



# Full wwPDB X-ray Structure Validation Report

May 16, 2020 – 08:53 am BST

PDB ID : 3AXL  
Title : Murine Valpha 10 Vbeta 8.1 T-cell receptor  
Authors : Patel, O.; Rossjohn, J.  
Deposited on : 2011-04-11  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the  symbol.

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The following versions of software and data (see [references](#) ) were used in the production of this report:

MolProbity : 4.02b-467  
Xtrriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

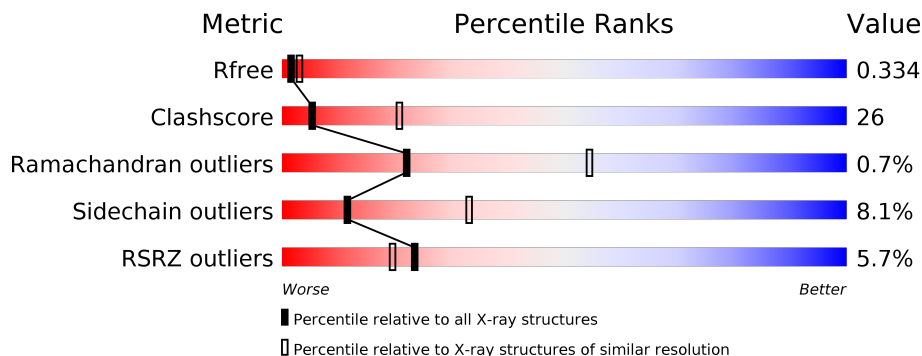
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	198	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 48%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 37%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">6% 48% 37% 7% • 8%</p>
1	G	198	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 35%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">2% 54% 35% 7% • •</p>
2	B	238	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 37%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 4%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">10% 59% 37% •</p>
2	H	238	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 66%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 32%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> </div> <p style="font-size: small; margin-top: 5px;">4% 66% 32% •</p>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6728 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 Valpha 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	183	1393	866	232	287	8	0	0	0
1	G	190	1437	890	240	299	8	0	0	0

- Molecule 2 is a protein called Vbeta 8.1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	238	1887	1193	330	358	6	0	0	0
2	H	238	1883	1189	330	358	6	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	28	Total 28	O 28	0	0
3	B	43	Total 43	O 43	0	0
3	G	27	Total 27	O 27	0	0
3	H	30	Total 30	O 30	0	0

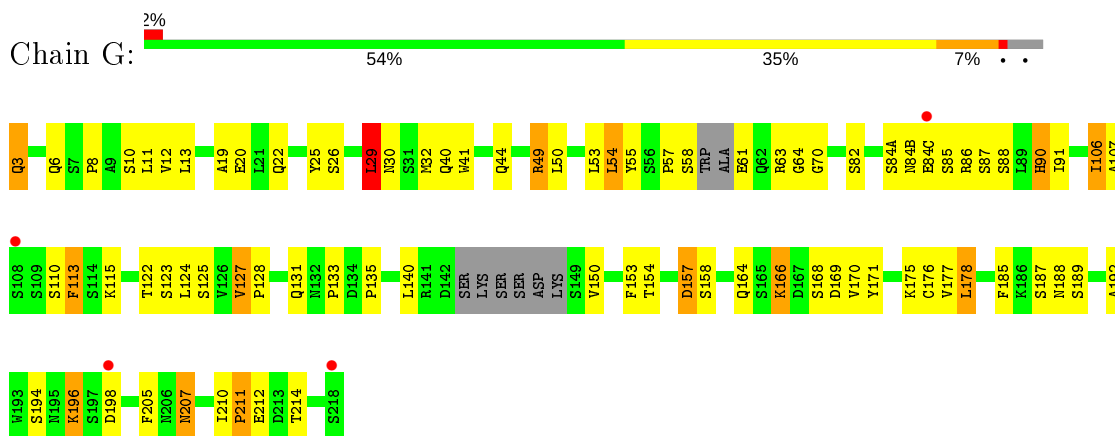
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

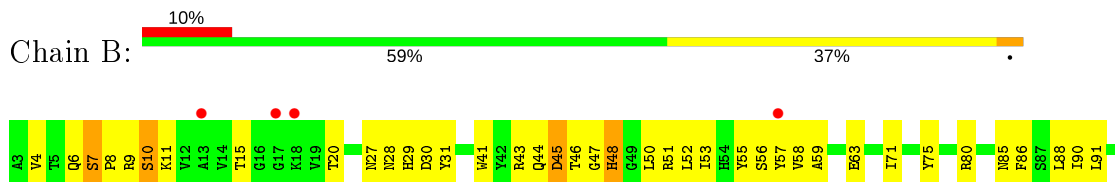
- Molecule 1: Valpha 10

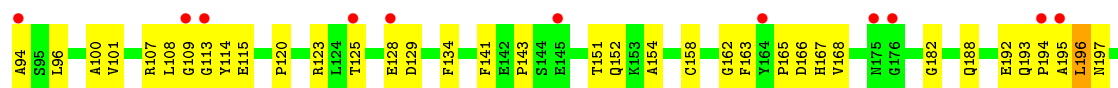


- Molecule 1: Valpha 10

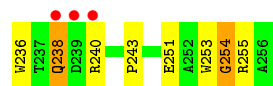
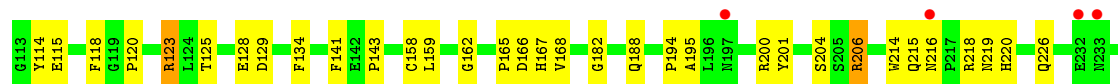
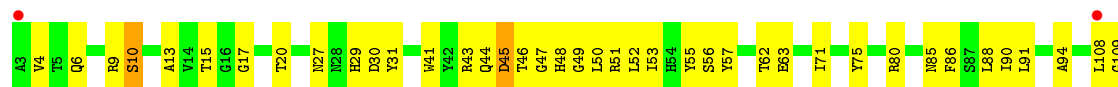


