P04578
A	139	THR	-	linker	UNP P04578
A	140	GLY	-	linker	UNP P04578
A	141	GLY	-	linker	UNP P04578
A	142	GLY	-	linker	UNP P04578
A	257	PRO	-	linker	UNP Q6WG00
A	258	GLY	-	linker	UNP Q6WG00
A	259	SER	-	linker	UNP Q6WG00
A	288	GLY	-	expression tag	UNP D9IEJ2
A	289	ARG	-	expression tag	UNP D9IEJ2
A	290	LEU	-	expression tag	UNP D9IEJ2
A	291	VAL	-	expression tag	UNP D9IEJ2
A	292	PRO	-	expression tag	UNP D9IEJ2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	293	ARG	-	expression tag	UNP D9IEJ2
A	294	GLY	-	expression tag	UNP D9IEJ2
A	295	SER	-	expression tag	UNP D9IEJ2
A	296	GLY	-	expression tag	UNP D9IEJ2
A	297	HIS	-	expression tag	UNP D9IEJ2
A	298	HIS	-	expression tag	UNP D9IEJ2
A	299	HIS	-	expression tag	UNP D9IEJ2
A	300	HIS	-	expression tag	UNP D9IEJ2
A	301	HIS	-	expression tag	UNP D9IEJ2
A	302	HIS	-	expression tag	UNP D9IEJ2

- Molecule 2 is a protein called CR6261 antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1643	1039	274	321	9			

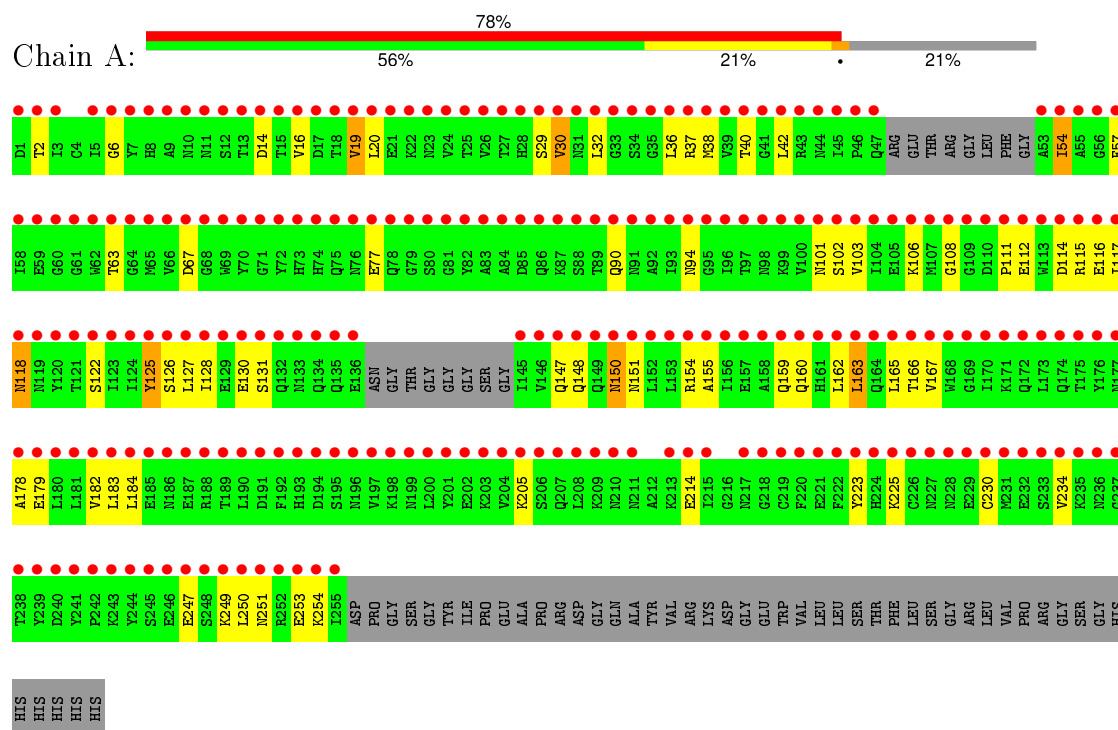
- Molecule 3 is a protein called CR6261 antibody light chain.

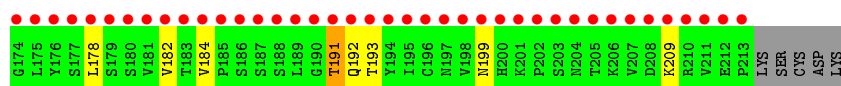
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	0	0
			1585	995	266	320	4			

