



# Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 04:23 AM GMT

PDB ID : 3HGT  
Title : Structural and functional studies of the yeast class II Hda1 HDAC complex  
Authors : Lee, J.H.; Maskos, K.; Huber, R.  
Deposited on : 2009-05-14  
Resolution : 2.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

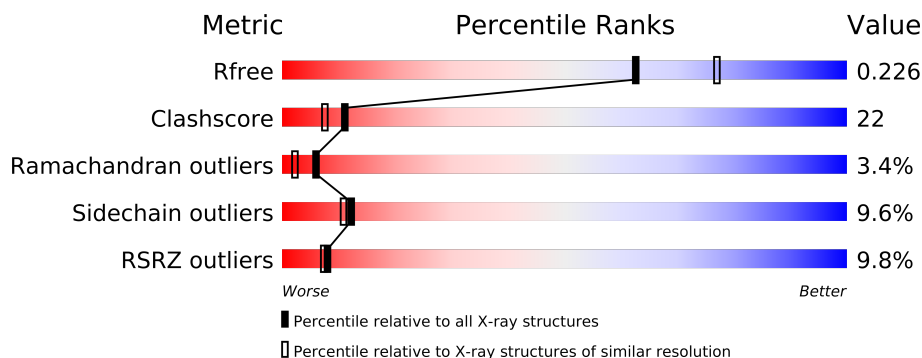
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	328	
1	B	328	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4813 atoms, of which 0 are hydrogen and 0 are deuterium.

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 HDA1 complex subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2332	1502	385	432	13			
1	B	286	Total	C	N	O	S	0	0	0
			2332	1502	385	432	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	ALA	LYS	ENGINEERED	UNP Q06623
A	169	ALA	GLN	ENGINEERED	UNP Q06623
A	170	ALA	LYS	ENGINEERED	UNP Q06623
B	168	ALA	LYS	ENGINEERED	UNP Q06623
B	169	ALA	GLN	ENGINEERED	UNP Q06623
B	170	ALA	LYS	ENGINEERED	UNP Q06623

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	66	Total	O	0	0
			66	66		
2	B	83	Total	O	0	0
			83	83		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.18Å 116.57Å 55.19Å 90.00° 97.42° 90.00°	Depositor
Resolution (Å)	19.98 – 2.20 49.53 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.5 (19.98-2.20) 95.4 (49.53-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.87 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.198 , 0.237 0.201 , 0.226	Depositor DCC
$R_{free}$ test set	1674 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.0	EDS
Estimated twinning fraction	0.296 for L,-K,H 0.278 for l,-k,h	Xtriage
Reported twinning fraction	0.296 for L,-K,H	Depositor
L-test for twinning	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 33474 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4813	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.36	0/2386	0.56	0/3239
1	B	0.35	0/2386	0.57	0/3239
All	All	0.35	0/4772	0.56	0/6478

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2332	0	2344	104	0
1	B	2332	0	2344	108	0
2	A	66	0	0	13	0
2	B	83	0	0	19	0
All	All	4813	0	4688	210	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (210) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:49:VAL:HA	1:B:77:MET:HE2	1.41	1.02