- Molecule 2: Vbeta 8.1





● Molecule 2: Vbeta 8.1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	148.84Å 65.80Å 97.38Å 90.00° 97.14° 90.00°	Depositor
Resolution (Å)	42.95 – 2.90 42.95 – 2.77	Depositor EDS
% Data completeness (in resolution range)	96.4 (42.95-2.90) 97.2 (42.95-2.77)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.77Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.254 , 0.327 0.257 , 0.334	Depositor DCC
$R_{free}$ test set	1185 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtrriage
Anisotropy	0.464	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 57.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	6728	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.50% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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	0.53	0/1417	0.73	1/1921 (0.1%)
1	G	0.54	0/1463	0.71	1/1986 (0.1%)
2	B	0.53	0/1940	0.75	1/2644 (0.0%)
2	H	0.59	0/1936	0.98	3/2638 (0.1%)
All	All	0.55	0/6756	0.81	6/9189 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	29	LEU	CA-CB-CG	6.96	131.30	115.30
1	A	29	LEU	CA-CB-CG	6.44	130.12	115.30
2	B	7	SER	C-N-CD	-6.05	107.28	120.60
2	H	123	ARG	CA-CB-CG	5.28	125.02	113.40
2	H	159	LEU	CA-CB-CG	5.20	127.25	115.30
2	H	49	GLY	N-CA-C	-5.04	100.51	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	7	SER	Peptide

## 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	1393	0	1312	85	0
1	G	1437	0	1348	90	0
2	B	1887	0	1788	114	0
2	H	1883	0	1778	89	0
3	A	28	0	0	2	0
3	B	43	0	0	18	0
3	G	27	0	0	6	0
3	H	30	0	0	5	0
All	All	6728	0	6226	338	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 26.

