



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2023 – 01:41 AM EDT

PDB ID : 1HU8  
Title : CRYSTAL STRUCTURE OF THE MOUSE P53 CORE DNA-BINDING DOMAIN AT 2.7Å RESOLUTION  
Authors : Zhao, K.; Chai, X.; Johnston, K.; Clements, A.; Marmorstein, R.  
Deposited on : 2001-01-04  
Resolution : 2.70 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.34  
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) : 2.34

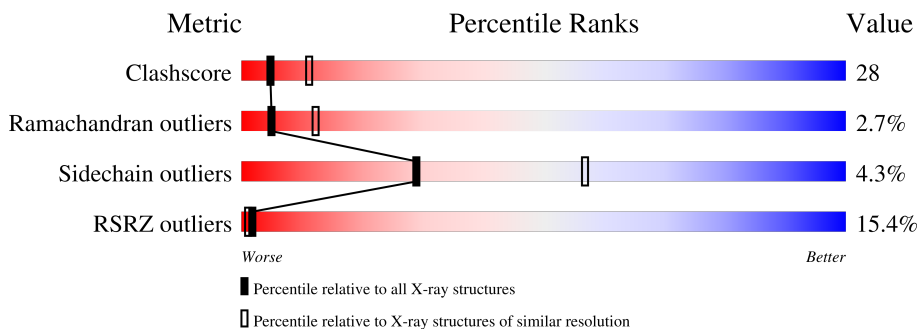
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 of 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	186	
1	B	186	
1	C	186	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4494 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 CELLULAR TUMOR ANTIGEN P53.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	186	1461	908	265	273	15	1	0	0
1	B	186	1461	908	265	273	15	0	0	0
1	C	186	1461	908	265	273	15	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	ALA	TYR	engineered mutation	UNP P02340
B	199	ALA	TYR	engineered mutation	UNP P02340
C	199	ALA	TYR	engineered mutation	UNP P02340

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	48	Total	O	0	0
			48	48		
3	B	41	Total	O	0	0
			41	41		

*Continued on next page...*

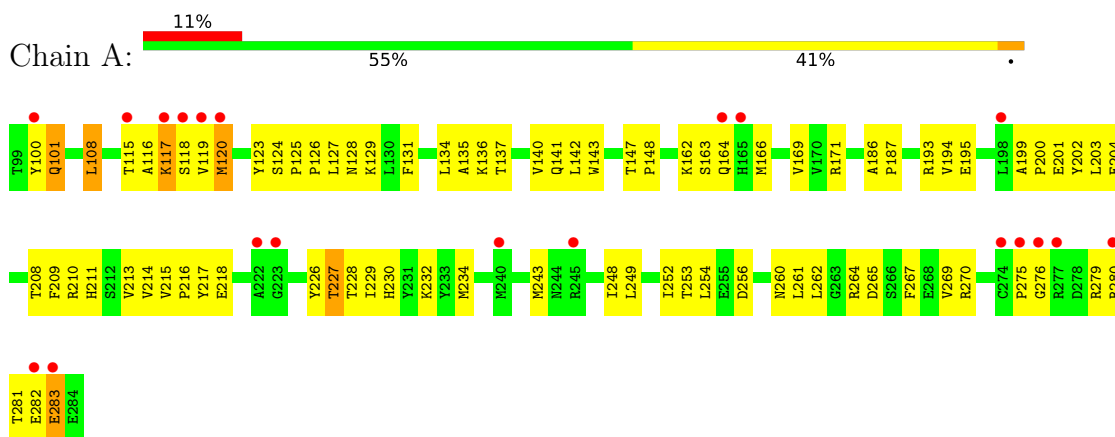
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	C	19	Total	O	0	0
			19	19		