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:49:VAL:HA	1:A:77:MET:HE2	1.46	0.96
1:A:56:ILE:HD11	1:A:77:MET:HE3	1.45	0.96
1:B:86:THR:HG22	1:B:115:LYS:HZ2	1.30	0.95
1:B:63:SER:O	1:B:64:HIS:HB2	1.69	0.92
1:A:63:SER:O	1:A:64:HIS:HB2	1.68	0.92
1:B:208:THR:HG22	2:B:374:HOH:O	1.73	0.87
1:B:86:THR:HB	2:B:397:HOH:O	1.76	0.86
1:A:234:PRO:HD2	2:A:371:HOH:O	1.75	0.86
1:A:49:VAL:HA	1:A:77:MET:CE	2.07	0.85
1:B:49:VAL:HA	1:B:77:MET:CE	2.06	0.85
1:A:86:THR:HG22	1:A:115:LYS:HZ2	1.43	0.84
1:A:198:ARG:HE	1:A:223:LYS:HD3	1.42	0.83
1:B:296:VAL:O	1:B:300:GLU:HG2	1.79	0.82
1:B:198:ARG:HE	1:B:223:LYS:HD3	1.45	0.82
1:B:56:ILE:HD11	1:B:77:MET:HE3	1.62	0.82
1:A:195:SER:O	1:A:196:LYS:HB2	1.79	0.81
1:B:195:SER:O	1:B:196:LYS:HB2	1.77	0.81
1:B:121:ASP:HA	1:B:291:LYS:HE3	1.62	0.81
1:B:86:THR:HG22	1:B:115:LYS:NZ	1.94	0.81
1:B:160:TYR:OH	1:B:179:HIS:HD2	1.63	0.81
1:A:121:ASP:HA	1:A:291:LYS:HE3	1.61	0.80
1:A:160:TYR:OH	1:A:179:HIS:HD2	1.63	0.80
1:A:296:VAL:O	1:A:300:GLU:HG2	1.82	0.79
1:A:27:THR:HB	1:A:31:TYR:HE1	1.47	0.79
1:A:86:THR:HG22	1:A:115:LYS:NZ	1.98	0.77
1:B:94:HIS:HA	2:B:362:HOH:O	1.87	0.75
1:B:27:THR:HB	1:B:31:TYR:HE1	1.50	0.75
1:A:233:ALA:HB1	2:A:371:HOH:O	1.85	0.74
1:A:158:LYS:HE2	2:A:392:HOH:O	1.86	0.74
1:A:45:THR:HG21	1:A:277:LEU:HD11	1.69	0.74
1:B:222:TYR:O	1:B:223:LYS:HB2	1.87	0.74
1:A:291:LYS:HD3	2:A:384:HOH:O	1.87	0.73
1:A:56:ILE:HD11	1:A:77:MET:CE	2.18	0.73
1:B:250:PHE:CE2	1:B:313:PRO:HA	2.24	0.73
1:B:186:ILE:O	1:B:187:ASN:HB3	1.88	0.73
1:A:201:MET:HA	2:A:371:HOH:O	1.89	0.72
1:B:199:PHE:HB2	2:B:399:HOH:O	1.88	0.71
1:A:250:PHE:CE2	1:A:313:PRO:HA	2.25	0.71
1:A:186:ILE:O	1:A:187:ASN:HB3	1.89	0.71
1:A:222:TYR:O	1:A:223:LYS:HB2	1.88	0.71
1:B:56:ILE:HD11	1:B:77:MET:CE	2.21	0.71
1:A:188:PHE:HE1	1:A:193:ILE:HD11	1.57	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:188:PHE:HE1	1:B:193:ILE:HD11	1.56	0.69
1:A:263:LEU:O	1:A:267:THR:HG23	1.92	0.69
1:B:72:GLU:O	1:B:76:THR:HG23	1.92	0.69
1:B:45:THR:HG21	1:B:277:LEU:HD11	1.72	0.69
1:A:89:TYR:OH	1:A:108:HIS:HE1	1.77	0.68
1:B:89:TYR:OH	1:B:108:HIS:HE1	1.77	0.68
1:B:131:THR:HG22	1:B:200:ASP:OD1	1.94	0.68
1:A:72:GLU:O	1:A:76:THR:HG23	1.93	0.67
1:B:263:LEU:O	1:B:267:THR:HG23	1.95	0.67
1:B:27:THR:HG21	2:B:382:HOH:O	1.94	0.67
1:B:66:LYS:HB2	1:B:71:LEU:HG	1.77	0.66
1:A:131:THR:HG22	1:A:200:ASP:OD1	1.94	0.66
1:B:198:ARG:HH21	1:B:223:LYS:HG2	1.59	0.66