### 3 Residue-property plots

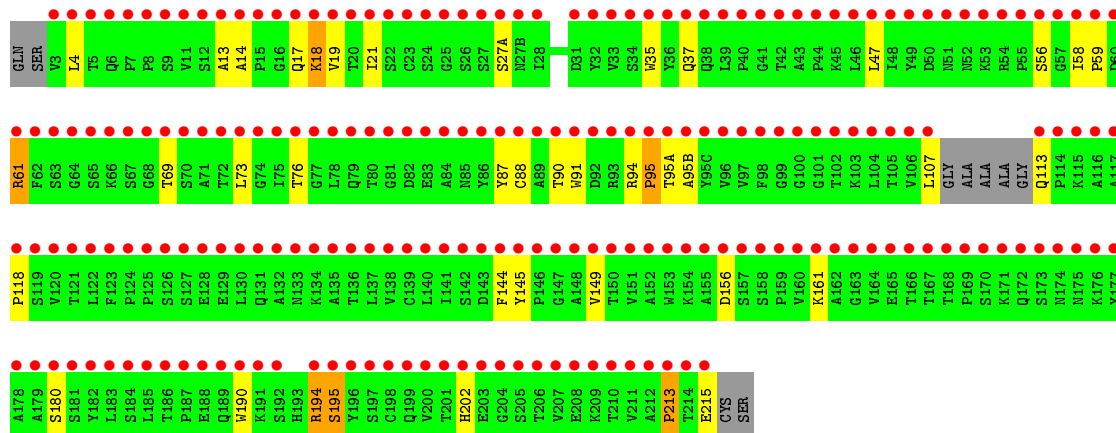
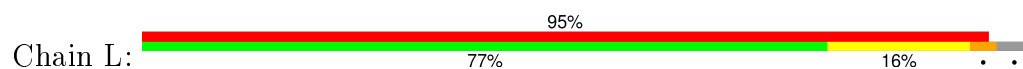
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Hemagglutinin, Envelope glycoprotein, Fibritin fusion protein





● Molecule 3: CR6261 antibody light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.65Å 101.65Å 186.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.06 – 4.30 27.06 – 4.30	Depositor EDS
% Data completeness (in resolution range)	99.0 (27.06-4.30) 99.1 (27.06-4.30)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 4.25Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2_1309)	Depositor
R, $R_{free}$	0.238 , 0.310 0.237 , 0.309	Depositor DCC
$R_{free}$ test set	240 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	166.1	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	508.12 , -10.0	EDS
Estimated twinning fraction	0.073 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 4799 reflections	Xtriage
$F_o, F_c$ correlation	0.65	EDS
Total number of atoms	5158	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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

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	0.30	0/1961	0.52	0/2650
2	H	0.27	0/1684	0.50	0/2292
3	L	0.26	0/1624	0.53	0/2220
All	All	0.28	0/5269	0.51	0/7162

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	1930	0	1850	50	0
2	H	1643	0	1625	36	0
3	L	1585	0	1547	20	0
All	All	5158	0	5022	89	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 9.

All (89) 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:90:GLN:NE2	2:H:31:SER:O	2.07	0.87