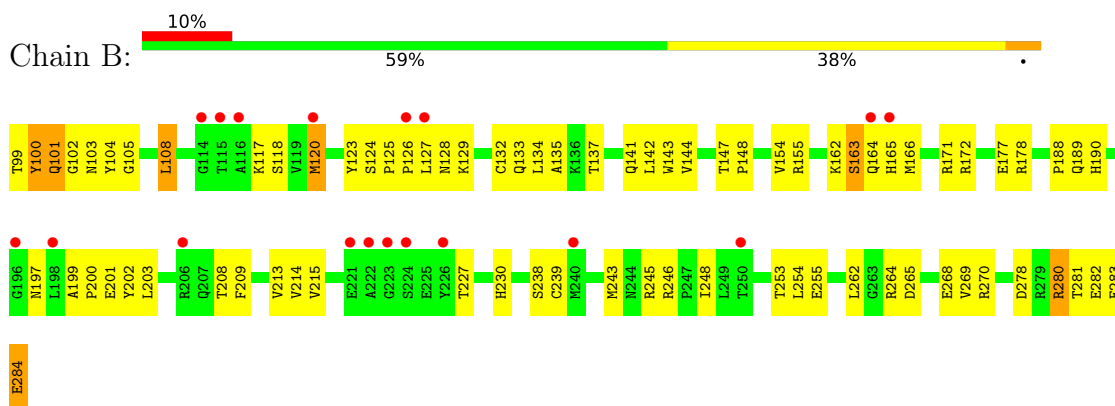
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

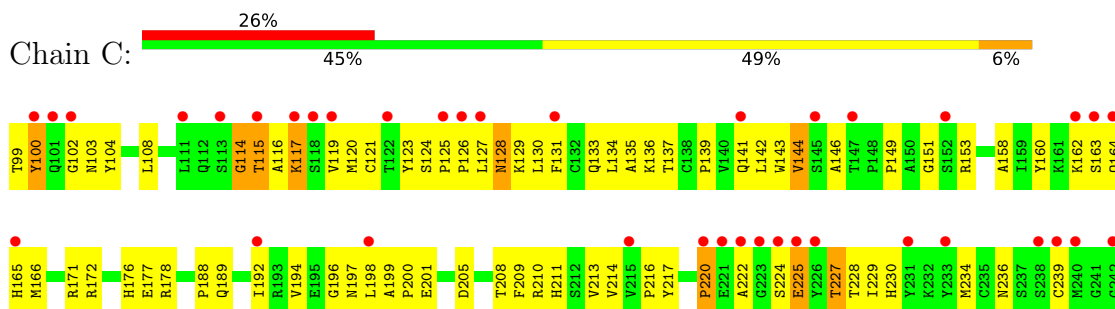
#### • Molecule 1: CELLULAR TUMOR ANTIGEN P53

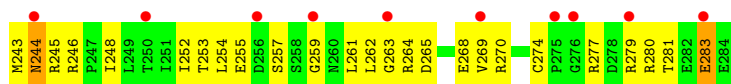


#### • Molecule 1: CELLULAR TUMOR ANTIGEN P53



#### • Molecule 1: CELLULAR TUMOR ANTIGEN P53





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.68Å 119.99Å 184.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70 30.95 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (10.00-2.70) 99.4 (30.95-2.70)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.19 (at 2.68Å)	Xtrriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.239 , 0.299 0.249 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.9	Xtrriage
Anisotropy	0.194	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 81.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4494	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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](#)

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

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	0.39	0/1497	0.64	0/2027
1	B	0.41	0/1497	0.64	0/2027
1	C	0.34	0/1497	0.62	0/2027
All	All	0.38	0/4491	0.63	0/6081

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 [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	1461	0	1419	70	0
1	B	1461	0	1419	68	0
1	C	1461	0	1420	105	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	48	0	0	4	0
3	B	41	0	0	4	0
3	C	19	0	0	7	0
All	All	4494	0	4258	240	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 28.

