



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:35 AM GMT

PDB ID : 2HRP  
Title : ANTIGEN-ANTIBODY COMPLEX  
Authors : Lescar, J.; Bentley, G.A.  
Deposited on : 1996-12-27  
Resolution : 2.20 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 : 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

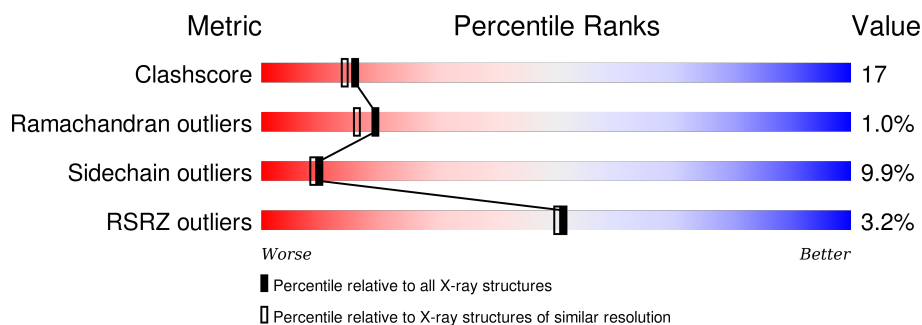
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	218	<div> <div>2%</div> <div>67% 28% . .</div> </div>
1	M	218	<div> <div>3%</div> <div>69% 26% 5%</div> </div>
2	H	226	<div> <div>4%</div> <div>64% 30% 6%</div> </div>
2	N	226	<div> <div>4%</div> <div>67% 28% . .</div> </div>
3	P	10	<div> <div>80% 10% 10%</div> </div>
3	Q	10	<div> <div>70% 30%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7246 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 MONOCLONAL ANTIBODY F11.2.32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	0	0
			1656	1034	281	333	8			
1	M	218	Total	C	N	O	S	0	0	0
			1659	1036	284	331	8			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	4	LEU	MET	CONFLICT	GB 600718
L	18	ARG	SER	CONFLICT	GB 600718
L	19	ALA	VAL	CONFLICT	GB 600718
L	27C	ASP	GLU	CONFLICT	GB 600718
L	30	LYS	THR	CONFLICT	GB 600718
L	32	PHE	LEU	CONFLICT	GB 600718
L	34	ASN	GLN	CONFLICT	GB 600718
L	36	PHE	TYR	CONFLICT	GB 600718
L	50	ALA	GLY	CONFLICT	GB 600718
L	54	GLN	VAL	CONFLICT	GB 600718
L	55	GLY	GLU	CONFLICT	GB 600718
L	74	HIS	ASN	CONFLICT	GB 600718
L	78	MET	VAL	CONFLICT	GB 600718
L	83	SER	ILE	CONFLICT	GB 600718
L	85	MET	ILE	CONFLICT	GB 600718
L	92	LYS	ARG	CONFLICT	GB 600718
L	93	GLU	LYS	CONFLICT	GB 600718
L	96	TRP	ALA	CONFLICT	GB 600718
L	100	GLY	SER	CONFLICT	GB 600718
M	4	LEU	MET	CONFLICT	GB 600718
M	18	ARG	SER	CONFLICT	GB 600718
M	19	ALA	VAL	CONFLICT	GB 600718
M	27C	ASP	GLU	CONFLICT	GB 600718
M	30	LYS	THR	CONFLICT	GB 600718
M	32	PHE	LEU	CONFLICT	GB 600718

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
M	34	ASN	GLN	CONFLICT	GB 600718
M	36	PHE	TYR	CONFLICT	GB 600718
M	50	ALA	GLY	CONFLICT	GB 600718
M	54	GLN	VAL	CONFLICT	GB 600718
M	55	GLY	GLU	CONFLICT	GB 600718
M	74	HIS	ASN	CONFLICT	GB 600718
M	78	MET	VAL	CONFLICT	GB 600718
M	83	SER	ILE	CONFLICT	GB 600718
M	85	MET	ILE	CONFLICT	GB 600718
M	92	LYS	ARG	CONFLICT	GB 600718
M	93	GLU	LYS	CONFLICT	GB 600718
M	96	TRP	ALA	CONFLICT	GB 600718
M	100	GLY	SER	CONFLICT	GB 600718

- Molecule 2 is a protein called MONOCLONAL ANTIBODY F11.2.32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	226	Total	C	N	O	S	0	0	0
			1706	1076	287	334	9			
2	N	224	Total	C	N	O	S	0	0	0
			1669	1055	280	325	9			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	5	VAL	LEU	CONFLICT	GB 600716
H	13	GLN	LYS	CONFLICT	GB 600716
H	18	ARG	LEU	CONFLICT	GB 600716
H	30	MET	SER	CONFLICT	GB 600716
H	31	ARG	ASP	CONFLICT	GB 600716
H	32	PHE	TYR	CONFLICT	GB 600716
H	74	PRO	ALA	CONFLICT	GB 600716
H	89	LEU	MET	CONFLICT	GB 600716
H	95	SER	-	INSERTION	GB 600716
H	96	GLY	-	INSERTION	GB 600716
H	97	GLY	TRP	CONFLICT	GB 600716
H	98	ILE	ASP	CONFLICT	GB 600716
H	99	GLU	THR	CONFLICT	GB 600716
H	100	ARG	THR	CONFLICT	GB 600716
H	100A	TYR	VAL	CONFLICT	GB 600716
H	100B	ASP	SER	CONFLICT	GB 600716
H	100D	THR	HIS	CONFLICT	GB 600716