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ASP:O	1:A:118:ASN:ND2	2.16	0.79
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.67	0.75
1:A:36:LEU:HD11	1:A:178:ALA:HB1	1.72	0.71
1:A:101:ASN:HD21	2:H:29:PHE:HB2	1.55	0.71
1:A:223:TYR:O	1:A:251:ASN:ND2	2.27	0.67
1:A:40:THR:HG21	2:H:53:ILE:HD12	1.76	0.67
1:A:30:VAL:HG23	2:H:74:PHE:CZ	2.30	0.66
1:A:36:LEU:HB3	1:A:182:VAL:HG21	1.78	0.66
1:A:127:LEU:HA	1:A:130:GLU:HG3	1.76	0.65
1:A:147:GLN:HA	1:A:150:ASN:HB2	1.78	0.65
3:L:113:GLN:HB2	3:L:145:TYR:CE1	2.32	0.64
3:L:13:ALA:O	3:L:107:LEU:N	2.29	0.64
1:A:102:SER:O	1:A:106:LYS:N	2.24	0.62
1:A:32:LEU:HD13	2:H:74:PHE:HE1	1.65	0.62
1:A:94:ASN:HA	2:H:31:SER:HB2	1.81	0.61
1:A:111:PRO:HA	1:A:114:ASP:HB2	1.84	0.59
3:L:18:LYS:HE3	3:L:18:LYS:H	1.68	0.59
3:L:21:ILE:HD12	3:L:73:LEU:HD23	1.85	0.58
2:H:61:PRO:HA	2:H:64:GLN:HB2	1.86	0.58
3:L:27(A):SER:HB2	3:L:94:ARG:HB2	1.86	0.57
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.88	0.55
2:H:159:LEU:HD13	2:H:182:VAL:HG21	1.88	0.55
1:A:101:ASN:ND2	2:H:29:PHE:HB2	2.22	0.55
1:A:90:GLN:OE1	2:H:98:TYR:HB3	2.07	0.54
3:L:149:VAL:HG12	3:L:202:HIS:HB2	1.90	0.54
1:A:250:LEU:HB3	1:A:254:LYS:HE2	1.89	0.53
1:A:114:ASP:O	1:A:116:GLU:N	2.42	0.53
3:L:118:PRO:HB3	3:L:144:PHE:HB3	1.91	0.52
1:A:247:GLU:O	1:A:251:ASN:ND2	2.42	0.52
1:A:127:LEU:O	1:A:130:GLU:HB2	2.10	0.52
1:A:16:VAL:HG12	1:A:37:ARG:HG2	1.91	0.52
1:A:118:ASN:O	1:A:122:SER:OG	2.16	0.52
1:A:90:GLN:OE1	1:A:90:GLN:HA	2.10	0.52
1:A:14:ASP:OD2	1:A:29:SER:OG	2.26	0.51
2:H:36:TRP:CE2	2:H:80:MET:HB2	2.45	0.51
1:A:205:LYS:NZ	1:A:214:GLU:OE2	2.43	0.51
2:H:61:PRO:HG3	3:L:95(A):THR:OG1	2.10	0.51
3:L:91:TRP:CZ2	3:L:95(B):ALA:HB1	2.45	0.51
1:A:125:TYR:HA	1:A:128:ILE:HB	1.92	0.51
2:H:123:PRO:HD3	2:H:209:LYS:HE2	1.91	0.50
2:H:94:LYS:HG2	2:H:102:VAL:HB	1.94	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLY:HA2	1:A:57:PHE:HB3	1.93	0.50
1:A:250:LEU:O	1:A:254:LYS:N	2.40	0.49
1:A:90:GLN:CD	2:H:98:TYR:HB3	2.33	0.49
2:H:182:VAL:HG22	2:H:184:VAL:HG13	1.95	0.48
1:A:179:GLU:O	1:A:183:LEU:HG	2.14	0.46
1:A:101:ASN:HD21	2:H:29:PHE:H	1.63	0.46
1:A:94:ASN:OD1	2:H:31:SER:HB2	2.16	0.46
3:L:27(A):SER:CB	3:L:94:ARG:HB2	2.46	0.46
1:A:38:MET:HE1	1:A:103:VAL:HG11	1.98	0.46
1:A:30:VAL:HG23	2:H:74:PHE:CE2	2.51	0.46
2:H:41:PRO:HA	2:H:42:GLY:HA2	1.51	0.45
3:L:35:TRP:CH2	3:L:88:CYS:HB3	2.52	0.44
1:A:19:VAL:HG22	1:A:20:LEU:HD12	1.99	0.44
2:H:48:MET:HG2	2:H:63:PHE:CE2	2.52	0.44
1:A:32:LEU:HB2	1:A:36:LEU:HB2	2.00	0.44
3:L:94:ARG:HB3	3:L:95:PRO:HD3	1.99	0.44
1:A:230:CYS:O	1:A:234:VAL:HG23	2.17	0.44
2:H:33:ALA:HB2	2:H:98:TYR:O	2.17	0.44
1:A:159:GLN:O	1:A:163:LEU:HB2	2.18	0.44
2:H:146:PHE:HA	2:H:147:PRO:HA	1.83	0.43
1:A:117:ILE:HG13	1:A:118:ASN:ND2	2.33	0.43
1:A:250:LEU:HD23	1:A:253:GLU:OE2	2.19	0.43
1:A:250:LEU:HA	1:A:253:GLU:HG2	2.00	0.43
2:H:150:VAL:HG12	2:H:178:LEU:HD21	2.01	0.43
1:A:90:GLN:HB2	2:H:98:TYR:CD2	2.54	0.42
2:H:64:GLN:NE2	2:H:64:GLN:HA	2.34	0.42
3:L:14:ALA:O	3:L:17:GLN:HB3	2.19	0.42
1:A:101:ASN:HD21	2:H:29:PHE:N	2.17	0.42
1:A:108:GLY:C	1:A:111:PRO:HD2	2.40	0.42
1:A:117:ILE:HD13	1:A:167:VAL:HG11	2.01	0.41
2:H:151:THR:HB	2:H:199:ASN:HB3	2.01	0.41
2:H:117:LYS:HG2	2:H:118:GLY:O	2.20	0.41
3:L:190:TRP:CZ2	3:L:213:PRO:HA	2.55	0.41
3:L:4:LEU:HD11	3:L:90:THR:HG22	2.02	0.41
2:H:52:ILE:HD12	2:H:98:TYR:O	2.20	0.41
1:A:32:LEU:HA	2:H:74:PHE:CE1	2.55	0.41
1:A:155:ALA:O	1:A:159:GLN:HG3	2.21	0.41
1:A:151:ASN:HA	1:A:154:ARG:HB2	2.03	0.41
1:A:77:GLU:OE2	1:A:225:LYS:NZ	2.39	0.41
3:L:61:ARG:HG2	3:L:76:THR:O	2.21	0.41
2:H:44:GLY:HA2	3:L:87:TYR:CE1	2.55	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:163:VAL:HG22	2:H:182:VAL:HB	2.02	0.41
1:A:151:ASN:HB3	1:A:154:ARG:NH2	2.35	0.41
2:H:191:THR:OG1	2:H:192:GLN:N	2.54	0.41
3:L:194:ARG:HD3	3:L:195:SER:HB3	2.03	0.40
3:L:58:ILE:HA	3:L:59:PRO:HD3	1.79	0.40
2:H:125:ALA:HA	2:H:126:PRO:HD3	1.98	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	236/305 (77%)	216 (92%)	18 (8%)	2 (1%)	24	70
2	H	219/226 (97%)	210 (96%)	7 (3%)	2 (1%)	21	67
3	L	208/221 (94%)	192 (92%)	13 (6%)	3 (1%)	14	59
All	All	663/752 (88%)	618 (93%)	38 (6%)	7 (1%)	17	64