All (240) 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:253:THR:HG22	1:A:264:ARG:HG3	1.37	1.07
1:A:117:LYS:HD3	1:A:118:SER:H	1.22	1.03
1:B:108:LEU:HD22	1:B:265:ASP:HB3	1.41	0.99
1:C:104:TYR:HA	1:C:146:ALA:HB3	1.47	0.93
1:B:141:GLN:HE21	1:B:143:TRP:HE1	1.12	0.93
1:C:261:LEU:HD13	1:C:263:GLY:H	1.37	0.87
1:B:141:GLN:NE2	1:B:143:TRP:HE1	1.75	0.84
1:C:143:TRP:O	1:C:144:VAL:HG13	1.77	0.84
1:A:117:LYS:HD3	1:A:118:SER:N	1.93	0.83
1:C:253:THR:HG22	1:C:264:ARG:HG3	1.61	0.83
1:A:141:GLN:HE21	1:A:143:TRP:HE1	1.27	0.82
1:A:208:THR:OG1	1:A:210:ARG:HG3	1.82	0.80
1:B:124:SER:OG	1:B:127:LEU:HD13	1.82	0.79
1:A:115:THR:HG23	1:A:280:ARG:HH21	1.47	0.79
1:B:120:MET:HB3	1:B:133:GLN:NE2	1.98	0.79
1:A:201:GLU:HB3	1:A:214:VAL:HG13	1.65	0.78
1:C:116:ALA:HB3	1:C:119:VAL:HG23	1.66	0.77
1:A:124:SER:HG	1:A:127:LEU:HD13	1.49	0.77
1:C:108:LEU:HD13	1:C:265:ASP:HB3	1.67	0.76
1:A:243:MET:SD	1:A:248:ILE:HD13	2.26	0.75
1:C:261:LEU:HD13	1:C:263:GLY:N	2.00	0.75
1:B:123:TYR:O	1:B:125:PRO:HD3	1.87	0.74
1:A:129:LYS:HE2	1:A:270:ARG:HB2	1.72	0.71
1:A:137:THR:HG23	1:A:230:HIS:HB3	1.71	0.70
1:A:204:GLU:HG2	1:A:211:HIS:ND1	2.06	0.70
1:B:253:THR:HG22	1:B:264:ARG:HG3	1.75	0.69
1:B:105:GLY:O	1:B:144:VAL:HA	1.93	0.68
1:A:124:SER:OG	1:A:127:LEU:HD13	1.94	0.68
1:A:142:LEU:HB2	1:A:227:THR:HG23	1.74	0.67
1:C:126:PRO:HG2	1:C:127:LEU:HD12	1.77	0.67
1:C:261:LEU:HD13	1:C:262:LEU:N	2.09	0.67
1:A:162:LYS:HB3	1:A:164:GLN:OE1	1.96	0.66
1:B:102:GLY:C	1:B:104:TYR:H	1.99	0.66
1:C:102:GLY:HA3	1:C:262:LEU:O	1.97	0.64
1:C:261:LEU:CD1	1:C:263:GLY:H	2.10	0.64
1:B:117:LYS:O	1:B:118:SER:HB3	1.97	0.64
1:C:120:MET:HA	1:C:133:GLN:HE21	1.61	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLN:NE2	1:A:143:TRP:HE1	1.93	0.64
1:A:194:VAL:HG23	1:A:213:VAL:HG11	1.78	0.64
1:B:264:ARG:HH11	1:B:264:ARG:HB3	1.63	0.63
1:B:172:ARG:HD3	1:B:188:PRO:O	1.98	0.63
1:C:208:THR:OG1	1:C:210:ARG:HG3	1.97	0.63
1:B:163:SER:HA	1:B:166:MET:HB2	1.81	0.63
1:C:171:ARG:HB3	3:C:66:HOH:O	1.98	0.62
1:A:171:ARG:NH1	1:B:178:ARG:HG2	2.14	0.62
1:B:264:ARG:HB3	1:B:264:ARG:NH1	2.15	0.62
1:A:120:MET:HG3	1:A:136:LYS:HG2	1.82	0.62
1:C:137:THR:HG23	1:C:230:HIS:HB3	1.82	0.62
1:A:129:LYS:HZ1	1:A:270:ARG:HD2	1.65	0.62
1:B:137:THR:HG21	1:B:230:HIS:HD2	1.65	0.61
1:B:201:GLU:HB3	1:B:214:VAL:HG13	1.82	0.61
1:C:127:LEU:HD12	1:C:127:LEU:H	1.64	0.61
1:B:280:ARG:HG2	1:B:281:THR:N	2.15	0.61
1:C:279:ARG:O	1:C:283:GLU:HB2	2.00	0.60
1:C:151:GLY:HA3	1:C:257:SER:HB3	1.83	0.60
1:A:115:THR:HG23	1:A:280:ARG:NH2	2.17	0.59
1:B:125:PRO:N	1:B:126:PRO:HD2	2.17	0.59
1:B:117:LYS:HG2	1:B:118:SER:H	1.67	0.59
1:B:155:ARG:HH12	1:B:203:LEU:HD12	1.68	0.58
1:A:163:SER:HA	1:A:166:MET:HB2	1.85	0.58