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
H	187	PRO	THR	CONFLICT	GB 600716
H	188	ARG	TRP	CONFLICT	GB 600716
H	191	GLU	GLN	CONFLICT	GB 600716
N	5	VAL	LEU	CONFLICT	GB 600716
N	13	GLN	LYS	CONFLICT	GB 600716
N	18	ARG	LEU	CONFLICT	GB 600716
N	30	MET	SER	CONFLICT	GB 600716
N	31	ARG	ASP	CONFLICT	GB 600716
N	32	PHE	TYR	CONFLICT	GB 600716
N	74	PRO	ALA	CONFLICT	GB 600716
N	89	LEU	MET	CONFLICT	GB 600716
N	95	SER	-	INSERTION	GB 600716
N	96	GLY	-	INSERTION	GB 600716
N	97	GLY	TRP	CONFLICT	GB 600716
N	98	ILE	ASP	CONFLICT	GB 600716
N	99	GLU	THR	CONFLICT	GB 600716
N	100	ARG	THR	CONFLICT	GB 600716
N	100A	TYR	VAL	CONFLICT	GB 600716
N	100B	ASP	SER	CONFLICT	GB 600716
N	100D	THR	HIS	CONFLICT	GB 600716
N	187	PRO	THR	CONFLICT	GB 600716
N	188	ARG	TRP	CONFLICT	GB 600716
N	191	GLU	GLN	CONFLICT	GB 600716

- Molecule 3 is a protein called HIV-1 PROTEASE PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	S	0	0	0
			80	52	15	12	1			
3	Q	10	Total	C	N	O	S	0	0	0
			80	52	15	12	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	92	Total	O	0	0
			92	92		
4	L	103	Total	O	0	0
			103	103		
4	M	99	Total	O	0	0
			99	99		
4	N	93	Total	O	0	0
			93	93		

*Continued on next page...*

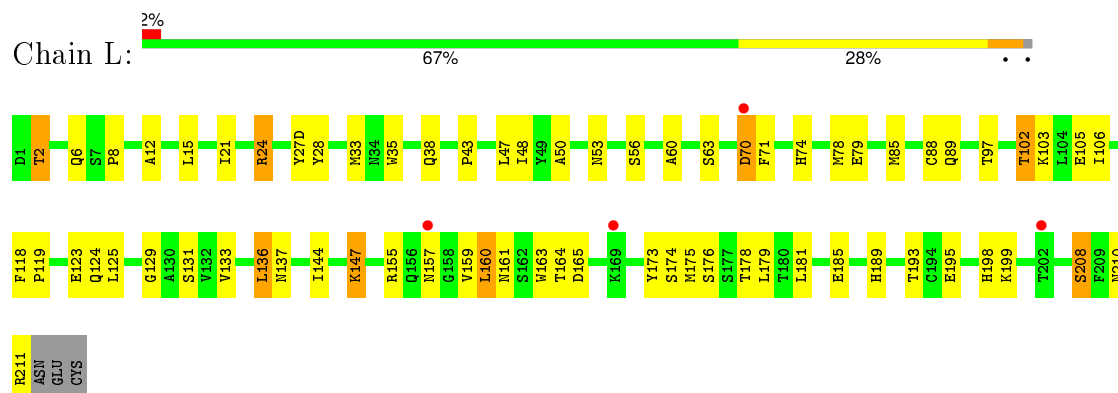
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	6	Total	O	0	0
			6	6		
4	Q	3	Total	O	0	0
			3	3		

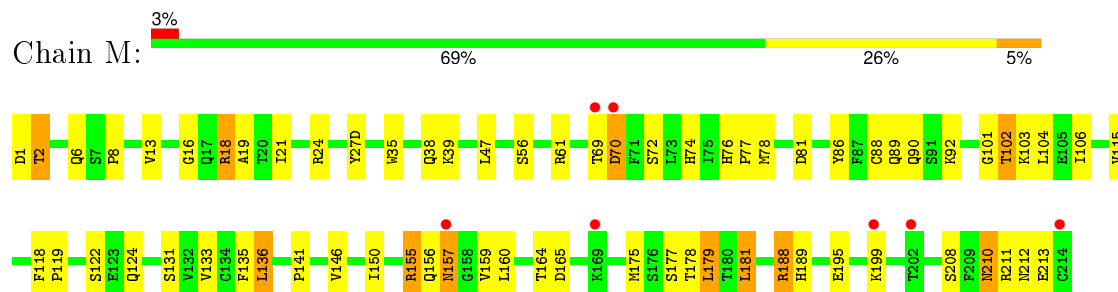
### 3 Residue-property plots

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.

