



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:56 PM UTC

PDB ID : 5KDM / pdb\_00005kdm  
Title : Crystal structure of EBV tegument protein BNRF1 in complex with histone chaperone DAXX and histones H3.3-H4  
Authors : Huang, H.; Patel, D.  
Deposited on : 2016-06-08  
Resolution : 3.50 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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

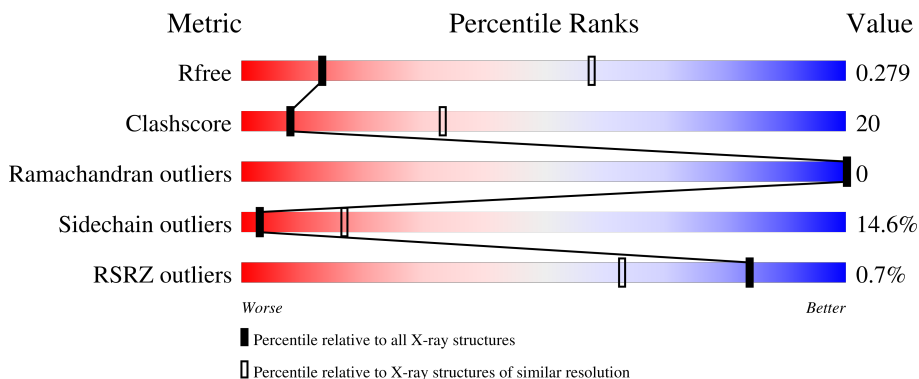
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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))
$R_{free}$	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	135	 3% 39% 28% 6% 27%
2	B	102	 46% 23% 7% 25%
3	C	212	 57% 33% 6% 6%
4	D	219	 3% 44% 30% 7% 18%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4341 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 Histone H3.3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	99	785	495	152	136	2	0	0	0

- Molecule 2 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	77	599	379	116	103	1	0	0	0

- Molecule 3 is a protein called Death domain-associated protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	205	1636	1022	303	305	6	0	0	0

- Molecule 4 is a protein called Major tegument protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	180	1321	851	217	244	9	0	0	0

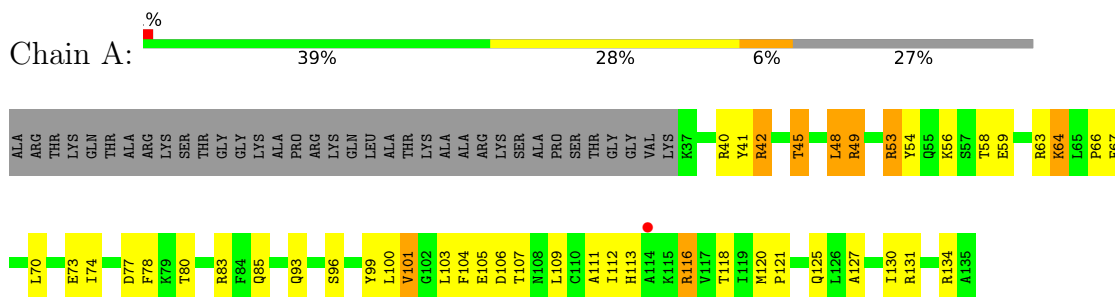
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	587	SER	ARG	conflict	UNP Q1HVJ0

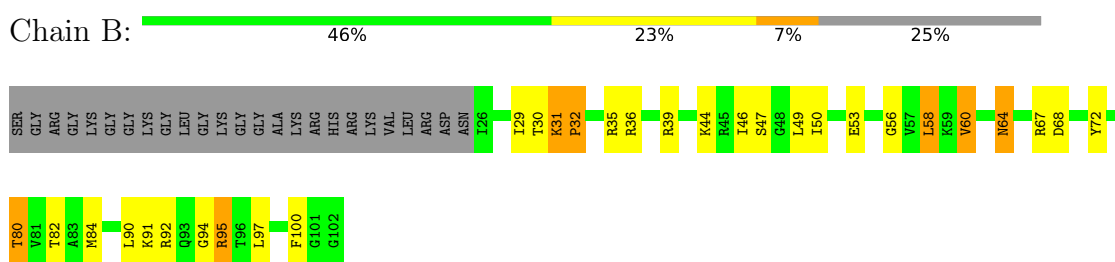
### 3 Residue-property plots [i](#)

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.