All (338) 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:H:17:GLY:HA3	3:H:275:HOH:O	1.69	0.93
2:B:58:VAL:HA	3:B:271:HOH:O	1.72	0.88
2:B:216:ASN:HB3	2:B:219:ASN:HD22	1.35	0.88
2:B:216:ASN:HB3	2:B:219:ASN:ND2	1.89	0.86
2:H:6:GLN:HG2	2:H:120:PRO:HD2	1.57	0.84
2:H:48:HIS:HD2	2:H:51:ARG:CZ	1.90	0.84
2:B:6:GLN:HG2	2:B:120:PRO:HD2	1.61	0.83
2:H:216:ASN:HB3	2:H:219:ASN:ND2	1.95	0.81
1:A:153:PHE:HB2	1:A:205:PHE:CZ	2.14	0.81
1:A:166:LYS:O	1:G:166:LYS:O	1.99	0.81
2:B:162:GLY:O	2:B:200:ARG:HD3	1.81	0.80
2:H:43:ARG:HG2	2:H:53:ILE:HD11	1.65	0.78
2:B:236:TRP:CH2	2:B:238:GLN:HG3	2.17	0.78
1:G:153:PHE:HB2	1:G:205:PHE:CZ	2.18	0.78
2:H:236:TRP:CH2	2:H:238:GLN:HG3	2.19	0.78
2:B:194:PRO:HG2	1:G:166:LYS:HG3	1.64	0.77
2:B:43:ARG:HG2	2:B:53:ILE:HD11	1.66	0.77
2:H:216:ASN:HB3	2:H:219:ASN:HD22	1.49	0.77
2:H:13:ALA:HA	3:H:270:HOH:O	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:PHE:HE2	1:A:187:SER:HB2	1.48	0.76
1:G:185:PHE:HE2	1:G:187:SER:HB2	1.51	0.75
2:B:6:GLN:HB2	3:B:279:HOH:O	1.86	0.74
2:B:31:TYR:CE1	2:B:57:TYR:CE1	2.77	0.72
2:H:167:HIS:HE1	3:H:69:HOH:O	1.71	0.72
2:H:134:PHE:HZ	2:H:240:ARG:HH22	1.34	0.72
2:H:31:TYR:CE1	2:H:57:TYR:CE1	2.78	0.71
2:B:123:ARG:NH1	3:B:289:HOH:O	2.23	0.71
2:H:162:GLY:O	2:H:200:ARG:HD3	1.90	0.71
2:B:134:PHE:HZ	2:B:240:ARG:HH22	1.35	0.70
2:B:162:GLY:C	2:B:200:ARG:HD3	2.13	0.70
1:G:84(A):SER:C	1:G:86:ARG:NH2	2.45	0.69
1:A:185:PHE:CE2	1:A:187:SER:HB2	2.28	0.68
1:A:110:SER:HB2	2:B:109:GLY:O	1.93	0.68
1:G:185:PHE:CE2	1:G:187:SER:HB2	2.28	0.68
1:A:113:PHE:HB2	2:B:31:TYR:OH	1.95	0.67
2:B:196:LEU:HD13	2:B:196:LEU:H	1.57	0.67
1:G:169:ASP:OD2	1:G:196:LYS:HD3	1.95	0.67
1:G:128:PRO:HG3	1:G:177:VAL:HG21	1.77	0.66
1:A:169:ASP:O	1:A:194:SER:HB2	1.95	0.66
2:B:193:GLN:HB3	2:B:196:LEU:HD11	1.77	0.66
2:B:196:LEU:HD13	2:B:196:LEU:N	2.11	0.66
2:H:134:PHE:CZ	2:H:240:ARG:NH2	2.60	0.66
2:H:15:THR:HA	2:H:94:ALA:O	1.96	0.66
1:G:110:SER:HB3	3:G:239:HOH:O	1.95	0.66
1:G:55:TYR:HE2	1:G:57:PRO:HG3	1.61	0.66
2:H:215:GLN:HA	2:H:255:ARG:O	1.95	0.66
2:H:162:GLY:C	2:H:200:ARG:HD3	2.16	0.65
2:B:31:TYR:HE1	2:B:57:TYR:CE1	2.15	0.65
1:G:55:TYR:CE2	1:G:57:PRO:HG3	2.31	0.65
1:A:29:LEU:HB3	1:A:106:ILE:HD13	1.78	0.65
2:B:220:HIS:HE1	2:B:251:GLU:HB2	1.62	0.65
1:A:44:GLN:HB2	1:A:50:LEU:HD23	1.78	0.65
1:A:153:PHE:HB2	1:A:205:PHE:CE2	2.32	0.64
1:A:169:ASP:OD2	1:A:196:LYS:HD3	1.98	0.64
1:A:20:GLU:OE2	1:A:90:HIS:CG	2.50	0.64
2:B:193:GLN:CB	2:B:196:LEU:HD11	2.26	0.64
1:A:18:ASN:HB3	3:A:73:HOH:O	1.98	0.64
2:B:196:LEU:HD23	2:B:197:ASN:O	1.97	0.64
2:B:215:GLN:HA	2:B:255:ARG:O	1.98	0.64
2:B:48:HIS:HD2	2:B:51:ARG:CZ	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PHE:HB2	2:B:31:TYR:CZ	2.33	0.64
2:H:31:TYR:HE1	2:H:57:TYR:CE1	2.16	0.64
1:A:25:TYR:CD1	1:A:26:SER:N	2.66	0.63
1:A:40:GLN:NE2	2:B:115:GLU:HG3	2.13	0.63
1:G:169:ASP:O	1:G:194:SER:HB2	1.97	0.63
1:G:44:GLN:HB2	1:G:50:LEU:HD23	1.80	0.63
1:G:140:LEU:HB3	2:H:141:PHE:HB3	1.81	0.63
1:G:110:SER:HB2	2:H:109:GLY:O	1.98	0.63
1:A:207:ASN:ND2	2:H:195:ALA:HB2	2.14	0.62
2:H:91:LEU:N	2:H:91:LEU:HD12	2.14	0.62
2:B:59:ALA:N	3:B:271:HOH:O	2.31	0.62
1:A:166:LYS:HG3	2:H:194:PRO:HG2	1.81	0.62
2:H:48:HIS:CD2	2:H:51:ARG:CZ	2.79	0.62
2:H:10:SER:HB2	2:H:167:HIS:HD2	1.65	0.61
2:B:158:CYS:O	2:B:204:SER:HA	2.00	0.61
1:G:19:ALA:HB3	1:G:91:ILE:HB	1.83	0.61
1:A:212:GLU:HG2	3:A:233:HOH:O	2.01	0.61
2:B:15:THR:HA	2:B:94:ALA:O	1.99	0.61
1:A:135:PRO:HB2	1:A:214:THR:HA	1.82	0.60
1:G:170:VAL:HA	1:G:194:SER:HB3	1.83	0.60
1:G:128:PRO:HG3	1:G:177:VAL:CG2	2.31	0.60
1:A:113:PHE:H	1:A:113:PHE:HD2	1.48	0.60
2:H:134:PHE:CE1	2:H:240:ARG:NH2	2.70	0.60
2:H:31:TYR:HA	2:H:56:SER:O	2.02	0.60
1:G:25:TYR:CD1	1:G:26:SER:N	2.70	0.60