1:B:248:ILE:HG13	1:B:269:VAL:HG13	1.84	0.58
1:C:124:SER:HG	1:C:127:LEU:HD13	1.69	0.58
1:C:220:PRO:HG2	3:C:45:HOH:O	2.03	0.58
1:C:141:GLN:HE21	1:C:143:TRP:HE1	1.52	0.58
1:B:108:LEU:HD22	1:B:265:ASP:CB	2.25	0.58
1:A:125:PRO:N	1:A:126:PRO:HD2	2.19	0.57
1:B:209:PHE:CE1	1:C:188:PRO:HD3	2.39	0.57
1:A:249:LEU:HD12	1:A:267:PHE:C	2.24	0.57
1:C:253:THR:HB	1:C:261:LEU:HD21	1.87	0.57
1:C:160:TYR:OH	1:C:243:MET:HA	2.05	0.57
1:A:117:LYS:O	1:A:118:SER:HB3	2.05	0.57
1:C:129:LYS:HE3	1:C:268:GLU:HG2	1.87	0.56
1:C:172:ARG:HD3	1:C:188:PRO:O	2.04	0.56
1:C:201:GLU:HB3	1:C:214:VAL:HG13	1.86	0.56
1:A:137:THR:CG2	1:A:230:HIS:HB3	2.36	0.56
1:C:126:PRO:HG2	1:C:127:LEU:CD1	2.35	0.56
1:C:189:GLN:HB2	3:C:49:HOH:O	2.05	0.55
1:A:279:ARG:O	1:A:283:GLU:HB2	2.05	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:LEU:HD12	1:B:127:LEU:N	2.22	0.55
1:C:120:MET:HG2	1:C:133:GLN:NE2	2.22	0.55
1:A:227:THR:HG22	3:A:537:HOH:O	2.07	0.55
1:C:124:SER:OG	1:C:127:LEU:HD13	2.07	0.55
1:A:129:LYS:NZ	1:A:270:ARG:HD2	2.21	0.55
1:B:280:ARG:HG2	1:B:281:THR:H	1.72	0.54
1:C:116:ALA:HB3	1:C:119:VAL:CG2	2.35	0.54
1:B:248:ILE:HG13	1:B:269:VAL:CG1	2.38	0.54
1:C:127:LEU:HD12	1:C:127:LEU:N	2.21	0.54
1:B:162:LYS:HB3	1:B:164:GLN:OE1	2.07	0.53
1:C:217:TYR:HE1	1:C:227:THR:HG21	1.74	0.53
1:C:196:GLY:O	1:C:198:LEU:HD22	2.09	0.53
1:A:218:GLU:HG2	3:A:540:HOH:O	2.08	0.53
1:B:137:THR:CG2	1:B:230:HIS:HD2	2.21	0.53
1:C:124:SER:C	1:C:126:PRO:HD2	2.28	0.53
1:C:153:ARG:HG2	1:C:216:PRO:HA	1.90	0.53
1:C:163:SER:HA	1:C:166:MET:HB2	1.91	0.53
1:C:119:VAL:HG12	1:C:120:MET:N	2.23	0.52
1:A:108:LEU:HD21	1:A:252:ILE:HG13	1.91	0.52
1:B:264:ARG:HG2	1:B:265:ASP:N	2.24	0.52
1:B:284:GLU:O	1:B:284:GLU:OE1	2.27	0.52
1:C:280:ARG:O	1:C:283:GLU:N	2.41	0.52
1:A:256:ASP:OD2	1:A:260:ASN:N	2.40	0.51
1:B:215:VAL:HG13	3:B:508:HOH:O	2.10	0.51
1:B:248:ILE:CG1	1:B:269:VAL:HG13	2.40	0.51
1:C:244:ASN:C	1:C:246:ARG:H	2.14	0.51
1:C:120:MET:HB3	1:C:136:LYS:HG2	1.93	0.51
1:C:129:LYS:HA	1:C:268:GLU:O	2.10	0.51
1:C:225:GLU:H	1:C:225:GLU:CD	2.14	0.51
1:B:99:THR:O	1:B:100:TYR:HB2	2.11	0.51
1:B:102:GLY:HA3	1:B:262:LEU:O	2.11	0.50
1:C:162:LYS:HB3	1:C:164:GLN:OE1	2.11	0.50
1:C:253:THR:HG23	3:C:57:HOH:O	2.11	0.50
1:B:102:GLY:C	1:B:104:TYR:N	2.65	0.50
1:C:205:ASP:OD2	1:C:208:THR:HG23	2.12	0.50
1:C:153:ARG:HD2	1:C:214:VAL:HG22	1.94	0.50
1:C:117:LYS:HD3	1:C:280:ARG:NH1	2.27	0.50
1:C:280:ARG:HG3	1:C:281:THR:N	2.27	0.49
1:A:127:LEU:HD12	1:A:127:LEU:N	2.27	0.49
1:B:208:THR:O	1:B:209:PHE:HB2	2.11	0.49
1:C:220:PRO:HG3	1:C:227:THR:HG22	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:LEU:HD21	1:B:154:VAL:HG21	1.95	0.49
1:C:127:LEU:H	1:C:127:LEU:CD1	2.26	0.49