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	ARG
3	L	95	PRO
1	A	54	ILE
2	H	133	GLY
3	L	213	PRO
3	L	156	ASP
2	H	126	PRO

### 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	213/260 (82%)	192 (90%)	21 (10%)	10	42
2	H	184/189 (97%)	175 (95%)	9 (5%)	31	68
3	L	178/182 (98%)	168 (94%)	10 (6%)	26	65
All	All	575/631 (91%)	535 (93%)	40 (7%)	19	58

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	19	VAL
1	A	30	VAL
1	A	42	LEU
1	A	54	ILE
1	A	63	THR
1	A	67	ASP
1	A	112	GLU
1	A	118	ASN
1	A	125	TYR
1	A	126	SER
1	A	131	SER
1	A	148	GLN
1	A	150	ASN
1	A	160	GLN
1	A	162	LEU
1	A	163	LEU
1	A	165	LEU
1	A	166	THR
1	A	184	LEU
1	A	249	LYS
2	H	4	LEU
2	H	64	GLN
2	H	98	TYR
2	H	116	THR
2	H	130	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	H	150	VAL
2	H	164	HIS
2	H	191	THR
2	H	193	THR
3	L	18	LYS
3	L	19	VAL
3	L	56	SER
3	L	61	ARG
3	L	69	THR
3	L	161	LYS
3	L	180	SER
3	L	194	ARG
3	L	195	SER
3	L	215	GLU

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

Mol	Chain	Res	Type
1	A	101	ASN
1	A	118	ASN
1	A	147	GLN

### 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 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	A	242/305 (79%)	10.53	239 (98%) <b>0</b> <b>0</b>	25, 75, 165, 251	0
2	H	221/226 (97%)	9.13	214 (96%) <b>0</b> <b>0</b>	23, 61, 140, 194	0
3	L	212/221 (95%)	9.73	209 (98%) <b>0</b> <b>0</b>	37, 93, 177, 253	0
All	All	675/752 (89%)	9.82	662 (98%) <b>0</b> <b>0</b>	23, 77, 168, 253	0

All (662) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233	SER	43.2
1	A	226	CYS	40.4
1	A	109	GLY	33.2
3	L	50	ASP	32.6
1	A	79	GLY	32.5
1	A	80	SER	32.3
1	A	102	SER	32.1
3	L	13	ALA	29.6
1	A	236	ASN	29.1
1	A	95	GLY	27.3
2	H	203	SER	26.0
1	A	112	GLU	25.8
2	H	118	GLY	25.7
1	A	245	SER	25.4
1	A	248	SER	25.2
3	L	52	ASN	25.2
3	L	14	ALA	24.7
3	L	174	ASN	24.0
3	L	53	LYS	23.9
3	L	115	LYS	23.7
1	A	195	SER	23.6
2	H	43	GLN	23.2
1	A	111	PRO	23.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	192	GLN	22.8
1	A	27	THR	22.7
3	L	49	TYR	22.7
1	A	199	ASN	22.6
3	L	51	ASN	22.3
3	L	204	GLY	22.3
1	A	119	ASN	22.1
1	A	230	CYS	21.9
3	L	175	ASN	21.8
1	A	78	GLN	21.7
1	A	98	ASN	21.4
1	A	105	GLU	21.3
3	L	147	GLY	21.2
1	A	246	GLU	21.2
2	H	85	GLU	21.0
3	L	205	SER	21.0
2	H	162	GLY	20.4
1	A	108	GLY	20.4
3	L	27(A)	SER	20.3
2	H	204	ASN	20.2
2	H	160	THR	20.0
2	H	115	SER	19.7
3	L	55	PRO	19.6
1	A	76	ASN	19.3
1	A	133	ASN	19.2
2	H	171	GLN	19.2
2	H	161	SER	19.1
3	L	54	ARG	19.1
3	L	12	SER	19.0
1	A	136	GLU	18.9
1	A	196	ASN	18.9
2	H	197	ASN	18.8
2	H	72	ASP	18.7
3	L	143	ASP	18.7
1	A	224	HIS	18.7
1	A	44	ASN	18.6
2	H	114	ALA	18.5
1	A	234	VAL	18.4
2	H	190	GLY	18.3
3	L	8	PRO	18.2
1	A	247	GLU	18.1
3	L	116	ALA	18.0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	172	SER	17.8
3	L	56	SER	17.5
3	L	133	ASN	17.5
3	L	148	ALA	17.4
3	L	77	GLY	17.3
1	A	174	GLN	17.2
2	H	21	SER	17.1
2	H	70	THR	16.9
1	A	26	VAL	16.9
1	A	115	ARG	16.9
1	A	94	ASN	16.7
1	A	238	THR	16.7
1	A	251	ASN	16.7
1	A	17	ASP	16.7
2	H	127	SER	16.7
2	H	207	VAL	16.5
1	A	225	LYS	16.5
1	A	103	VAL	16.3
3	L	163	GLY	16.3
2	H	9	ALA	16.0
1	A	134	GLN	15.9
2	H	117	LYS	15.7
1	A	88	SER	15.6
1	A	14	ASP	15.4
2	H	144	ASP	15.4
3	L	41	GLY	15.4
2	H	158	ALA	15.3
2	H	81	GLU	15.3
1	A	81	GLY	15.3
2	H	18	VAL	15.3
1	A	232	GLU	15.3
2	H	153	SER	15.2
1	A	46	PRO	15.2
3	L	40	PRO	15.1
1	A	135	GLN	15.1
2	H	71	ALA	14.9
3	L	17	GLN	14.8
3	L	155	ALA	14.8
3	L	119	SER	14.7
1	A	249	LYS	14.7
2	H	196	CYS	14.6
1	A	116	GLU	14.6