1:G:113:PHE:HD2	1:G:113:PHE:H	1.50	0.59
1:G:135:PRO:HB2	1:G:214:THR:HA	1.85	0.59
2:B:236:TRP:N	3:B:273:HOH:O	2.36	0.59
1:A:3:GLN:HB3	1:A:25:TYR:HE1	1.66	0.59
1:G:29:LEU:HB3	1:G:106:ILE:HD13	1.83	0.58
1:A:170:VAL:HA	1:A:194:SER:HB3	1.85	0.58
1:G:178:LEU:HD23	3:G:240:HOH:O	2.03	0.58
2:B:91:LEU:N	2:B:91:LEU:HD12	2.18	0.58
1:G:153:PHE:HB2	1:G:205:PHE:CE2	2.39	0.58
1:G:40:GLN:NE2	2:H:115:GLU:HG3	2.18	0.58
2:H:220:HIS:HE1	2:H:251:GLU:HB2	1.67	0.58
2:B:128:GLU:OE1	2:B:128:GLU:HA	2.03	0.57
2:B:236:TRP:CZ2	2:B:238:GLN:HB2	2.39	0.57
2:B:134:PHE:CZ	2:B:240:ARG:NH2	2.64	0.57
2:B:216:ASN:HB2	3:B:112:HOH:O	2.04	0.57
2:B:48:HIS:CD2	2:B:51:ARG:CZ	2.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:ALA:HB3	1:A:91:ILE:HB	1.87	0.56
2:B:100:ALA:C	3:B:289:HOH:O	2.43	0.56
2:B:10:SER:HB2	2:B:167:HIS:HD2	1.69	0.56
2:B:31:TYR:CE1	2:B:57:TYR:CD1	2.93	0.56
1:G:20:GLU:OE2	1:G:90:HIS:CG	2.59	0.56
1:A:32:MET:HE1	1:A:41:TRP:HE1	1.70	0.56
1:A:175:LYS:HA	1:A:189:SER:O	2.05	0.56
2:B:134:PHE:CE1	2:B:240:ARG:NH2	2.73	0.56
2:H:158:CYS:O	2:H:204:SER:HA	2.05	0.56
1:G:63:ARG:C	1:G:70:GLY:H	2.10	0.55
1:G:178:LEU:HD13	2:H:182:GLY:HA2	1.86	0.55
2:H:31:TYR:CE1	2:H:57:TYR:CD1	2.93	0.55
2:B:108:LEU:HB3	2:B:114:TYR:HB2	1.89	0.55
2:B:143:PRO:HB3	2:B:154:ALA:HB1	1.88	0.55
2:B:27:ASN:HB3	2:B:29:HIS:CD2	2.42	0.55
1:G:22:GLN:OE1	1:G:88:SER:CB	2.53	0.55
1:G:53:LEU:O	1:G:54:LEU:CD1	2.54	0.55
2:H:30:ASP:OD2	2:H:31:TYR:CE2	2.60	0.55
1:G:3:GLN:HB3	1:G:25:TYR:HE1	1.73	0.54
1:A:110:SER:O	2:B:109:GLY:C	2.46	0.54
1:A:128:PRO:HG3	1:A:177:VAL:HG21	1.90	0.54
1:G:127:VAL:CG1	1:G:158:SER:HB3	2.39	0.53
1:A:63:ARG:C	1:A:70:GLY:H	2.12	0.53
2:B:216:ASN:CB	2:B:219:ASN:ND2	2.66	0.53
2:B:41:TRP:HH2	3:B:279:HOH:O	1.91	0.53
1:G:175:LYS:HA	1:G:189:SER:O	2.08	0.53
2:H:243:PRO:HA	3:H:282:HOH:O	2.06	0.53
1:G:113:PHE:HB2	2:H:31:TYR:OH	2.09	0.53
2:H:55:TYR:CE1	2:H:63:GLU:HG3	2.43	0.53
2:B:30:ASP:OD2	2:B:31:TYR:CE2	2.61	0.53
1:G:49:ARG:NH1	2:H:118:PHE:O	2.42	0.53
2:B:48:HIS:HD2	2:B:51:ARG:NE	2.07	0.52
2:H:13:ALA:CA	3:H:270:HOH:O	2.51	0.52
1:A:110:SER:HB2	2:B:113:GLY:CA	2.40	0.52
1:A:128:PRO:HG3	1:A:177:VAL:CG2	2.39	0.52
2:B:55:TYR:CE1	2:B:63:GLU:HG3	2.43	0.52
1:G:53:LEU:O	1:G:54:LEU:HD13	2.09	0.52
2:H:20:THR:HG23	2:H:90:ILE:CD1	2.40	0.52
2:B:254:GLY:O	2:B:255:ARG:HG3	2.10	0.52
1:G:188:ASN:N	3:G:220:HOH:O	2.20	0.52
2:B:166:ASP:HB3	2:B:201:TYR:CG	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:TRP:HD1	2:B:86:PHE:CE2	2.28	0.52
1:G:189:SER:OG	2:H:206:ARG:HD2	2.10	0.52
2:B:27:ASN:CB	2:B:29:HIS:CD2	2.94	0.51
2:H:236:TRP:CZ2	2:H:238:GLN:HB2	2.46	0.51
2:H:128:GLU:HA	2:H:128:GLU:OE1	2.10	0.51
2:B:162:GLY:HA2	2:B:200:ARG:CD	2.41	0.51
1:G:40:GLN:HE22	2:H:115:GLU:HG3	1.76	0.51
1:A:166:LYS:CE	1:G:168:SER:HA	2.41	0.51
2:B:27:ASN:HB3	2:B:29:HIS:NE2	2.26	0.51
1:A:22:GLN:OE1	1:A:88:SER:CB	2.60	0.50
1:G:30:ASN:HB3	1:G:107:ALA:O	2.12	0.50
1:G:61:GLU:N	3:G:222:HOH:O	2.43	0.50
1:A:110:SER:HA	2:B:113:GLY:HA2	1.92	0.50
1:G:11:LEU:N	1:G:11:LEU:HD23	2.26	0.50
2:B:20:THR:HG23	2:B:90:ILE:CD1	2.42	0.50
1:A:178:LEU:HD12	1:A:178:LEU:C	2.32	0.50
1:G:8:PRO:O	1:G:122:THR:HG23	2.12	0.50
1:G:22:GLN:OE1	1:G:88:SER:HB2	2.12	0.50
1:G:32:MET:HE1	1:G:41:TRP:HE1	1.77	0.50
1:A:110:SER:O	2:B:113:GLY:N	2.45	0.49
2:B:31:TYR:HA	2:B:56:SER:O	2.13	0.49
1:A:176:CYS:SG	2:B:206:ARG:NH1	2.86	0.49
1:G:29:LEU:HD13	1:G:29:LEU:H	1.78	0.49
1:G:171:TYR:O	1:G:192:ALA:HA	2.13	0.49
2:H:44:GLN:HB2	2:H:50:LEU:HD23	1.93	0.49
1:A:11:LEU:N	1:A:11:LEU:HD23	2.28	0.49
1:A:150:VAL:HG22	1:A:193:TRP:HB3	1.95	0.49
1:G:113:PHE:HB2	2:H:31:TYR:CZ	2.48	0.49
1:A:115:LYS:HA	2:B:107:ARG:HH12	1.77	0.49
1:A:171:TYR:O	1:A:192:ALA:HA	2.13	0.49
1:A:113:PHE:CB	2:B:31:TYR:OH	2.59	0.49