1:B:194:LYS:HB2	1:B:194:LYS:NZ	2.11	0.66
1:B:294:TYR:HB2	2:B:340:HOH:O	1.96	0.65
1:A:194:LYS:NZ	1:A:194:LYS:HB2	2.10	0.65
1:A:66:LYS:HB2	1:A:71:LEU:HG	1.78	0.64
1:A:198:ARG:HE	1:A:223:LYS:CD	2.11	0.64
1:A:198:ARG:HH21	1:A:223:LYS:HG2	1.60	0.64
1:B:67:GLU:HG3	1:B:70:ILE:HB	1.80	0.63
1:B:60:PHE:HB3	1:B:319:SER:OG	1.99	0.63
1:A:138:ARG:HB3	1:A:208:THR:HG21	1.80	0.63
1:B:186:ILE:O	1:B:187:ASN:CB	2.46	0.63
1:A:67:GLU:HG3	1:A:70:ILE:HB	1.81	0.63
1:B:87:HIS:HD2	1:B:89:TYR:H	1.46	0.63
1:A:60:PHE:HB3	1:A:319:SER:OG	1.98	0.63
1:A:186:ILE:O	1:A:187:ASN:CB	2.47	0.62
1:B:138:ARG:HB3	1:B:208:THR:HG21	1.82	0.62
1:B:123:ILE:HA	1:B:126:VAL:HG12	1.81	0.61
1:A:188:PHE:CE1	1:A:193:ILE:HD11	2.36	0.60
1:A:273:LEU:HD11	1:A:314:LEU:HD22	1.83	0.60
1:B:188:PHE:CE1	1:B:193:ILE:HD11	2.36	0.60
1:B:183:SER:OG	1:B:208:THR:HG23	2.01	0.60
1:B:276:ARG:HD2	2:B:403:HOH:O	2.00	0.60
1:B:209:VAL:HG23	2:B:374:HOH:O	2.00	0.60
1:A:256:ASP:HB2	2:A:373:HOH:O	2.00	0.60
1:B:198:ARG:HE	1:B:223:LYS:CD	2.13	0.59
1:A:123:ILE:HA	1:A:126:VAL:HG12	1.84	0.59
1:B:27:THR:CG2	2:B:382:HOH:O	2.48	0.59
1:A:87:HIS:HD2	1:A:89:TYR:H	1.51	0.59
1:B:146:LEU:HD13	1:B:180:LEU:HD22	1.84	0.58
1:A:183:SER:OG	1:A:208:THR:HG23	2.04	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:155:VAL:HG11	1:B:178:VAL:HG23	1.85	0.58
1:A:127:GLN:NE2	1:A:153:ASN:HB3	2.19	0.57
1:B:273:LEU:HD11	1:B:314:LEU:HD22	1.87	0.56
1:A:89:TYR:OH	1:A:108:HIS:CE1	2.58	0.56
1:B:155:VAL:CG1	1:B:178:VAL:HG23	2.35	0.56
1:A:324:ARG:O	1:A:328:THR:HG23	2.05	0.56
1:B:324:ARG:O	1:B:328:THR:HG23	2.06	0.56
1:A:194:LYS:HZ2	1:A:194:LYS:HB2	1.69	0.55
1:A:160:TYR:OH	1:A:179:HIS:CD2	2.53	0.55
1:B:222:TYR:HD1	2:B:395:HOH:O	1.89	0.55
1:B:233:ALA:N	2:B:381:HOH:O	2.39	0.55
1:A:27:THR:HB	1:A:31:TYR:CE1	2.34	0.55
1:B:89:TYR:OH	1:B:108:HIS:CE1	2.58	0.55
1:B:203:ILE:HG12	1:B:236:VAL:CG1	2.37	0.55
1:B:127:GLN:NE2	1:B:153:ASN:HB3	2.22	0.55
1:B:158:LYS:NZ	2:B:379:HOH:O	2.38	0.55
1:B:121:ASP:CG	1:B:291:LYS:HG2	2.27	0.54
1:B:233:ALA:CB	2:B:399:HOH:O	2.56	0.54
1:B:121:ASP:CA	1:B:291:LYS:HE3	2.35	0.54
1:A:155:VAL:CG1	1:A:178:VAL:HG23	2.38	0.54
1:A:301:ASN:O	1:A:304:VAL:HB	2.08	0.53
1:A:40:TYR:HB2	1:B:40:TYR:HB2	1.89	0.53
1:A:155:VAL:HG11	1:A:178:VAL:HG23	1.90	0.53
1:B:27:THR:HB	1:B:31:TYR:CE1	2.37	0.53
1:A:121:ASP:CG	1:A:291:LYS:HG2	2.29	0.53
1:A:32:TRP:CE2	1:A:311:ILE:HA	2.44	0.53