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	L	131	GLN	14.6
3	L	106	VAL	14.6
3	L	59	PRO	14.6
3	L	178	ALA	14.5
3	L	69	THR	14.5
2	H	208	ASP	14.4
3	L	114	PRO	14.4
3	L	172	GLN	14.4
3	L	18	LYS	14.4
1	A	22	LYS	14.4
2	H	56	THR	14.2
3	L	64	GLY	14.2
2	H	107	THR	14.2
2	H	128	SER	14.1
2	H	82(B)	SER	14.1
3	L	107	LEU	14.0
2	H	84	SER	14.0
1	A	210	ASN	14.0
2	H	199	ASN	13.9
1	A	169	GLY	13.6
3	L	213	PRO	13.6
2	H	133	GLY	13.6
2	H	31	SER	13.6
3	L	149	VAL	13.6
2	H	64	GLN	13.6
3	L	173	SER	13.6
2	H	10	GLU	13.5
1	A	113	TRP	13.5
2	H	17	SER	13.5
3	L	206	THR	13.4
1	A	1	ASP	13.4
2	H	183	THR	13.3
3	L	158	SER	13.3
3	L	15	PRO	13.3
2	H	78	VAL	13.1
1	A	75	GLN	13.1
1	A	25	THR	13.0
2	H	134	GLY	13.0
2	H	202	PRO	13.0
1	A	237	GLY	12.9
1	A	191	ASP	12.9
3	L	9	SER	12.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	61	PRO	12.9
3	L	94	ARG	12.9
1	A	172	GLN	12.8
3	L	60	ASP	12.8
2	H	201	LYS	12.7
3	L	130	LEU	12.7
2	H	113	SER	12.7
2	H	116	THR	12.6
1	A	185	GLU	12.6
3	L	144	PHE	12.6
1	A	23	ASN	12.6
1	A	29	SER	12.5
1	A	107	MET	12.5
3	L	65	SER	12.5
2	H	82(C)	LEU	12.5
3	L	61	ARG	12.5
2	H	57	THR	12.4
1	A	77	GLU	12.4
1	A	18	THR	12.3
3	L	179	ALA	12.2
2	H	210	ARG	12.2
1	A	47	GLN	12.2
1	A	21	GLU	12.1
3	L	70	SER	12.1
1	A	189	THR	12.1
3	L	210	THR	12.0
1	A	129	GLU	12.0
1	A	231	MET	12.0
3	L	129	GLU	12.0
3	L	118	PRO	12.0
3	L	142	SER	12.0
2	H	119	PRO	12.0
2	H	173	SER	11.9
3	L	57	GLY	11.9
2	H	60	ALA	11.7
2	H	42	GLY	11.7
1	A	209	LYS	11.7
2	H	193	THR	11.7
1	A	170	ILE	11.7
1	A	178	ALA	11.6
2	H	86	ASP	11.6
3	L	105	THR	11.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	L	76	THR	11.5
3	L	156	ASP	11.5
3	L	25	GLY	11.5
2	H	112	SER	11.5
1	A	114	ASP	11.5
1	A	255	ILE	11.4
3	L	203	GLU	11.4
1	A	13	THR	11.4
1	A	244	TYR	11.4
2	H	159	LEU	11.3
1	A	194	ASP	11.3
2	H	168	ALA	11.3
3	L	139	CYS	11.3
3	L	150	THR	11.3
2	H	184	VAL	11.3
3	L	42	THR	11.2
2	H	22	CYS	11.2
1	A	64	GLY	11.2
1	A	235	LYS	11.2
1	A	104	ILE	11.1
2	H	8	GLY	11.1
3	L	195	SER	11.1
2	H	143	LYS	11.1
1	A	148	GLN	11.1
1	A	166	THR	11.1
1	A	99	LYS	11.0
1	A	211	ASN	11.0
1	A	167	VAL	11.0
1	A	87	LYS	11.0
3	L	32	TYR	11.0
3	L	102	THR	11.0
2	H	106	GLY	11.0
1	A	12	SER	10.9
2	H	205	THR	10.9
1	A	130	GLU	10.9
1	A	175	THR	10.9
1	A	158	ALA	10.9
1	A	192	PHE	10.8
3	L	24	SER	10.8
1	A	177	ASN	10.8
3	L	95	PRO	10.8
1	A	220	PHE	10.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	145	TYR	10.8
3	L	66	LYS	10.8
1	A	151	ASN	10.8
3	L	162	ALA	10.8
3	L	95(B)	ALA	10.7
1	A	74	HIS	10.7
1	A	254	LYS	10.7
3	L	202	HIS	10.7
1	A	118	ASN	10.7
2	H	87	THR	10.6
3	L	176	LYS	10.6
2	H	19	LYS	10.6
1	A	149	GLN	10.6
3	L	120	VAL	10.6
2	H	16	SER	10.6
2	H	27	GLY	10.5