2:B:4:VAL:O	2:B:120:PRO:HD3	2.12	0.48
1:G:44:GLN:HA	3:G:233:HOH:O	2.13	0.48
2:H:141:PHE:N	2:H:141:PHE:CD2	2.81	0.48
1:A:29:LEU:HB3	1:A:106:ILE:CD1	2.42	0.48
1:G:3:GLN:NE2	1:G:26:SER:HB2	2.28	0.48
1:A:207:ASN:HD22	2:H:195:ALA:HB2	1.77	0.48
2:B:129:ASP:C	2:B:129:ASP:OD1	2.52	0.48
2:B:52:LEU:O	2:B:71:ILE:HG12	2.13	0.48
1:A:127:VAL:CG1	1:A:158:SER:HB3	2.42	0.48
2:B:193:GLN:HB2	2:B:196:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:84(B):ASN:N	1:G:86:ARG:HH21	2.12	0.48
1:A:210:ILE:O	1:A:211:PRO:C	2.51	0.48
1:A:7:SER:HB3	1:A:22:GLN:HB2	1.95	0.48
1:A:13:LEU:HD23	1:G:8:PRO:HB3	1.95	0.48
2:H:41:TRP:CD1	2:H:86:PHE:CD2	3.02	0.48
2:H:41:TRP:HD1	2:H:86:PHE:CE2	2.32	0.48
1:A:40:GLN:HE22	2:B:115:GLU:HG3	1.77	0.48
2:B:88:LEU:C	2:B:90:ILE:HD13	2.34	0.48
2:H:114:TYR:N	2:H:114:TYR:CD2	2.81	0.48
2:H:27:ASN:HB3	2:H:29:HIS:CD2	2.49	0.48
2:H:75:TYR:HB3	2:H:88:LEU:HD11	1.96	0.48
1:A:29:LEU:HD13	1:A:29:LEU:H	1.79	0.47
1:G:84(A):SER:C	1:G:86:ARG:HH22	2.15	0.47
1:A:54:LEU:HA	1:A:54:LEU:HD12	1.59	0.47
2:H:45:ASP:OD1	2:H:45:ASP:N	2.47	0.47
2:H:48:HIS:HD2	2:H:51:ARG:NE	2.12	0.47
1:A:46:PRO:HG3	3:B:285:HOH:O	2.15	0.47
1:A:178:LEU:HD13	2:B:182:GLY:HA2	1.97	0.47
1:G:40:GLN:HG3	1:G:54:LEU:O	2.14	0.47
1:A:30:ASN:HB3	1:A:107:ALA:O	2.15	0.47
1:G:84(B):ASN:N	1:G:86:ARG:NH2	2.63	0.47
2:H:30:ASP:OD2	2:H:31:TYR:CD2	2.68	0.47
1:A:3:GLN:NE2	1:A:26:SER:HB2	2.29	0.47
2:B:41:TRP:CD1	2:B:86:PHE:CD2	3.01	0.47
1:G:210:ILE:O	1:G:211:PRO:C	2.53	0.47
1:G:22:GLN:OE1	1:G:88:SER:HB3	2.13	0.47
2:H:168:VAL:HA	2:H:226:GLN:O	2.15	0.47
1:G:29:LEU:H	1:G:29:LEU:CD1	2.27	0.47
1:A:3:GLN:HB3	1:A:25:TYR:CE1	2.49	0.47
2:H:4:VAL:O	2:H:120:PRO:HD3	2.14	0.47
2:B:43:ARG:NH1	3:B:268:HOH:O	2.47	0.47
1:G:57:PRO:O	1:G:58:SER:O	2.33	0.46
1:A:29:LEU:H	1:A:29:LEU:CD1	2.28	0.46
1:G:3:GLN:HB3	1:G:25:TYR:CE1	2.50	0.46
2:H:125:THR:HG21	2:H:165:PRO:CG	2.45	0.46
1:A:168:SER:HA	1:G:166:LYS:CE	2.46	0.46
1:A:22:GLN:OE1	1:A:88:SER:HB2	2.15	0.46
1:G:63:ARG:O	1:G:70:GLY:N	2.48	0.46
2:H:162:GLY:HA2	2:H:200:ARG:CD	2.46	0.46
2:H:46:THR:HA	2:H:47:GLY:HA2	1.73	0.46
1:A:8:PRO:O	1:A:122:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:113:PHE:CB	2:H:31:TYR:OH	2.64	0.46
2:B:53:ILE:N	2:B:53:ILE:HD12	2.31	0.46
1:G:29:LEU:HB3	1:G:106:ILE:CD1	2.43	0.46
2:H:108:LEU:HB3	2:H:114:TYR:HB2	1.98	0.46
2:B:101:VAL:HG23	3:B:289:HOH:O	2.15	0.46
2:B:236:TRP:CZ2	2:B:238:GLN:HG3	2.51	0.46
1:G:196:LYS:N	3:G:228:HOH:O	2.48	0.46
1:A:133:PRO:HB3	1:A:157:ASP:HB3	1.98	0.45
1:G:54:LEU:HD12	1:G:54:LEU:HA	1.67	0.45
2:B:28:ASN:ND2	3:B:278:HOH:O	2.49	0.45
2:B:235:GLU:HA	3:B:273:HOH:O	2.16	0.45
1:A:63:ARG:O	1:A:70:GLY:N	2.49	0.45
2:H:134:PHE:CE1	2:H:240:ARG:NH1	2.85	0.45
2:H:254:GLY:O	2:H:255:ARG:HG3	2.16	0.45
2:H:51:ARG:HB3	2:H:71:ILE:CD1	2.46	0.45
2:B:195:ALA:HB2	1:G:207:ASN:ND2	2.32	0.45
1:G:178:LEU:CD1	2:H:182:GLY:HA2	2.47	0.45
1:G:127:VAL:HG11	1:G:158:SER:HB3	1.99	0.45
2:H:88:LEU:C	2:H:90:ILE:HD13	2.37	0.45
2:B:226:GLN:NE2	3:B:266:HOH:O	2.46	0.45
1:G:84(C):GLU:O	1:G:86:ARG:N	2.49	0.45
1:A:82:SER:O	1:A:87:SER:HA	2.17	0.45
1:G:176:CYS:SG	2:H:206:ARG:NH1	2.89	0.45
2:B:192:GLU:HG3	2:B:200:ARG:O	2.17	0.45
2:B:216:ASN:ND2	2:B:219:ASN:ND2	2.65	0.45
1:G:84(A):SER:C	1:G:86:ARG:HH21	2.18	0.44
2:H:218:ARG:O	2:H:253:TRP:HZ3	2.00	0.44
2:H:10:SER:HA	2:H:123:ARG:O	2.17	0.44
2:H:236:TRP:CZ2	2:H:238:GLN:HG3	2.51	0.44
2:B:11:LYS:NZ	3:B:288:HOH:O	2.39	0.44
2:B:151:THR:O	2:B:152:GLN:HB2	2.17	0.44
2:B:162:GLY:CA	2:B:200:ARG:HD3	2.48	0.44
2:B:216:ASN:O	2:B:254:GLY:HA3	2.16	0.44
2:B:75:TYR:HB3	2:B:88:LEU:HD11	1.99	0.44
1:G:113:PHE:HB2	2:H:31:TYR:CE1	2.53	0.44
1:A:8:PRO:HB2	1:G:12:VAL:O	2.16	0.44
2:B:143:PRO:CB	2:B:154:ALA:HB1	2.48	0.44