1:C:261:LEU:CD1	1:C:263:GLY:N	2.72	0.49
1:C:127:LEU:O	1:C:128:ASN:HB3	2.12	0.49
1:C:222:ALA:C	1:C:224:SER:H	2.16	0.49
1:A:169:VAL:HG12	1:A:171:ARG:HG3	1.93	0.49
1:B:278:ASP:O	1:B:282:GLU:HG3	2.13	0.48
1:C:123:TYR:O	1:C:125:PRO:HD3	2.13	0.48
1:A:134:LEU:HD23	1:A:135:ALA:HB2	1.95	0.48
1:C:143:TRP:O	1:C:144:VAL:CG1	2.56	0.48
1:C:197:ASN:OD1	1:C:199:ALA:N	2.31	0.48
1:A:280:ARG:C	1:A:282:GLU:H	2.17	0.48
1:A:232:LYS:NZ	3:A:538:HOH:O	2.47	0.48
1:B:171:ARG:HD2	3:B:521:HOH:O	2.14	0.47
1:C:119:VAL:HG12	1:C:120:MET:H	1.78	0.47
1:A:134:LEU:HD23	1:A:134:LEU:C	2.35	0.47
1:C:158:ALA:HB2	1:C:192:ILE:HD11	1.96	0.47
1:B:197:ASN:ND2	3:B:508:HOH:O	2.47	0.47
1:C:208:THR:O	1:C:209:PHE:HB2	2.14	0.47
1:C:125:PRO:N	1:C:126:PRO:HD2	2.29	0.47
1:A:101:GLN:O	1:A:101:GLN:HG2	2.14	0.47
1:B:202:TYR:CE2	1:B:213:VAL:HG13	2.49	0.47
1:C:165:HIS:CD2	1:C:246:ARG:HH11	2.33	0.47
1:A:186:ALA:HB2	1:A:202:TYR:CZ	2.50	0.47
1:B:102:GLY:O	1:B:104:TYR:N	2.47	0.47
1:C:194:VAL:HG23	1:C:213:VAL:HG11	1.97	0.47
1:C:269:VAL:CG2	1:C:270:ARG:N	2.78	0.47
1:B:134:LEU:HD23	1:B:135:ALA:HB2	1.96	0.46
1:C:239:CYS:O	1:C:244:ASN:HA	2.16	0.46
1:A:127:LEU:HD13	1:A:283:GLU:OE1	2.16	0.46
1:B:99:THR:O	1:B:100:TYR:CB	2.63	0.46
1:B:117:LYS:HG2	1:B:118:SER:N	2.30	0.46
1:B:199:ALA:N	1:B:200:PRO:CD	2.79	0.46
1:C:120:MET:HA	1:C:133:GLN:NE2	2.29	0.46
1:C:255:GLU:OE2	1:C:259:GLY:HA2	2.16	0.46
1:B:123:TYR:OH	1:B:128:ASN:ND2	2.43	0.46
1:C:244:ASN:O	1:C:246:ARG:N	2.48	0.46
1:B:129:LYS:HG3	1:B:268:GLU:HG2	1.98	0.46
1:C:177:GLU:O	1:C:177:GLU:HG2	2.16	0.46
1:C:199:ALA:N	1:C:200:PRO:CD	2.78	0.46
1:A:209:PHE:CE1	1:B:188:PRO:HD3	2.49	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:LEU:CD2	1:B:265:ASP:HB3	2.29	0.46
1:C:176:HIS:C	1:C:178:ARG:H	2.19	0.46
1:C:243:MET:O	1:C:246:ARG:HB2	2.16	0.46
1:B:201:GLU:OE2	1:B:203:LEU:HD21	2.16	0.45
1:A:123:TYR:OH	1:A:128:ASN:ND2	2.49	0.45
1:C:99:THR:HG22	3:C:91:HOH:O	2.15	0.45
1:B:177:GLU:HG3	1:B:189:GLN:HG2	1.99	0.45
1:B:254:LEU:O	1:B:262:LEU:HB2	2.16	0.45
1:C:115:THR:HB	1:C:279:ARG:HD3	1.97	0.45
1:C:274:CYS:HB3	1:C:277:ARG:HB3	1.97	0.45
1:C:130:LEU:HD12	1:C:131:PHE:H	1.82	0.45
1:C:176:HIS:CE1	1:C:239:CYS:SG	3.10	0.45
1:A:147:THR:HA	1:A:148:PRO:HD3	1.88	0.45
1:A:215:VAL:HG13	1:A:216:PRO:HD2	1.99	0.45
1:C:176:HIS:C	1:C:178:ARG:N	2.71	0.44
1:A:137:THR:HG21	1:A:230:HIS:HD2	1.83	0.44
1:B:101:GLN:NE2	3:B:530:HOH:O	2.49	0.44
1:B:238:SER:HB3	1:B:245:ARG:NH1	2.32	0.44
1:B:264:ARG:HG2	1:B:265:ASP:H	1.81	0.44
1:A:215:VAL:HG13	3:A:533:HOH:O	2.18	0.44
1:A:129:LYS:CE	1:A:270:ARG:HB2	2.42	0.44
1:A:186:ALA:HA	1:A:187:PRO:HD3	1.89	0.44
1:C:137:THR:HG22	1:C:139:PRO:HD3	2.00	0.44
1:C:255:GLU:HB2	1:C:259:GLY:C	2.38	0.44