1:B:160:TYR:OH	1:B:179:HIS:CD2	2.54	0.52
1:A:121:ASP:CA	1:A:291:LYS:HE3	2.34	0.52
1:B:301:ASN:O	1:B:304:VAL:HB	2.09	0.52
1:B:257:LYS:HB3	2:B:383:HOH:O	2.09	0.52
1:A:127:GLN:NE2	1:A:154:LYS:H	2.07	0.52
1:B:31:TYR:O	1:B:237:ARG:HG3	2.10	0.52
1:B:291:LYS:O	1:B:291:LYS:HD3	2.11	0.51
1:A:281:PRO:HG2	1:A:312:TYR:CE1	2.45	0.51
1:A:42:LYS:HD3	1:B:95:TYR:CD1	2.46	0.51
1:A:146:LEU:HD13	1:A:180:LEU:HD22	1.93	0.51
1:B:88:PRO:HG2	2:B:384:HOH:O	2.11	0.51
1:B:195:SER:O	1:B:196:LYS:CB	2.55	0.50
1:B:155:VAL:HG11	1:B:178:VAL:CG2	2.40	0.50
1:B:65:TYR:C	1:B:66:LYS:HG2	2.32	0.50
1:B:127:GLN:NE2	1:B:154:LYS:H	2.09	0.50
1:A:203:ILE:HG12	1:A:236:VAL:CG1	2.41	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:194:LYS:HB2	1:B:194:LYS:HZ2	1.75	0.50
1:A:37:MET:CE	1:A:85:ALA:HA	2.41	0.50
1:A:31:TYR:O	1:A:237:ARG:HG3	2.11	0.50
1:A:93:ASP:OD1	1:A:141:ARG:NH1	2.44	0.50
1:A:291:LYS:CD	2:A:384:HOH:O	2.54	0.49
1:B:32:TRP:CE2	1:B:311:ILE:HA	2.47	0.49
1:B:37:MET:CE	1:B:85:ALA:HA	2.41	0.49
1:B:93:ASP:OD1	1:B:141:ARG:NH1	2.44	0.49
1:B:194:LYS:NZ	1:B:194:LYS:CB	2.76	0.49
1:A:194:LYS:NZ	1:A:194:LYS:CB	2.76	0.49
1:A:30:ASP:OD2	1:A:237:ARG:NH1	2.46	0.49
1:A:65:TYR:C	1:A:66:LYS:HG2	2.33	0.49
1:B:96:MET:CE	1:B:100:LEU:HD21	2.43	0.48
1:B:281:PRO:HG2	1:B:312:TYR:CE1	2.48	0.48
1:B:52:HIS:HB2	1:B:77:MET:HE3	1.94	0.48
1:B:271:VAL:O	1:B:274:ARG:HB3	2.14	0.48
1:A:45:THR:CG2	1:A:277:LEU:HD11	2.41	0.48
1:A:234:PRO:CD	2:A:371:HOH:O	2.49	0.48
1:A:291:LYS:O	1:A:291:LYS:HD3	2.14	0.48
1:B:30:ASP:OD2	1:B:237:ARG:NH1	2.47	0.47
1:A:274:ARG:HE	1:A:274:ARG:HB3	1.48	0.47
1:A:47:GLN:O	1:A:51:LEU:HD13	2.15	0.47
1:A:236:VAL:HB	2:A:376:HOH:O	2.14	0.47
1:A:155:VAL:HG11	1:A:178:VAL:CG2	2.44	0.46
1:B:37:MET:HE1	1:B:85:ALA:HA	1.98	0.46
1:A:318:THR:HG22	2:A:375:HOH:O	2.14	0.46
1:B:274:ARG:HB3	1:B:274:ARG:HE	1.48	0.46
1:A:123:ILE:CG2	1:A:155:VAL:HG21	2.46	0.46
1:A:58:ARG:HH12	1:A:62:THR:HG21	1.81	0.46
1:B:58:ARG:HH12	1:B:62:THR:HG21	1.80	0.45
1:A:113:SER:HB3	1:A:116:PHE:HB2	1.98	0.45
1:A:306:TRP:HA	1:A:307:PRO:HD3	1.67	0.45
1:B:45:THR:CG2	1:B:277:LEU:HD11	2.44	0.45
1:A:96:MET:CE	1:A:100:LEU:HD21	2.47	0.45
1:B:61:GLU:HG3	1:B:62:THR:N	2.31	0.45
1:B:123:ILE:CG2	1:B:155:VAL:HG21	2.47	0.45
1:A:132:GLU:HG3	1:A:195:SER:OG	2.18	0.44
1:A:275:ASP:HB3	2:A:395:HOH:O	2.16	0.44
1:A:61:GLU:HG3	1:A:62:THR:N	2.33	0.44