2:B:163:PHE:CE2	2:B:201:TYR:HB2	2.51	0.44
2:B:80:ARG:HD2	2:B:85:ASN:O	2.17	0.44
2:B:134:PHE:CE1	2:B:240:ARG:NH1	2.86	0.44
1:G:169:ASP:N	1:G:169:ASP:OD1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:129:ASP:OD1	2:H:129:ASP:C	2.56	0.44
2:B:141:PHE:N	2:B:141:PHE:CD2	2.85	0.43
1:A:53:LEU:O	1:A:54:LEU:CD1	2.66	0.43
1:A:140:LEU:HB3	2:B:141:PHE:HB3	2.00	0.43
2:H:10:SER:HB2	2:H:167:HIS:CD2	2.49	0.43
2:B:125:THR:HG21	2:B:165:PRO:CG	2.49	0.43
2:B:41:TRP:CD1	2:B:86:PHE:CE2	3.06	0.43
2:H:166:ASP:HB3	2:H:201:TYR:CG	2.54	0.43
2:H:216:ASN:CB	2:H:219:ASN:ND2	2.76	0.43
1:A:113:PHE:HB2	2:B:31:TYR:CE1	2.53	0.43
1:A:12:VAL:O	1:G:8:PRO:HB2	2.18	0.43
1:A:180:MET:HE1	1:A:183:MET:SD	2.59	0.43
2:B:96:LEU:HD11	2:B:128:GLU:OE2	2.19	0.43
1:G:178:LEU:HD12	1:G:178:LEU:C	2.38	0.43
2:H:166:ASP:HB3	2:H:201:TYR:CD2	2.54	0.43
2:H:219:ASN:O	2:H:253:TRP:HA	2.19	0.43
2:H:53:ILE:N	2:H:53:ILE:HD12	2.33	0.43
2:H:52:LEU:O	2:H:71:ILE:HG12	2.19	0.43
2:H:27:ASN:CB	2:H:29:HIS:CD2	3.02	0.43
2:B:101:VAL:CG2	3:B:289:HOH:O	2.66	0.43
1:G:84(B):ASN:O	1:G:84(C):GLU:C	2.56	0.43
1:A:72:LEU:N	1:A:72:LEU:HD12	2.34	0.42
2:H:41:TRP:CD1	2:H:86:PHE:CE2	3.07	0.42
2:H:91:LEU:N	2:H:91:LEU:CD1	2.82	0.42
2:B:218:ARG:O	2:B:253:TRP:HZ3	2.02	0.42
1:A:29:LEU:CB	1:A:106:ILE:HD13	2.47	0.42
1:G:53:LEU:O	1:G:54:LEU:HD12	2.18	0.42
1:A:212:GLU:O	1:A:212:GLU:HG2	2.19	0.42
1:A:53:LEU:O	1:A:54:LEU:HD13	2.18	0.42
1:G:6:GLN:HA	1:G:22:GLN:O	2.20	0.42
1:A:105:ALA:HB2	1:A:118:PHE:CD1	2.55	0.42
2:B:168:VAL:HA	2:B:226:GLN:O	2.20	0.42
2:H:27:ASN:HB3	2:H:29:HIS:NE2	2.35	0.42
1:A:21:LEU:HD22	1:A:122:THR:HG21	2.02	0.42
2:B:10:SER:HB2	2:B:167:HIS:CD2	2.51	0.42
2:B:216:ASN:HD22	2:B:219:ASN:HD21	1.68	0.42
1:A:45:ARG:HG3	1:A:46:PRO:O	2.19	0.41
2:B:43:ARG:HH21	2:B:100:ALA:HB2	1.85	0.41
2:B:45:ASP:N	2:B:45:ASP:OD1	2.52	0.41
2:B:196:LEU:N	2:B:196:LEU:CD1	2.81	0.41
1:A:113:PHE:N	1:A:113:PHE:CD2	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ARG:C	1:A:72:LEU:HD12	2.40	0.41
2:B:30:ASP:OD2	2:B:31:TYR:CD2	2.73	0.41
1:G:210:ILE:HG13	1:G:210:ILE:O	2.18	0.41
2:B:255:ARG:HB3	3:B:290:HOH:O	2.20	0.41
2:B:43:ARG:NH2	2:B:100:ALA:HB2	2.36	0.41
2:H:236:TRP:CZ2	2:H:243:PRO:HD3	2.56	0.41
2:B:227:PHE:O	2:B:245:THR:HG23	2.20	0.41
2:B:255:ARG:NH1	3:B:270:HOH:O	2.53	0.41
1:G:127:VAL:HG13	1:G:158:SER:OG	2.20	0.41
1:G:82:SER:O	1:G:87:SER:HA	2.20	0.41
1:G:11:LEU:HD21	1:G:124:LEU:HD13	2.03	0.41
1:G:29:LEU:N	1:G:29:LEU:CD1	2.84	0.41
2:B:114:TYR:HB3	2:B:115:GLU:H	1.61	0.41
1:G:12:VAL:HA	1:G:125:SER:O	2.21	0.41
1:G:131:GLN:O	1:G:133:PRO:HD3	2.21	0.41
2:H:162:GLY:CA	2:H:200:ARG:HD3	2.51	0.41
2:H:143:PRO:HD2	2:H:214:TRP:CE2	2.56	0.41
2:B:244:VAL:O	2:B:246:GLN:HG2	2.20	0.41
1:G:133:PRO:HB3	1:G:157:ASP:HB3	2.03	0.41
1:A:42:PHE:CD1	1:A:52:SER:HA	2.56	0.41
2:B:46:THR:HA	2:B:47:GLY:HA2	1.74	0.41
2:H:80:ARG:HD2	2:H:85:ASN:O	2.21	0.41
1:A:134:ASP:O	1:A:135:PRO:C	2.58	0.40
1:A:166:LYS:HE2	1:G:168:SER:HA	2.02	0.40
1:A:169:ASP:OD1	1:A:169:ASP:N	2.53	0.40
1:A:3:GLN:HE21	1:A:3:GLN:HB3	1.69	0.40
2:B:44:GLN:HB2	2:B:50:LEU:HD23	2.04	0.40
2:B:219:ASN:O	2:B:253:TRP:HA	2.22	0.40
2:H:51:ARG:CB	2:H:71:ILE:HD11	2.52	0.40
2:H:62:THR:HG22	2:H:63:GLU:N	2.36	0.40
1:A:137:VAL:O	1:A:217:PRO:HD2	2.21	0.40
1:A:43:TYR:C	1:A:43:TYR:CD2	2.94	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	175/198 (88%)	162 (93%)	12 (7%)	1 (1%)	25	58
1	G	184/198 (93%)	170 (92%)	12 (6%)	2 (1%)	14	42
2	B	236/238 (99%)	222 (94%)	12 (5%)	2 (1%)	19	51
2	H	236/238 (99%)	225 (95%)	10 (4%)	1 (0%)	34	66
All	All	831/872 (95%)	779 (94%)	46 (6%)	6 (1%)	22	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	GLY
2	B	254	GLY
2	H	254	GLY
2	B	8	PRO
1	G	64	GLY
1	G	211	PRO