1:C:104:TYR:CD2	1:C:104:TYR:N	2.86	0.44
1:C:114:GLY:O	1:C:116:ALA:N	2.48	0.43
1:A:117:LYS:C	1:A:119:VAL:H	2.20	0.43
1:A:143:TRP:CE2	1:A:226:TYR:HB3	2.53	0.43
1:B:127:LEU:HD11	1:B:283:GLU:HA	2.00	0.43
1:C:135:ALA:HB2	1:C:234:MET:CE	2.48	0.43
1:C:228:THR:CG2	1:C:229:ILE:N	2.81	0.43
1:A:134:LEU:HD23	1:A:135:ALA:N	2.33	0.43
1:A:264:ARG:HG2	1:A:265:ASP:N	2.33	0.43
1:C:100:TYR:CZ	1:C:102:GLY:HA2	2.54	0.43
1:B:129:LYS:HE2	1:B:270:ARG:HB2	2.00	0.43
1:A:280:ARG:HG3	1:A:281:THR:N	2.34	0.43
1:B:147:THR:HA	1:B:148:PRO:HD3	1.91	0.43
1:B:165:HIS:CD2	1:B:246:ARG:HH11	2.37	0.43
1:A:123:TYR:HE1	1:A:128:ASN:HD22	1.66	0.42
1:A:193:ARG:NE	1:A:234:MET:HG3	2.34	0.42
1:B:190:HIS:CE1	1:B:202:TYR:HB3	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:MET:CE	1:C:136:LYS:HZ2	2.33	0.42
1:C:141:GLN:C	1:C:142:LEU:HD12	2.39	0.42
1:A:141:GLN:C	1:A:142:LEU:HD12	2.40	0.42
1:C:269:VAL:HG22	1:C:270:ARG:N	2.34	0.42
1:C:243:MET:SD	1:C:248:ILE:HG21	2.60	0.42
1:A:208:THR:CB	1:A:210:ARG:HG3	2.49	0.42
1:A:248:ILE:HG13	1:A:269:VAL:HG13	2.02	0.42
1:A:261:LEU:C	1:A:261:LEU:HD13	2.40	0.42
1:C:130:LEU:HD12	1:C:131:PHE:N	2.34	0.41
1:B:120:MET:O	1:B:132:CYS:HA	2.21	0.41
1:C:114:GLY:C	1:C:116:ALA:H	2.21	0.41
1:C:119:VAL:HG12	1:C:121:CYS:H	1.84	0.41
1:A:117:LYS:NZ	1:A:117:LYS:HA	2.35	0.41
1:C:217:TYR:CE1	1:C:227:THR:HG21	2.53	0.41
1:A:194:VAL:HG12	1:A:195:GLU:N	2.34	0.41
1:C:99:THR:O	1:C:100:TYR:CB	2.68	0.41
1:C:225:GLU:HA	3:C:61:HOH:O	2.20	0.41
1:A:254:LEU:O	1:A:262:LEU:HB2	2.20	0.41
1:C:100:TYR:HD1	3:C:46:HOH:O	2.04	0.41
1:C:141:GLN:NE2	1:C:143:TRP:HE1	2.17	0.41
1:C:142:LEU:HB2	1:C:227:THR:HG23	2.01	0.41
1:C:208:THR:CB	1:C:210:ARG:HG3	2.51	0.41
1:C:134:LEU:HD11	1:C:176:HIS:CD2	2.56	0.41
1:A:129:LYS:HD3	1:A:131:PHE:CZ	2.55	0.41
1:B:141:GLN:NE2	1:B:143:TRP:NE1	2.57	0.41
1:B:243:MET:SD	1:B:248:ILE:HD13	2.61	0.41
1:C:134:LEU:HD12	1:C:236:ASN:ND2	2.36	0.41
1:C:153:ARG:HB3	1:C:214:VAL:HG23	2.02	0.41
1:A:201:GLU:HG2	1:A:203:LEU:HD21	2.01	0.41
1:A:275:PRO:HG2	1:A:276:GLY:H	1.85	0.41
1:B:125:PRO:CD	1:B:126:PRO:HD2	2.51	0.41
1:C:134:LEU:HD23	1:C:134:LEU:C	2.41	0.41
1:A:228:THR:HG22	1:A:229:ILE:N	2.36	0.40
1:A:261:LEU:HD13	1:A:262:LEU:N	2.36	0.40
1:C:108:LEU:HD21	1:C:252:ILE:HG13	2.04	0.40
1:A:148:PRO:HD2	1:A:217:TYR:CE2	2.56	0.40
1:B:117:LYS:O	1:B:118:SER:CB	2.65	0.40
1:A:199:ALA:N	1:A:200:PRO:CD	2.84	0.40
1:B:127:LEU:N	1:B:127:LEU:CD1	2.85	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	184/186 (99%)	166 (90%)	16 (9%)	2 (1%)	14	34
1	B	184/186 (99%)	156 (85%)	24 (13%)	4 (2%)	6	17
1	C	184/186 (99%)	149 (81%)	26 (14%)	9 (5%)	2	4
All	All	552/558 (99%)	471 (85%)	66 (12%)	15 (3%)	5	12