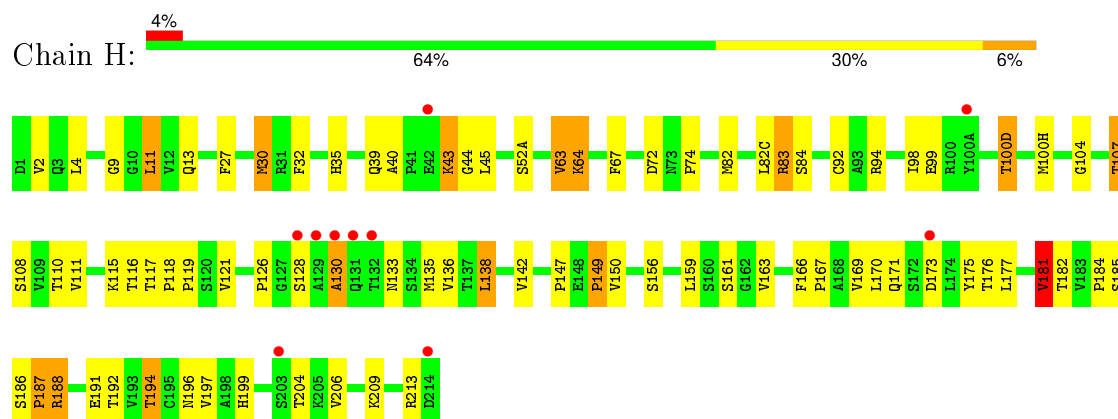
#### • Molecule 1: MONOCLONAL ANTIBODY F11.2.32



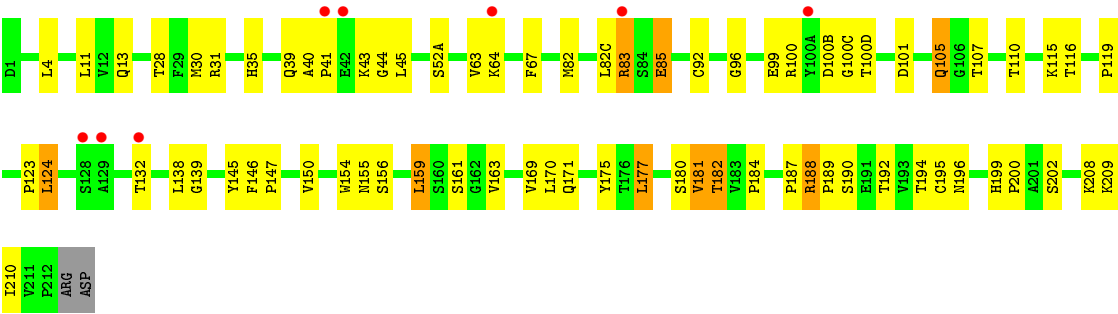
#### • Molecule 1: MONOCLONAL ANTIBODY F11.2.32



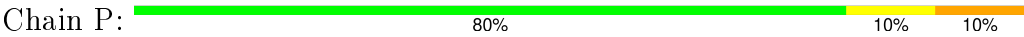
#### • Molecule 2: MONOCLONAL ANTIBODY F11.2.32



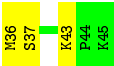
#### • Molecule 2: MONOCLONAL ANTIBODY F11.2.32



● Molecule 3: HIV-1 PROTEASE PEPTIDE



● Molecule 3: HIV-1 PROTEASE PEPTIDE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.30 Å 96.31 Å 105.86 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20 19.77 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.0 (7.00-2.20) 99.6 (19.77-2.10)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.57 (at 2.09 Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.198 , 0.289 0.212 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	21.5	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 83.3	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	3 of 49538 reflections (0.006%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7246	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.20 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.8236e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	L	0.54	0/1697	0.76	1/2302 (0.0%)
1	M	0.52	0/1700	0.78	1/2305 (0.0%)
2	H	0.54	0/1750	0.82	1/2385 (0.0%)
2	N	0.54	0/1712	0.82	1/2338 (0.0%)
3	P	0.54	0/83	0.66	0/110
3	Q	0.51	0/83	0.74	0/110
All	All	0.53	0/7025	0.80	4/9550 (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	H	181	VAL	CB-CA-C	-6.03	99.94	111.40
1	M	181	LEU	CA-CB-CG	5.52	128.01	115.30
2	N	177	LEU	CA-CB-CG	5.49	127.93	115.30
1	L	136	LEU	CA-CB-CG	5.01	126.83	115.30

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	L	1656	0	1577	53	0
1	M	1659	0	1571	64	0
2	H	1706	0	1665	61	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	1669	0	1623	59	0
3	P	80	0	79	2	0
3	Q	80	0	79	1	0
4	H	92	0	0	6	0
4	L	103	0	0	9	0
4	M	99	0	0	7	0
4	N	93	0	0	6	0
4	P	6	0	0	0	0
4	Q	3	0	0	0	0
All	All	7246	0	6594	228	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 17.