### 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	160/177 (90%)	138 (86%)	22 (14%)	3	10
1	G	166/177 (94%)	143 (86%)	23 (14%)	3	10
2	B	202/205 (98%)	194 (96%)	8 (4%)	31	65
2	H	201/205 (98%)	195 (97%)	6 (3%)	41	75
All	All	729/764 (95%)	670 (92%)	59 (8%)	11	33

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	10	SER
1	A	13	LEU
1	A	29	LEU
1	A	49	ARG
1	A	54	LEU
1	A	85	SER
1	A	90	HIS
1	A	106	ILE
1	A	113	PHE
1	A	115	LYS
1	A	123	SER
1	A	127	VAL
1	A	154	THR
1	A	157	ASP
1	A	164	GLN
1	A	166	LYS
1	A	178	LEU
1	A	196	LYS
1	A	198	ASP
1	A	207	ASN
1	A	212	GLU
2	B	9	ARG
2	B	10	SER
2	B	45	ASP
2	B	48	HIS
2	B	188	GLN
2	B	196	LEU
2	B	206	ARG
2	B	238	GLN
1	G	3	GLN
1	G	10	SER
1	G	13	LEU
1	G	29	LEU
1	G	49	ARG
1	G	54	LEU
1	G	85	SER
1	G	90	HIS
1	G	106	ILE
1	G	113	PHE
1	G	115	LYS
1	G	123	SER
1	G	127	VAL