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	ALA
1	B	100	TYR
1	C	100	TYR
1	B	103	ASN
1	B	163	SER
1	C	115	THR
1	C	245	ARG
1	C	117	LYS
1	B	239	CYS
1	C	244	ASN
1	A	100	TYR
1	C	114	GLY
1	C	144	VAL
1	C	149	PRO
1	C	220	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	162/162 (100%)	155 (96%)	7 (4%)	29	57
1	B	162/162 (100%)	155 (96%)	7 (4%)	29	57
1	C	162/162 (100%)	155 (96%)	7 (4%)	29	57
All	All	486/486 (100%)	465 (96%)	21 (4%)	29	57

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	108	LEU
1	A	117	LYS
1	A	120	MET
1	A	140	VAL
1	A	227	THR
1	A	283	GLU
1	B	101	GLN
1	B	108	LEU
1	B	120	MET
1	B	227	THR
1	B	255	GLU
1	B	280	ARG
1	B	284	GLU
1	C	103	ASN
1	C	128	ASN
1	C	211	HIS
1	C	225	GLU
1	C	227	THR
1	C	254	LEU
1	C	283	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	128	ASN
1	A	133	GLN
1	A	141	GLN
1	A	189	GLN
1	A	207	GLN
1	A	230	HIS
1	B	101	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	107	HIS
1	B	128	ASN
1	B	133	GLN
1	B	141	GLN
1	B	165	HIS
1	B	189	GLN
1	B	207	GLN
1	B	230	HIS
1	C	101	GLN
1	C	128	ASN
1	C	133	GLN
1	C	141	GLN
1	C	175	HIS
1	C	189	GLN
1	C	207	GLN
1	C	230	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [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	186/186 (100%)	0.54	20 (10%) <b>5</b> <b>4</b>	28, 51, 96, 104	1 (0%)
1	B	186/186 (100%)	0.51	18 (9%) <b>7</b> <b>6</b>	24, 51, 95, 106	0
1	C	186/186 (100%)	1.42	48 (25%) <b>0</b> <b>0</b>	36, 82, 118, 134	0
All	All	558/558 (100%)	0.82	86 (15%) <b>2</b> <b>1</b>	24, 58, 107, 134	1 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	222	ALA	8.0
1	C	119	VAL	7.5
1	C	222	ALA	5.3
1	C	223	GLY	5.3
1	B	223	GLY	5.1
1	B	115	THR	5.1
1	C	126	PRO	5.0
1	C	118	SER	4.9
1	A	164	GLN	4.8
1	C	164	GLN	4.8
1	C	122	THR	4.8
1	C	221	GLU	4.7
1	C	263	GLY	4.6
1	C	224	SER	4.5
1	A	245	ARG	4.4
1	A	240	MET	4.4
1	C	111	LEU	4.2
1	A	115	THR	4.1
1	C	240	MET	4.1
1	C	100	TYR	4.1
1	A	280	ARG	4.0
1	A	119	VAL	4.0
1	C	102	GLY	3.9