All (228) 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:N:163:VAL:HG22	2:N:181:VAL:HG12	1.55	0.87
2:H:156:SER:H	2:H:196:ASN:HD21	1.24	0.82
1:M:157:ASN:HA	4:M:227:HOH:O	1.79	0.82
2:H:184:PRO:O	2:H:187:PRO:HD2	1.81	0.80
2:H:121:VAL:HG21	2:H:206:VAL:HG11	1.64	0.79
1:M:24:ARG:HH11	1:M:70:ASP:HA	1.47	0.79
2:H:63:VAL:HG13	2:H:67:PHE:HB2	1.62	0.79
2:N:156:SER:H	2:N:196:ASN:HD21	1.32	0.77
1:M:210:ASN:HD22	1:M:212:ASN:H	1.34	0.74
1:M:199:LYS:HG3	4:M:248:HOH:O	1.87	0.74
1:M:8:PRO:O	1:M:102:THR:HB	1.86	0.74
4:H:284:HOH:O	2:N:182:THR:HG21	1.87	0.73
2:N:63:VAL:HG13	2:N:67:PHE:HB2	1.69	0.73
1:L:8:PRO:O	1:L:102:THR:HB	1.89	0.72
2:N:163:VAL:HG22	2:N:181:VAL:CG1	2.18	0.72
2:H:194:THR:HG23	4:H:251:HOH:O	1.89	0.72
1:M:61:ARG:HD2	1:M:77:PRO:O	1.90	0.72
2:N:154:TRP:CZ3	2:N:210:ILE:HD11	2.24	0.72
1:L:33:MET:HE1	1:L:89:GLN:H	1.55	0.71
1:L:33:MET:CE	1:L:88:CYS:HB2	2.21	0.71
2:N:184:PRO:HB2	2:N:187:PRO:HD2	1.72	0.71
2:N:154:TRP:HZ3	2:N:210:ILE:HD11	1.56	0.70
1:M:210:ASN:ND2	1:M:212:ASN:H	1.88	0.70
2:N:184:PRO:HB2	2:N:187:PRO:CD	2.22	0.70