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Mol	Chain	Res	Type
1	G	150	VAL
1	G	154	THR
1	G	157	ASP
1	G	164	GLN
1	G	166	LYS
1	G	178	LEU
1	G	196	LYS
1	G	198	ASP
1	G	207	ASN
1	G	212	GLU
2	H	9	ARG
2	H	10	SER
2	H	45	ASP
2	H	188	GLN
2	H	206	ARG
2	H	238	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	159	GLN
1	A	195	ASN
2	B	44	GLN
2	B	48	HIS
2	B	132	ASN
2	B	167	HIS
2	B	219	ASN
2	B	220	HIS
1	G	3	GLN
1	G	44	GLN
1	G	159	GLN
1	G	195	ASN
2	H	44	GLN
2	H	48	HIS
2	H	167	HIS
2	H	219	ASN
2	H	220	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	183/198 (92%)	0.27	11 (6%) 21 18	10, 29, 55, 82	0
1	G	190/198 (95%)	0.15	4 (2%) 63 61	11, 28, 56, 83	0
2	B	238/238 (100%)	0.60	24 (10%) 7 5	20, 35, 63, 98	0
2	H	238/238 (100%)	0.28	9 (3%) 40 36	17, 33, 61, 98	0
All	All	849/872 (97%)	0.34	48 (5%) 23 19	10, 32, 58, 98	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	240	ARG	4.2
1	G	198	ASP	4.2
2	B	240	ARG	3.7
2	B	237	THR	3.6
1	G	218	SER	3.4
2	B	239	ASP	3.4
1	A	165	SER	3.3
2	B	57	TYR	3.2
2	H	239	ASP	3.1
2	B	241	ALA	3.0
1	A	183	MET	3.0
2	B	164	TYR	2.9
2	B	236	TRP	2.9
2	B	109	GLY	2.9
1	A	182	SER	2.8
2	B	234	ASP	2.8
1	A	113	PHE	2.8
2	H	233	ASN	2.7
1	A	24	THR	2.6
2	H	216	ASN	2.6
2	H	197	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	108	SER	2.6
2	B	94	ALA	2.6
1	A	210	ILE	2.5
1	G	84(C)	GLU	2.5
2	B	176	GLY	2.5
2	B	18	LYS	2.4
2	B	175	ASN	2.4
1	A	131	GLN	2.3
2	B	215	GLN	2.3
2	B	113	GLY	2.3
2	H	3	ALA	2.3
2	H	108	LEU	2.3
1	A	85	SER	2.3
1	A	83	ALA	2.3
1	A	141	ARG	2.3
2	B	17	GLY	2.3
2	H	232	GLU	2.2
2	B	145	GLU	2.2
2	H	238	GLN	2.2
2	B	195	ALA	2.2
2	B	194	PRO	2.1
1	A	198	ASP	2.1
2	B	128	GLU	2.1
2	B	13	ALA	2.0
2	B	217	PRO	2.0
2	B	125	THR	2.0
2	B	242	LYS	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

There are no such residues in this entry.