1	A	30	VAL	10.5
3	L	23	CYS	10.5
1	A	126	SER	10.5
1	A	250	LEU	10.5
3	L	95(C)	TYR	10.4
2	H	126	PRO	10.4
1	A	91	ASN	10.4
1	A	160	GLN	10.3
1	A	106	LYS	10.3
1	A	241	TYR	10.3
2	H	148	GLU	10.3
1	A	159	GLN	10.3
3	L	141	ILE	10.3
3	L	85	ASN	10.2
2	H	83	ARG	10.2
3	L	157	SER	10.2
2	H	206	LYS	10.2
3	L	146	PRO	10.2
2	H	135	THR	10.1
1	A	28	HIS	10.1
1	A	202	GLU	10.1
3	L	92	ASP	10.1
2	H	130	SER	10.0
2	H	20	VAL	10.0
2	H	176	TYR	10.0
1	A	206	SER	10.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	L	164	VAL	9.9
2	H	92	CYS	9.9
2	H	120	SER	9.9
3	L	188	GLU	9.9
2	H	104	GLY	9.9
1	A	163	LEU	9.8
3	L	68	GLY	9.8
3	L	78	LEU	9.8
3	L	96	VAL	9.8
2	H	26	GLY	9.7
1	A	110	ASP	9.7
2	H	1	GLU	9.7
2	H	75	ALA	9.7
1	A	86	GLN	9.6
2	H	62	LYS	9.6
1	A	227	ASN	9.6
2	H	44	GLY	9.6
3	L	184	SER	9.6
2	H	164	HIS	9.6
1	A	242	PRO	9.5
1	A	2	THR	9.5
1	A	171	LYS	9.5
3	L	27	SER	9.5
1	A	200	LEU	9.5
1	A	188	ARG	9.5
3	L	215	GLU	9.5
1	A	190	LEU	9.5
1	A	61	GLY	9.5
3	L	58	ILE	9.5
3	L	177	TYR	9.4
1	A	165	LEU	9.4
2	H	82	LEU	9.4
3	L	5	THR	9.3
3	L	103	LYS	9.3
2	H	37	VAL	9.3
2	H	175	LEU	9.3
1	A	65	MET	9.2
2	H	7	SER	9.2
3	L	26	SER	9.2
1	A	132	GLN	9.2
3	L	117	ALA	9.2
3	L	95(A)	THR	9.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	156	SER	9.2
1	A	10	ASN	9.2
2	H	200	HIS	9.1
3	L	208	GLU	9.1
1	A	85	ASP	9.1
1	A	122	SER	9.1
2	H	79	TYR	9.0
1	A	31	ASN	9.0
2	H	45	PRO	9.0
2	H	65	GLY	8.9
3	L	101	GLY	8.9
3	L	183	LEU	8.9
2	H	105	LYS	8.9
1	A	162	LEU	8.9
2	H	68	THR	8.9
2	H	2	VAL	8.9
3	L	19	VAL	8.9
1	A	243	LYS	8.8
1	A	186	ASN	8.8
1	A	179	GLU	8.8
2	H	129	LYS	8.8
3	L	27(B)	ASN	8.8
3	L	6	GLN	8.7
2	H	191	THR	8.7
2	H	195	ILE	8.7
1	A	168	TRP	8.7
2	H	82(A)	SER	8.7
1	A	252	ARG	8.7
1	A	45	ILE	8.7
2	H	77	THR	8.7
2	H	66	ARG	8.7
2	H	165	THR	8.7
3	L	186	THR	8.6
1	A	173	LEU	8.6
2	H	170	LEU	8.6
2	H	63	PHE	8.6
1	A	60	GLY	8.6
3	L	145	TYR	8.6
1	A	93	ILE	8.6
3	L	126	SER	8.6
3	L	38	GLN	8.5
1	A	43	ARG	8.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	177	SER	8.5
2	H	100(C)	THR	8.5
2	H	73	ASP	8.5
3	L	214	THR	8.4
2	H	194	TYR	8.4
3	L	151	VAL	8.4
3	L	128	GLU	8.4
2	H	101	ASP	8.4
1	A	187	GLU	8.4
3	L	166	THR	8.3
1	A	101	ASN	8.3
3	L	39	LEU	8.3
3	L	134	LYS	8.3
1	A	67	ASP	8.2
2	H	55	GLY	8.2
1	A	164	GLN	8.1
2	H	152	VAL	8.1
1	A	89	THR	8.1
1	A	184	LEU	8.1
1	A	228	ASN	8.1
2	H	149	PRO	8.1
2	H	13	LYS	8.1
3	L	81	GLY	8.1
1	A	96	ILE	8.0
1	A	59	GLU	8.0
1	A	66	VAL	8.0
2	H	157	GLY	8.0
2	H	198	VAL	8.0
3	L	165	GLU	7.9
3	L	127	SER	7.9
1	A	205	LYS	7.9
2	H	188	SER	7.9
2	H	174	GLY	7.9
3	L	44	PRO	7.9
2	H	47	TRP	7.9
1	A	161	HIS	7.8
3	L	33	VAL	7.8
2	H	30	ARG	7.8
3	L	7	PRO	7.8
2	H	169	VAL	7.8
1	A	152	LEU	7.7
3	L	93	ARG	7.7