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:43:LYS:HD2	2:H:44:GLY:H	1.56	0.70
2:N:115:LYS:HE3	2:N:116:THR:O	1.92	0.69
1:M:164:THR:HG22	1:M:165:ASP:O	1.93	0.69
1:M:141:PRO:HG2	1:M:199:LYS:HD3	1.72	0.69
2:N:44:GLY:HA3	4:N:224:HOH:O	1.92	0.69
2:N:147:PRO:O	2:N:199:HIS:HE1	1.75	0.69
2:H:32:PHE:CD2	2:H:94:ARG:HD3	2.28	0.68
2:N:85:GLU:HG3	4:N:296:HOH:O	1.95	0.67
2:H:9:GLY:H	2:H:107:THR:HG21	1.60	0.66
1:L:50:ALA:HB3	1:L:53:ASN:HD22	1.60	0.66
2:N:40:ALA:H	2:N:43:LYS:HE2	1.60	0.66
1:L:33:MET:HE2	1:L:88:CYS:HB2	1.78	0.66
2:N:63:VAL:CG1	2:N:67:PHE:HB2	2.25	0.65
2:H:199:HIS:HB3	2:H:204:THR:HB	1.77	0.65
2:H:43:LYS:HD2	2:H:44:GLY:N	2.12	0.65
1:M:160:LEU:HD21	2:N:171:GLN:HG3	1.78	0.65
1:L:189:HIS:O	1:L:211:ARG:HD3	1.98	0.64
1:M:24:ARG:NH1	1:M:70:ASP:HA	2.14	0.63
2:H:156:SER:H	2:H:196:ASN:ND2	1.96	0.63
1:L:70:ASP:HB2	4:L:257:HOH:O	1.98	0.63
1:M:78:MET:CE	1:M:106:ILE:HD13	2.29	0.63
2:H:186:SER:OG	2:H:187:PRO:HD3	1.99	0.63
2:H:192:THR:HG23	2:H:209:LYS:HE3	1.79	0.62
2:H:135:MET:HB3	2:H:182:THR:HG22	1.82	0.62
2:N:192:THR:HG23	2:N:209:LYS:NZ	2.15	0.62
1:M:115:VAL:HA	1:M:135:PHE:O	2.00	0.61
1:M:27(D):TYR:HB2	1:M:92:LYS:HD2	1.82	0.61
1:M:135:PHE:CE2	2:N:180:SER:HB3	2.36	0.61
1:L:27(D):TYR:HH	3:P:36:MET:N	1.99	0.60
1:L:6:GLN:HE21	1:L:102:THR:HG23	1.66	0.60
1:L:38:GLN:HE22	2:H:39:GLN:HE22	1.50	0.60
2:N:194:THR:HG22	4:N:300:HOH:O	2.01	0.59
2:H:100(D):THR:HG23	3:P:43:LYS:HB3	1.84	0.59
1:M:18:ARG:CZ	1:M:18:ARG:HB3	2.33	0.59
2:H:184:PRO:C	2:H:187:PRO:HD2	2.22	0.59
1:M:6:GLN:NE2	1:M:102:THR:HG22	2.18	0.59
1:L:6:GLN:HE21	1:L:102:THR:CG2	2.15	0.58
1:M:18:ARG:HB2	1:M:76:HIS:HB2	1.85	0.58
2:N:200:PRO:HG2	4:N:220:HOH:O	2.04	0.58
1:M:210:ASN:HD22	1:M:212:ASN:N	2.01	0.58
2:H:187:PRO:HA	2:H:191:GLU:HG2	1.85	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:78:MET:HE1	1:M:104:LEU:HG	1.86	0.57
2:H:2:VAL:HG21	2:H:94:ARG:HH21	1.68	0.57
2:H:119:PRO:HD2	2:H:204:THR:HG21	1.86	0.57
2:H:149:PRO:HD2	4:H:230:HOH:O	2.04	0.57
1:M:189:HIS:O	1:M:211:ARG:HD3	2.04	0.57
1:M:6:GLN:HE21	1:M:102:THR:CG2	2.17	0.56
2:N:188:ARG:HD2	2:N:189:PRO:HA	1.87	0.56
2:N:192:THR:HG22	4:N:300:HOH:O	2.05	0.56
2:N:124:LEU:HB2	2:N:139:GLY:C	2.25	0.56
2:H:135:MET:HB3	2:H:182:THR:CG2	2.35	0.56
2:N:63:VAL:HG13	2:N:67:PHE:CG	2.40	0.56
2:H:121:VAL:CG2	2:H:206:VAL:HG11	2.36	0.56
1:L:50:ALA:HB3	1:L:53:ASN:ND2	2.22	0.55
1:M:6:GLN:HE21	1:M:102:THR:HG22	1.72	0.55
2:N:63:VAL:HG13	2:N:67:PHE:CB	2.37	0.55
2:H:64:LYS:HD3	4:H:297:HOH:O	2.08	0.54
1:M:78:MET:HE3	1:M:106:ILE:HD13	1.89	0.54
2:H:99:GLU:OE1	2:H:100(D):THR:HB	2.07	0.54
2:N:105:GLN:HG3	2:N:105:GLN:O	2.08	0.53
2:H:163:VAL:HG22	2:H:181:VAL:HG13	1.90	0.53
1:M:155:ARG:HD2	1:M:157:ASN:OD1	2.08	0.53
2:H:147:PRO:O	2:H:199:HIS:HE1	1.91	0.53
1:L:159:VAL:HA	1:L:178:THR:O	2.08	0.53
1:M:24:ARG:HA	1:M:69:THR:O	2.08	0.53
1:L:33:MET:HE1	1:L:88:CYS:HB2	1.91	0.53
2:H:2:VAL:HG21	2:H:94:ARG:NH2	2.24	0.53
1:L:2:THR:HG21	4:L:258:HOH:O	2.09	0.52
1:L:155:ARG:NH2	4:L:278:HOH:O	2.43	0.52
1:M:78:MET:HE2	1:M:106:ILE:HD13	1.92	0.52
2:H:128:SER:C	2:H:130:ALA:H	2.12	0.52