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	C	225	GLU	3.8
1	C	115	THR	3.8
1	B	114	GLY	3.7
1	C	279	ARG	3.6
1	C	131	PHE	3.5
1	C	259	GLY	3.5
1	B	116	ALA	3.4
1	C	165	HIS	3.4
1	C	283	GLU	3.4
1	A	222	ALA	3.4
1	B	206	ARG	3.2
1	A	223	GLY	3.2
1	C	125	PRO	3.2
1	C	198	LEU	3.2
1	A	165	HIS	3.2
1	C	127	LEU	3.2
1	C	276	GLY	3.1
1	B	198	LEU	3.1
1	C	250	THR	3.1
1	A	118	SER	3.0
1	A	274	CYS	3.0
1	C	220	PRO	2.9
1	A	277	ARG	2.9
1	C	275	PRO	2.9
1	C	226	TYR	2.8
1	C	145	SER	2.8
1	C	242	GLY	2.8
1	B	226	TYR	2.8
1	C	192	ILE	2.7
1	C	239	CYS	2.7
1	C	256	ASP	2.7
1	C	101	GLN	2.7
1	C	231	TYR	2.7
1	B	126	PRO	2.6
1	C	233	TYR	2.6
1	B	120	MET	2.6
1	C	147	THR	2.5
1	A	276	GLY	2.5
1	C	163	SER	2.5
1	B	250	THR	2.5
1	C	113	SER	2.5
1	C	244	ASN	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	164	GLN	2.5
1	C	162	LYS	2.4
1	A	100	TYR	2.4
1	C	269	VAL	2.4
1	A	120	MET	2.4
1	B	240	MET	2.4
1	B	165	HIS	2.3
1	C	117	LYS	2.3
1	A	198	LEU	2.3
1	C	238	SER	2.3
1	A	117	LYS	2.2
1	B	224	SER	2.2
1	B	196	GLY	2.2
1	A	283	GLU	2.2
1	C	152	SER	2.1
1	C	215	VAL	2.1
1	C	141	GLN	2.1
1	A	275	PRO	2.1
1	B	221	GLU	2.1
1	B	127	LEU	2.0
1	A	282	GLU	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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ZN	C	503	1/1	0.98	0.09	66,66,66,66	0
2	ZN	B	502	1/1	0.99	0.13	53,53,53,53	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	501	1/1	0.99	0.09	60,60,60,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.