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	221	GLU	7.7
3	L	209	LYS	7.7
1	A	198	LYS	7.7
3	L	16	GLY	7.7
3	L	67	SER	7.6
3	L	82	ASP	7.6
1	A	97	THR	7.6
3	L	207	VAL	7.6
2	H	51	ILE	7.5
3	L	194	ARG	7.5
1	A	123	ILE	7.5
1	A	63	THR	7.5
2	H	11	VAL	7.5
2	H	93	ALA	7.4
1	A	240	ASP	7.4
1	A	73	HIS	7.4
1	A	213	LYS	7.4
2	H	132	SER	7.3
2	H	131	THR	7.3
3	L	48	ILE	7.3
1	A	3	ILE	7.3
1	A	32	LEU	7.3
1	A	176	TYR	7.3
3	L	45	LYS	7.3
2	H	111	VAL	7.3
2	H	140	CYS	7.2
1	A	197	VAL	7.2
2	H	103	TRP	7.2
1	A	229	GLU	7.1
3	L	83	GLU	7.1
2	H	182	VAL	7.1
3	L	73	LEU	7.1
2	H	67	VAL	7.1
3	L	180	SER	7.1
1	A	121	THR	7.0
1	A	131	SER	6.9
2	H	74	PHE	6.9
2	H	142	VAL	6.9
1	A	193	HIS	6.9
2	H	185	PRO	6.9
3	L	72	THR	6.9
2	H	100(B)	GLU	6.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	3	GLN	6.8
1	A	5	ILE	6.7
2	H	15	GLY	6.7
2	H	121	VAL	6.7
3	L	199	GLN	6.6
3	L	171	LYS	6.5
1	A	157	GLU	6.5
3	L	86	TYR	6.5
3	L	11	VAL	6.5
3	L	161	LYS	6.5
1	A	150	ASN	6.5
3	L	181	SER	6.5
1	A	145	ILE	6.5
3	L	43	ALA	6.5
3	L	4	LEU	6.5
3	L	132	ALA	6.5
2	H	48	MET	6.4
1	A	207	GLN	6.4
3	L	189	GLN	6.4
2	H	25	SER	6.3
2	H	108	THR	6.3
2	H	91	TYR	6.3
2	H	189	LEU	6.3
3	L	212	ALA	6.3
2	H	163	VAL	6.2
3	L	169	PRO	6.2
3	L	135	ALA	6.2
3	L	79	GLN	6.2
3	L	20	THR	6.2
3	L	121	THR	6.2
1	A	82	TYR	6.2
2	H	49	GLY	6.2
1	A	19	VAL	6.2
2	H	52	ILE	6.2
1	A	53	ALA	6.2
3	L	185	LEU	6.1
1	A	24	VAL	6.1
2	H	76	GLY	6.1
3	L	138	VAL	6.1
2	H	80	MET	6.1
3	L	159	PRO	6.1
2	H	5	VAL	6.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	102	VAL	6.1
3	L	113	GLN	6.1
1	A	239	TYR	6.0
2	H	123	PRO	6.0
2	H	32	TYR	5.9
3	L	34	SER	5.9
2	H	181	VAL	5.9
1	A	40	THR	5.9
1	A	181	LEU	5.9
2	H	167	PRO	5.8
2	H	14	PRO	5.8
3	L	37	GLN	5.8
1	A	16	VAL	5.8
2	H	94	LYS	5.8
2	H	95	HIS	5.8
2	H	180	SER	5.7
3	L	88	CYS	5.7
1	A	92	ALA	5.7
3	L	22	SER	5.7
1	A	15	THR	5.6
1	A	180	LEU	5.6
1	A	37	ARG	5.6
3	L	46	LEU	5.6
3	L	47	LEU	5.6
2	H	110	THR	5.5
1	A	146	VAL	5.5
1	A	201	TYR	5.5
1	A	90	GLN	5.5
2	H	53	ILE	5.4
3	L	84	ALA	5.4
3	L	200	VAL	5.4
3	L	35	TRP	5.4
1	A	54	ILE	5.4
3	L	74	GLY	5.4
2	H	52(A)	PRO	5.4
1	A	100	VAL	5.4
1	A	11	ASN	5.3
3	L	125	PRO	5.3
1	A	42	LEU	5.3
2	H	100(D)	MET	5.3
2	H	209	LYS	5.3
3	L	71	ALA	5.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	183	LEU	5.3
2	H	154	TRP	5.3
1	A	253	GLU	5.2
1	A	71	GLY	5.2