2:H:121:VAL:HG21	2:H:206:VAL:CG1	2.39	0.52
2:N:123:PRO:HD3	2:N:208:LYS:HD2	1.91	0.52
1:L:60:ALA:HB2	4:L:267:HOH:O	2.10	0.52
1:L:163:TRP:HD1	4:L:262:HOH:O	1.92	0.51
2:N:83:ARG:HB3	2:N:85:GLU:HG2	1.93	0.51
2:H:30:MET:O	2:H:52(A):SER:HB2	2.11	0.51
2:H:83:ARG:HA	2:H:83:ARG:NE	2.25	0.51
2:H:197:VAL:HB	2:H:206:VAL:CG1	2.41	0.51
2:N:31:ARG:NH1	4:N:237:HOH:O	2.44	0.51
2:N:156:SER:H	2:N:196:ASN:ND2	2.05	0.50
1:L:21:ILE:HG23	1:L:102:THR:HG21	1.91	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:33:MET:HG2	1:L:71:PHE:CG	2.45	0.50
2:H:72:ASP:OD1	2:H:74:PRO:HD2	2.11	0.50
2:N:138:LEU:HB3	2:N:210:ILE:HD13	1.92	0.50
1:M:18:ARG:HH11	1:M:18:ARG:HG2	1.75	0.50
1:M:188:ARG:NH1	4:M:220:HOH:O	2.44	0.50
2:H:40:ALA:H	2:H:43:LYS:NZ	2.09	0.50
1:M:18:ARG:CG	1:M:18:ARG:HH11	2.25	0.50
2:N:192:THR:HG23	2:N:209:LYS:HZ2	1.77	0.49
1:L:155:ARG:HH12	1:L:181:LEU:HD22	1.77	0.49
1:M:86:TYR:O	1:M:101:GLY:HA2	2.12	0.49
2:H:94:ARG:O	2:H:100(H):MET:HA	2.12	0.49
2:N:30:MET:O	2:N:52(A):SER:HB2	2.13	0.49
2:H:184:PRO:HB2	2:H:187:PRO:CD	2.42	0.49
1:L:160:LEU:HD23	1:L:178:THR:HB	1.94	0.49
2:H:138:LEU:HD21	2:H:188:ARG:HG3	1.93	0.49
1:L:125:LEU:HD23	1:L:129:GLY:O	2.12	0.49
2:N:124:LEU:HB2	2:N:139:GLY:O	2.13	0.49
2:H:136:VAL:HG13	2:H:185:SER:HA	1.94	0.49
1:L:173:TYR:HB3	4:L:262:HOH:O	2.13	0.48
1:L:43:PRO:HB3	2:H:104:GLY:O	2.13	0.48
2:N:96:GLY:HA3	2:N:101:ASP:OD2	2.13	0.48
2:H:84:SER:HA	2:H:111:VAL:HB	1.95	0.48
2:N:67:PHE:CZ	2:N:82:MET:HE2	2.48	0.48
1:L:33:MET:HE1	1:L:89:GLN:N	2.27	0.48
1:M:38:GLN:HE22	2:N:39:GLN:HE22	1.62	0.48
1:L:133:VAL:HG22	1:L:178:THR:HG23	1.96	0.47
4:M:275:HOH:O	3:Q:36:MET:HB2	2.14	0.47
2:H:170:LEU:HB2	2:H:175:TYR:CE1	2.48	0.47
2:N:195:CYS:SG	2:N:208:LYS:HB3	2.54	0.47
1:L:161:ASN:O	2:H:169:VAL:HG21	2.14	0.47
4:L:270:HOH:O	2:H:176:THR:HG21	2.13	0.47
1:L:160:LEU:CD2	1:L:178:THR:HB	2.44	0.47
1:L:124:GLN:HE22	1:L:131:SER:H	1.63	0.47
1:M:159:VAL:HA	1:M:178:THR:O	2.13	0.47
2:H:11:LEU:HD23	2:H:110:THR:O	2.15	0.47
1:M:160:LEU:HD13	2:N:169:VAL:HG23	1.97	0.47
1:L:210:ASN:ND2	4:L:315:HOH:O	2.47	0.47
2:H:67:PHE:CZ	2:H:82:MET:HE2	2.49	0.47
1:L:185:GLU:OE1	1:L:189:HIS:HE1	1.98	0.47
1:M:118:PHE:HA	1:M:119:PRO:HD3	1.67	0.47
2:H:133:ASN:HB2	4:H:260:HOH:O	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:192:THR:CG2	2:H:209:LYS:HE3	2.45	0.46
1:L:144:ILE:HG13	1:L:198:HIS:HB2	1.96	0.46
1:M:160:LEU:HD13	2:N:169:VAL:CG2	2.45	0.46
1:L:24:ARG:NH2	1:L:70:ASP:HA	2.31	0.46
1:M:18:ARG:HB3	1:M:18:ARG:NH1	2.31	0.46
1:L:79:GLU:OE2	1:M:61:ARG:NH1	2.49	0.46
1:M:18:ARG:HG2	1:M:19:ALA:N	2.30	0.46
1:L:163:TRP:HB3	4:L:262:HOH:O	2.16	0.46
1:M:39:LYS:NZ	4:M:313:HOH:O	2.47	0.46
1:L:118:PHE:HA	1:L:119:PRO:HD3	1.66	0.46
2:H:197:VAL:HB	2:H:206:VAL:HG13	1.98	0.46
1:M:18:ARG:CB	1:M:76:HIS:HB2	2.45	0.45
2:N:115:LYS:HG2	2:N:116:THR:N	2.32	0.45
2:H:170:LEU:HD11	2:H:173:ASP:HA	1.97	0.45
2:N:184:PRO:O	2:N:187:PRO:HD2	2.16	0.45
1:M:78:MET:HE3	1:M:106:ILE:CD1	2.46	0.45
1:M:81:ASP:CB	4:M:313:HOH:O	2.65	0.45
1:M:150:ILE:HD11	1:M:179:LEU:HD11	1.99	0.45
1:M:156:GLN:O	1:M:157:ASN:HB3	2.17	0.45