1:A:94:HIS:O	1:A:95:TYR:HB2	2.18	0.44
1:B:302:PRO:HG2	2:B:335:HOH:O	2.17	0.44
1:B:44:LEU:O	1:B:48:ILE:HG13	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:136:VAL:HG12	1:B:209:VAL:HG22	1.99	0.43
1:B:205:LEU:HD12	1:B:238:LEU:HD12	2.00	0.43
1:B:86:THR:CG2	1:B:115:LYS:HZ2	2.17	0.43
1:B:47:GLN:O	1:B:51:LEU:HD13	2.17	0.43
1:A:44:LEU:O	1:A:48:ILE:HG13	2.18	0.43
1:B:183:SER:OG	1:B:208:THR:CG2	2.67	0.43
1:B:94:HIS:O	1:B:95:TYR:HB2	2.18	0.43
1:A:96:MET:HE2	1:A:100:LEU:HD21	2.01	0.43
1:B:306:TRP:HA	1:B:307:PRO:HD3	1.69	0.43
1:A:84:VAL:CG2	1:A:91:LEU:HD22	2.48	0.43
1:B:84:VAL:CG2	1:B:91:LEU:HD22	2.49	0.43
1:A:58:ARG:HH12	1:A:62:THR:CG2	2.31	0.43
1:B:222:TYR:CA	2:B:395:HOH:O	2.66	0.43
1:B:113:SER:HB3	1:B:116:PHE:HB2	1.99	0.43
1:A:136:VAL:HG12	1:A:209:VAL:HG22	2.00	0.43
1:B:66:LYS:HD2	1:B:71:LEU:HD11	2.01	0.42
1:B:155:VAL:HG12	1:B:156:HIS:O	2.19	0.42
1:A:37:MET:HE1	1:A:85:ALA:HA	2.00	0.42
1:B:58:ARG:HH12	1:B:62:THR:CG2	2.32	0.42
1:A:124:ASN:HA	1:A:124:ASN:HD22	1.65	0.42
1:A:268:ALA:O	1:A:272:ILE:HD12	2.20	0.42
1:B:132:GLU:HG3	1:B:195:SER:OG	2.20	0.41
1:B:78:CYS:SG	1:B:270:MET:CE	3.08	0.41
1:A:251:PHE:HA	1:A:254:LYS:HB2	2.02	0.41
1:A:163:HIS:O	1:A:164:SER:HB2	2.20	0.41
1:B:194:LYS:HB3	2:B:404:HOH:O	2.19	0.41
1:B:222:TYR:O	1:B:223:LYS:CB	2.61	0.41
1:A:274:ARG:HG2	1:A:274:ARG:O	2.20	0.41
1:A:253:LYS:HB2	1:A:254:LYS:H	1.64	0.41
1:A:66:LYS:HD2	1:A:71:LEU:HD11	2.01	0.41
1:B:247:CYS:HA	1:B:314:LEU:HD12	2.02	0.41
1:A:198:ARG:NE	1:A:223:LYS:HD3	2.24	0.41
1:A:127:GLN:HE22	1:A:153:ASN:HB3	1.84	0.41
1:A:205:LEU:HD12	1:A:238:LEU:HD12	2.02	0.41
1:A:311:ILE:HG22	2:A:348:HOH:O	2.20	0.41
1:A:291:LYS:CE	2:A:384:HOH:O	2.68	0.40
1:B:257:LYS:CB	2:B:383:HOH:O	2.67	0.40
1:B:253:LYS:HB2	1:B:254:LYS:H	1.66	0.40
1:A:271:VAL:O	1:A:274:ARG:HB3	2.20	0.40
1:A:198:ARG:NH2	1:A:223:LYS:HG2	2.33	0.40
1:A:31:TYR:CE1	1:A:306:TRP:HB2	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	280/328 (85%)	257 (92%)	13 (5%)	10 (4%)	5	2
1	B	280/328 (85%)	257 (92%)	14 (5%)	9 (3%)	6	2
All	All	560/656 (85%)	514 (92%)	27 (5%)	19 (3%)	6	2

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	187	ASN
1	A	254	LYS
1	B	64	HIS
1	B	187	ASN
1	B	254	LYS
1	A	164	SER
1	A	195	SER
1	A	253	LYS
1	B	195	SER
1	B	253	LYS
1	B	257	LYS
1	A	66	LYS
1	A	257	LYS
1	B	66	LYS
1	B	164	SER
1	A	256	ASP
1	B	256	ASP
1	A	65	TYR