1	A	153	LEU	5.2
1	A	203	LYS	5.2
1	A	35	GLY	5.2
3	L	140	LEU	5.2
1	A	6	GLY	5.1
2	H	96	MET	5.1
1	A	214	GLU	5.1
2	H	69	ILE	5.1
3	L	63	SER	5.1
1	A	156	ILE	5.1
2	H	12	LYS	5.1
2	H	100	VAL	5.1
1	A	83	ALA	5.0
2	H	89	MET	5.0
1	A	62	TRP	5.0
2	H	28	PRO	5.0
2	H	178	LEU	5.0
3	L	152	ALA	5.0
2	H	29	PHE	4.9
2	H	59	TYR	4.9
2	H	211	VAL	4.9
1	A	223	TYR	4.9
3	L	87	TYR	4.9
2	H	6	GLU	4.9
2	H	125	ALA	4.8
1	A	182	VAL	4.8
3	L	182	TYR	4.8
2	H	150	VAL	4.8
2	H	151	THR	4.8
1	A	208	LEU	4.8
2	H	136	ALA	4.8
3	L	3	VAL	4.8
3	L	198	CYS	4.7
1	A	127	LEU	4.7
1	A	125	TYR	4.6
3	L	62	PHE	4.6
2	H	179	SER	4.6
3	L	124	PRO	4.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
3	L	104	LEU	4.5
2	H	124	LEU	4.5
2	H	50	GLY	4.4
1	A	7	TYR	4.4
1	A	84	ALA	4.4
2	H	141	LEU	4.4
2	H	187	SER	4.3
3	L	97	VAL	4.3
1	A	39	VAL	4.3
3	L	154	LYS	4.2
3	L	196	TYR	4.2
2	H	186	SER	4.2
2	H	122	PHE	4.2
1	A	57	PHE	4.2
3	L	137	LEU	4.2
3	L	100	GLY	4.2
3	L	31	ASP	4.2
3	L	167	THR	4.1
1	A	204	VAL	4.1
3	L	197	SER	4.1
2	H	166	PHE	4.1
1	A	222	PHE	4.1
2	H	213	PRO	4.1
3	L	168	THR	4.0
2	H	100(A)	ARG	4.0
3	L	187	PRO	4.0
3	L	75	ILE	4.0
2	H	36	TRP	3.9
1	A	218	GLY	3.9
1	A	117	ILE	3.9
1	A	38	MET	3.8
1	A	8	HIS	3.8
2	H	46	GLU	3.7
3	L	28	ILE	3.7
1	A	147	GLN	3.7
3	L	160	VAL	3.7
1	A	72	TYR	3.6
1	A	70	TYR	3.6
1	A	34	SER	3.6
2	H	33	ALA	3.6
3	L	211	VAL	3.6
2	H	139	GLY	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	138	LEU	3.6
2	H	54	PHE	3.6
1	A	58	ILE	3.6
3	L	80	THR	3.6
3	L	99	GLY	3.6
1	A	219	CYS	3.5
3	L	36	TYR	3.5
3	L	136	THR	3.5
2	H	155	ASN	3.5
3	L	89	ALA	3.5
2	H	109	VAL	3.4
2	H	35	SER	3.4
3	L	191	LYS	3.4
3	L	201	THR	3.4
1	A	120	TYR	3.3
2	H	90	TYR	3.3
1	A	68	GLY	3.3
3	L	98	PHE	3.2
2	H	88	ALA	3.2
3	L	122	LEU	3.1
2	H	41	PRO	3.1
2	H	212	GLU	3.0
2	H	40	ALA	3.0
1	A	69	TRP	3.0
1	A	55	ALA	2.9
3	L	170	SER	2.9
3	L	21	ILE	2.9
2	H	24	ALA	2.9
1	A	20	LEU	2.8
1	A	9	ALA	2.8
1	A	33	GLY	2.8
3	L	190	TRP	2.8
3	L	91	TRP	2.8
2	H	34	ILE	2.7
2	H	4	LEU	2.7
1	A	41	GLY	2.7
2	H	137	ALA	2.7
1	A	124	ILE	2.6
2	H	58	LYS	2.6
3	L	153	TRP	2.5
1	A	36	LEU	2.4
1	A	154	ARG	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	215	ILE	2.3
2	H	147	PRO	2.2
1	A	155	ALA	2.2
1	A	217	ASN	2.2
1	A	128	ILE	2.1
3	L	192	SER	2.1
3	L	90	THR	2.1
3	L	123	PHE	2.0
1	A	56	GLY	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.