1:M:72:SER:HB3	1:M:74:HIS:CE1	2.52	0.44
1:L:124:GLN:NE2	1:L:131:SER:H	2.14	0.44
1:M:2:THR:HG21	4:M:238:HOH:O	2.17	0.44
2:H:117:THR:HA	2:H:118:PRO:HD3	1.77	0.44
1:M:16:GLY:HA2	1:M:77:PRO:HB3	1.99	0.44
1:L:78:MET:HE3	1:L:106:ILE:CD1	2.48	0.44
2:N:83:ARG:HE	2:N:83:ARG:HA	1.83	0.44
1:M:159:VAL:HG12	1:M:179:LEU:HD23	2.00	0.44
2:N:192:THR:HG23	2:N:209:LYS:HZ3	1.83	0.44
1:L:70:ASP:OD1	1:L:70:ASP:N	2.50	0.43
1:M:89:GLN:HG2	1:M:90:GLN:N	2.33	0.43
2:N:35:HIS:O	2:N:92:CYS:HA	2.18	0.43
2:N:199:HIS:HD2	2:N:202:SER:OG	2.01	0.43
1:M:21:ILE:CG2	1:M:102:THR:HG21	2.49	0.43
2:N:155:ASN:CG	2:N:159:LEU:HD22	2.39	0.43
2:N:28:THR:O	2:N:31:ARG:HB2	2.18	0.43
2:N:170:LEU:HB2	2:N:175:TYR:CE1	2.53	0.43
1:M:21:ILE:HG23	1:M:102:THR:HG21	2.00	0.43
2:N:100(B):ASP:N	2:N:100(B):ASP:OD1	2.52	0.43
2:H:184:PRO:HB2	2:H:187:PRO:HD2	2.00	0.43
1:M:35:TRP:CH2	1:M:88:CYS:HB3	2.54	0.43
1:M:146:VAL:HA	1:M:195:GLU:O	2.17	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:133:VAL:HG22	1:M:178:THR:HG23	2.02	0.42
1:L:193:THR:OG1	1:L:208:SER:HB3	2.19	0.42
1:L:27(D):TYR:CZ	1:L:28:TYR:CD1	3.07	0.42
1:L:164:THR:HG22	1:L:165:ASP:N	2.35	0.42
2:N:40:ALA:HB1	2:N:41:PRO:CD	2.49	0.42
2:H:98:ILE:O	2:H:100(D):THR:HA	2.20	0.42
1:M:124:GLN:NE2	1:M:131:SER:H	2.17	0.42
2:H:35:HIS:O	2:H:92:CYS:HA	2.19	0.42
1:L:137:ASN:HD22	1:L:174:SER:HB3	1.85	0.42
2:H:2:VAL:HG22	2:H:27:PHE:HB3	2.01	0.42
1:L:63:SER:OG	1:L:74:HIS:HB2	2.20	0.42
1:M:160:LEU:O	1:M:177:SER:HA	2.20	0.42
2:N:100:ARG:N	2:N:100(C):GLY:O	2.50	0.42
2:H:163:VAL:HG22	2:H:181:VAL:CG1	2.50	0.41
2:N:119:PRO:HB3	2:N:145:TYR:HB3	2.01	0.41
2:H:126:PRO:O	2:H:213:ARG:HD2	2.20	0.41
2:H:194:THR:HB	2:H:209:LYS:HA	2.01	0.41
1:L:12:ALA:HA	1:L:105:GLU:O	2.20	0.41
1:L:175:MET:HG2	1:L:176:SER:N	2.34	0.41
2:N:184:PRO:C	2:N:187:PRO:HD2	2.41	0.41
2:N:116:THR:HA	2:N:146:PHE:O	2.21	0.41
1:M:24:ARG:HD2	1:M:70:ASP:OD1	2.21	0.41
1:L:89:GLN:HA	1:L:97:THR:O	2.21	0.41
2:H:40:ALA:H	2:H:43:LYS:HZ2	1.68	0.41
2:N:199:HIS:HA	2:N:200:PRO:HD2	1.91	0.41
1:M:103:LYS:HD2	1:M:103:LYS:HA	1.90	0.41
2:H:166:PHE:HA	2:H:167:PRO:HD3	1.93	0.41
2:N:11:LEU:HD22	2:N:110:THR:O	2.20	0.41
1:L:48:ILE:HA	1:L:53:ASN:O	2.21	0.40
1:L:147:LYS:HE2	1:L:195:GLU:O	2.20	0.40
1:M:61:ARG:HH11	1:M:61:ARG:HG3	1.86	0.40
1:M:13:VAL:HG21	1:M:19:ALA:HB2	2.03	0.40
2:N:188:ARG:HA	2:N:189:PRO:HA	1.83	0.40
1:L:85:MET:SD	1:L:103:LYS:HG2	2.61	0.40
1:M:18:ARG:CG	1:M:18:ARG:NH1	2.84	0.40
1:L:35:TRP:CZ3	1:L:88:CYS:HB3	2.57	0.40
1:M:160:LEU:HD21	2:N:171:GLN:CG	2.48	0.40
1:M:115:VAL:HG22	1:M:136:LEU:HD13	2.03	0.40
2:H:130:ALA:HA	4:H:262:HOH:O	2.21	0.40
1:L:15:LEU:HD23	1:L:106:ILE:HD12	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	L	213/218 (98%)	201 (94%)	9 (4%)	3 (1%)	14	10
1	M	216/218 (99%)	207 (96%)	6 (3%)	3 (1%)	14	10
2	H	224/226 (99%)	212 (95%)	10 (4%)	2 (1%)	21	19
2	N	222/226 (98%)	209 (94%)	12 (5%)	1 (0%)	34	35
3	P	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
3	Q	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
All	All	891/908 (98%)	842 (94%)	40 (4%)	9 (1%)	19	16

