W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:10 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)

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 (i)

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	Percentile Ranks	Value
Rfree		0.235
Clashscore		22
Ramachandran outliers		3.4%
Sidechain outliers		9.6%
RSRZ outliers		9.3%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▐ Percentile relative to X-ray structures of similar resolution
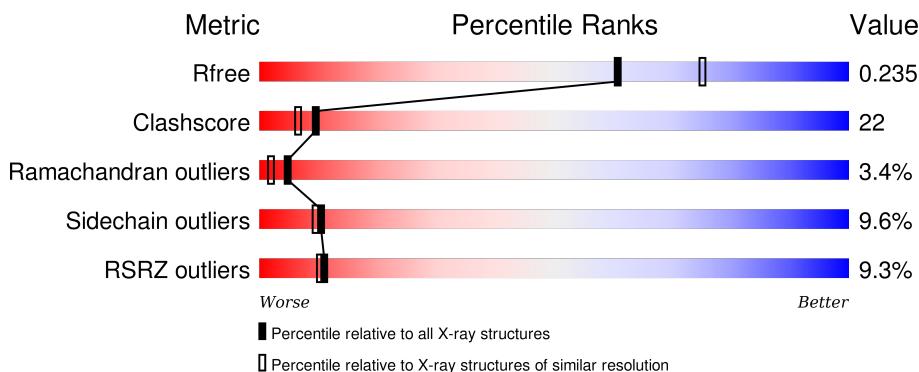
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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 >=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 <=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	328	9% / 47% / 34% / 5% / 13%
1	B	328	7% / 47% / 35% / 5% / 13%

Full wwPDB X-ray Structure Validation Report
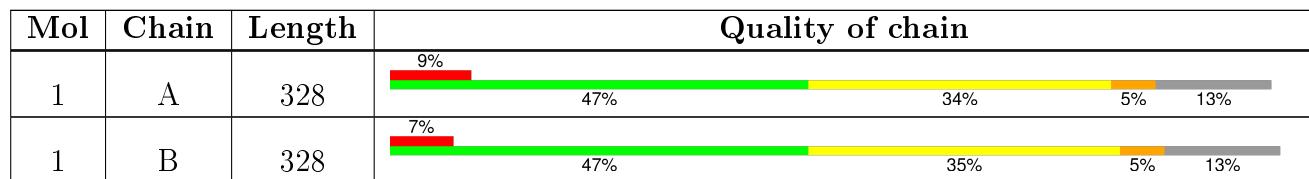
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4813 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 HDA1 complex subunit 3.

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

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 66	O 66	0	0
2	B	83	Total 83	O 83	0	0

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: HDA1 complex subunit 3
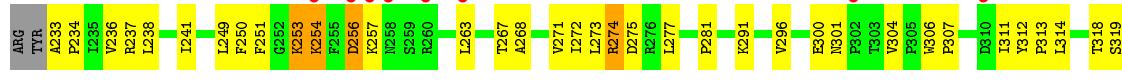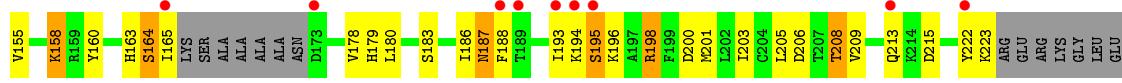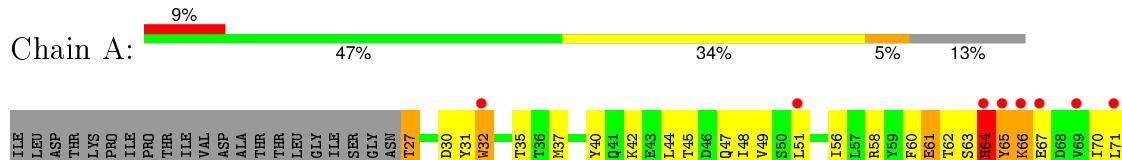
- Molecule 1: HDA1 complex subunit 3
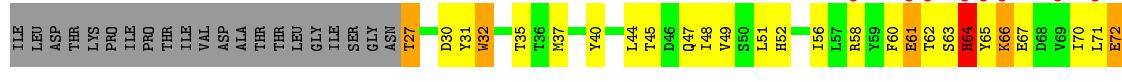
T328 GLU VAL HIS PHE LYS

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	8.87 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.198 , 0.237 0.199 , 0.235	Depositor DCC
R_{free} test set	1673 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 35.3	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[2]	$< |L| > = 0.44$, $< L^2 > = 0.26$	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^2)	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z| > 5$	RMSZ	#$|Z| > 5$
1	A	0.36	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 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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 22.

All (210) 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:B:49:VAL:HA	1:B:77:MET:HE2	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:PHE:HE1	1:A:193:ILE:HD11	1.57	0.69
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	280/328 (85%)	257 (92%)	13 (5%)	10 (4%)	4	2
1	B	280/328 (85%)	257 (92%)	14 (5%)	9 (3%)	5	2
All	All	560/656 (85%)	514 (92%)	27 (5%)	19 (3%)	5	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

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Mol	Chain	Res	Type
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 (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	267/301 (89%)	241 (90%)	26 (10%)	10	9
1	B	267/301 (89%)	242 (91%)	25 (9%)	11	10
All	All	534/602 (89%)	483 (90%)	51 (10%)	10	9

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 (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, 95th 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(Å²)	Q<0.9
1	A	286/328 (87%)	0.54	29 (10%)	9	8	17, 35, 67, 94	0
1	B	286/328 (87%)	0.56	24 (8%)	14	13	18, 36, 66, 92	0
All	All	572/656 (87%)	0.55	53 (9%)	11	10	17, 35, 67, 94	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	TYR	6.7
1	B	65	TYR	5.5
1	B	62	THR	5.0
1	B	66	LYS	4.3
1	A	66	LYS	4.0
1	B	258	ASN	4.0
1	B	173	ASP	3.9
1	A	69	VAL	3.7
1	A	328	THR	3.6
1	A	71	LEU	3.5
1	B	328	THR	3.5
1	A	263	LEU	3.4
1	B	98	LYS	3.4
1	B	256	ASP	3.3
1	A	64	HIS	3.3
1	A	213	GLN	3.3
1	B	257	LYS	3.2
1	A	173	ASP	3.1
1	A	130	GLU	3.1
1	A	320	MET	3.0
1	A	195	SER	2.9
1	A	165	ILE	2.7
1	A	51	LEU	2.7
1	A	189	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	58	ARG	2.6
1	A	256	ASP	2.6
1	A	258	ASN	2.6
1	B	222	TYR	2.6
1	B	194	LYS	2.5
1	A	32	TRP	2.5
1	B	71	LEU	2.5
1	A	194	LYS	2.4
1	A	310	ASP	2.4
1	B	223	LYS	2.4
1	B	61	GLU	2.3
1	B	261	GLU	2.3
1	A	302	PRO	2.2
1	B	255	PHE	2.2
1	A	193	ILE	2.2
1	B	64	HIS	2.2
1	B	69	VAL	2.2
1	B	301	ASN	2.2
1	B	304	VAL	2.2
1	B	195	SER	2.1
1	A	75	LYS	2.1
1	B	297	GLU	2.1
1	A	260	ARG	2.1
1	A	67	GLU	2.1
1	A	222	TYR	2.1
1	A	257	LYS	2.1
1	A	188	PHE	2.1
1	B	93	ASP	2.0
1	A	254	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 (i)

There are no such residues in this entry.