### 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	267/301 (89%)	241 (90%)	26 (10%)	12	10
1	B	267/301 (89%)	242 (91%)	25 (9%)	13	11
All	All	534/602 (89%)	483 (90%)	51 (10%)	12	11

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	32	TRP
1	A	35	THR
1	A	61	GLU
1	A	64	HIS
1	A	72	GLU
1	A	73	SER
1	A	82	SER
1	A	93	ASP
1	A	101	ILE
1	A	103	ARG
1	A	122	LEU
1	A	133	THR
1	A	146	LEU
1	A	149	LEU
1	A	158	LYS
1	A	165	ILE
1	A	198	ARG
1	A	206	ASP
1	A	208	THR
1	A	213	GLN
1	A	215	ASP
1	A	241	ILE
1	A	249	LEU
1	A	274	ARG
1	A	327	LEU
1	B	27	THR
1	B	32	TRP
1	B	35	THR
1	B	61	GLU
1	B	64	HIS
1	B	72	GLU
1	B	73	SER
1	B	93	ASP
1	B	101	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	103	ARG
1	B	122	LEU
1	B	133	THR
1	B	146	LEU
1	B	149	LEU
1	B	158	LYS
1	B	165	ILE
1	B	206	ASP
1	B	208	THR
1	B	213	GLN
1	B	215	ASP
1	B	241	ILE
1	B	249	LEU
1	B	274	ARG
1	B	291	LYS
1	B	327	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	87	HIS
1	A	108	HIS
1	A	112	ASN
1	A	127	GLN
1	A	179	HIS
1	A	213	GLN
1	B	47	GLN
1	B	87	HIS
1	B	108	HIS
1	B	112	ASN
1	B	127	GLN
1	B	163	HIS
1	B	179	HIS
1	B	213	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	286/328 (87%)	0.62	29 (10%) 7 7	17, 35, 67, 94	0
1	B	286/328 (87%)	0.65	27 (9%) 9 8	18, 36, 66, 92	0
All	All	572/656 (87%)	0.63	56 (9%) 8 7	17, 35, 67, 94	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	TYR	6.8
1	B	65	TYR	5.4
1	B	62	THR	4.8
1	B	66	LYS	4.1
1	B	258	ASN	4.1
1	B	173	ASP	4.0
1	A	66	LYS	4.0
1	B	328	THR	3.7
1	A	328	THR	3.6
1	A	69	VAL	3.6
1	A	71	LEU	3.5
1	B	256	ASP	3.5
1	B	257	LYS	3.4
1	B	98	LYS	3.3
1	A	213	GLN	3.3
1	A	173	ASP	3.3
1	A	130	GLU	3.2
1	A	263	LEU	3.2
1	A	320	MET	3.1
1	A	64	HIS	3.1
1	A	195	SER	3.0
1	A	165	ILE	2.8
1	A	189	THR	2.8
1	B	58	ARG	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	222	TYR	2.7
1	A	51	LEU	2.6
1	A	256	ASP	2.6
1	A	258	ASN	2.6
1	B	194	LYS	2.5
1	B	304	VAL	2.5
1	A	32	TRP	2.5
1	B	71	LEU	2.5
1	A	310	ASP	2.4
1	B	255	PHE	2.4
1	B	61	GLU	2.4
1	A	194	LYS	2.4
1	B	223	LYS	2.3
1	A	193	ILE	2.3
1	B	195	SER	2.3
1	A	302	PRO	2.3
1	B	301	ASN	2.2
1	A	222	TYR	2.2
1	B	261	GLU	2.2
1	A	67	GLU	2.2
1	A	75	LYS	2.2
1	A	188	PHE	2.2
1	B	64	HIS	2.1
1	B	69	VAL	2.1
1	A	254	LYS	2.1
1	A	260	ARG	2.1
1	B	93	ASP	2.1
1	B	297	GLU	2.1
1	B	165	ILE	2.1
1	B	254	LYS	2.1
1	B	283	ASP	2.1
1	A	62	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.