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	157	ASN
2	H	130	ALA
1	M	56	SER
1	M	213	GLU
2	N	64	LYS
1	L	56	SER
1	M	157	ASN
1	L	199	LYS
2	H	64	LYS

### 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	L	186/190 (98%)	175 (94%)	11 (6%)	24	27
1	M	183/190 (96%)	168 (92%)	15 (8%)	14	13
2	H	191/192 (100%)	165 (86%)	26 (14%)	5	3
2	N	185/192 (96%)	165 (89%)	20 (11%)	8	7
3	P	8/9 (89%)	7 (88%)	1 (12%)	6	4
3	Q	8/9 (89%)	6 (75%)	2 (25%)	1	0
All	All	761/782 (97%)	686 (90%)	75 (10%)	10	9

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	THR
1	L	24	ARG
1	L	47	LEU
1	L	70	ASP
1	L	102	THR
1	L	123	GLU
1	L	136	LEU
1	L	147	LYS
1	L	160	LEU
1	L	179	LEU
1	L	208	SER
2	H	4	LEU
2	H	11	LEU
2	H	13	GLN
2	H	30	MET
2	H	43	LYS
2	H	45	LEU
2	H	63	VAL
2	H	82(C)	LEU
2	H	83	ARG
2	H	100(D)	THR
2	H	107	THR
2	H	108	SER
2	H	115	LYS
2	H	116	THR
2	H	138	LEU
2	H	142	VAL
2	H	149	PRO
2	H	150	VAL
2	H	159	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	H	161	SER
2	H	171	GLN
2	H	177	LEU
2	H	181	VAL
2	H	187	PRO
2	H	188	ARG
2	H	194	THR
3	P	43	LYS
1	M	1	ASP
1	M	2	THR
1	M	18	ARG
1	M	47	LEU
1	M	70	ASP
1	M	102	THR
1	M	122	SER
1	M	136	LEU
1	M	155	ARG
1	M	175	MET
1	M	179	LEU
1	M	181	LEU
1	M	188	ARG
1	M	208	SER
1	M	210	ASN
2	N	4	LEU
2	N	13	GLN
2	N	45	LEU
2	N	82(C)	LEU
2	N	83	ARG
2	N	85	GLU
2	N	99	GLU
2	N	100(D)	THR
2	N	105	GLN
2	N	107	THR
2	N	124	LEU
2	N	132	THR
2	N	150	VAL
2	N	159	LEU
2	N	161	SER
2	N	177	LEU
2	N	181	VAL
2	N	182	THR
2	N	188	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	N	190	SER
3	Q	37	SER
3	Q	43	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	53	ASN
1	L	124	GLN
1	L	137	ASN
1	L	156	GLN
1	L	189	HIS
1	L	210	ASN
2	H	39	GLN
2	H	131	GLN
2	H	164	HIS
2	H	196	ASN
2	H	199	HIS
1	M	38	GLN
1	M	54	GLN
1	M	124	GLN
1	M	137	ASN
1	M	156	GLN
1	M	210	ASN
2	N	171	GLN
2	N	196	ASN
2	N	199	HIS

### 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	L	215/218 (98%)	-0.03	4 (1%) 70 68	9, 18, 33, 49	0
1	M	218/218 (100%)	0.04	7 (3%) 51 50	9, 18, 34, 44	0
2	H	226/226 (100%)	0.22	10 (4%) 38 37	9, 18, 41, 67	0
2	N	224/226 (99%)	0.06	8 (3%) 46 45	8, 17, 38, 55	0
3	P	10/10 (100%)	0.24	0 100 100	16, 20, 35, 42	0
3	Q	10/10 (100%)	0.26	0 100 100	18, 25, 31, 38	0
All	All	903/908 (99%)	0.08	29 (3%) 51 50	8, 18, 37, 67	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	130	ALA	8.8
2	N	41	PRO	5.5
2	H	128	SER	5.4
2	H	100(A)	TYR	5.2
2	H	129	ALA	5.0
2	H	214	ASP	4.5
2	H	132	THR	4.2
1	L	157	ASN	4.0
2	H	131	GLN	3.6
1	M	157	ASN	3.5
2	H	42	GLU	3.3
2	N	132	THR	3.2
1	M	202	THR	3.2
2	N	100(A)	TYR	3.1
1	M	69	THR	3.0
1	L	70	ASP	2.8
1	M	214	CYS	2.8
2	H	173	ASP	2.7
2	H	203	SER	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	N	129	ALA	2.6
2	N	42	GLU	2.5
2	N	64	LYS	2.5
1	M	199	LYS	2.5
1	L	169	LYS	2.4
1	L	202	THR	2.3
1	M	169	LYS	2.3
2	N	128	SER	2.3
2	N	83	ARG	2.1
1	M	70	ASP	2.1

## 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.