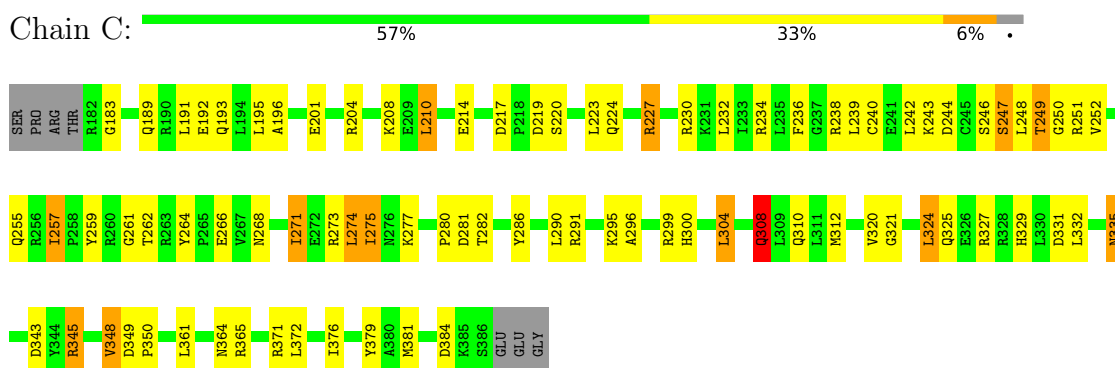
- Molecule 1: Histone H3.3



- Molecule 2: Histone H4



- Molecule 3: Death domain-associated protein 6



- Molecule 4: Major tegument protein





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	161.22Å 161.22Å 117.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.16 – 3.50 48.16 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.16-3.50) 87.0 (48.16-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.64 (at 3.48Å)	Xtrriage
Refinement program	PHENIX dev_1839	Depositor
R, $R_{free}$	0.234 , 0.280 0.236 , 0.279	Depositor DCC
$R_{free}$ test set	1135 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	114.8	Xtrriage
Anisotropy	0.056	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 89.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4341	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	130.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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	0.77	0/796	1.09	3/1072 (0.3%)
2	B	0.69	0/606	1.09	2/813 (0.2%)
3	C	0.70	0/1660	1.15	11/2239 (0.5%)
4	D	0.85	1/1356 (0.1%)	1.31	15/1851 (0.8%)
All	All	0.76	1/4418 (0.0%)	1.18	31/5975 (0.5%)

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
3	C	0	2
4	D	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	445	PRO	CA-C	5.47	1.57	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	568	ASP	N-CA-C	-8.16	98.16	108.45
4	D	489	GLY	CA-C-N	8.09	127.75	119.82
4	D	489	GLY	C-N-CA	8.09	127.75	119.82
3	C	264	TYR	CA-C-N	7.68	127.73	119.28
3	C	264	TYR	C-N-CA	7.68	127.73	119.28
3	C	308	GLN	N-CA-C	-7.43	103.68	112.89
3	C	274	LEU	N-CA-C	-7.41	102.15	112.45
3	C	183	GLY	N-CA-C	-7.40	105.48	114.66
4	D	389	ASP	N-CA-C	7.12	119.50	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	445	PRO	N-CA-C	6.63	118.78	110.70
1	A	113	HIS	N-CA-C	6.34	119.05	109.23
4	D	570	PHE	N-CA-C	6.02	123.62	110.80
4	D	388	TYR	N-CA-C	5.99	120.20	113.02
2	B	94	GLY	N-CA-C	-5.79	102.14	112.22
3	C	262	THR	N-CA-C	-5.72	103.15	110.53
3	C	249	THR	N-CA-C	5.62	118.02	108.02
3	C	371	ARG	N-CA-C	5.56	117.02	111.07
3	C	345	ARG	CA-C-N	5.55	125.17	119.56
3	C	345	ARG	C-N-CA	5.55	125.17	119.56
4	D	513	ARG	CA-C-N	-5.42	115.32	122.85
4	D	513	ARG	C-N-CA	-5.42	115.32	122.85
2	B	60	VAL	N-CA-C	-5.35	105.50	110.53
4	D	579	PRO	CA-C-N	5.21	126.35	119.84
4	D	579	PRO	C-N-CA	5.21	126.35	119.84
4	D	573	PHE	N-CA-C	-5.14	101.73	109.85
4	D	500	PHE	N-CA-C	5.12	119.22	112.92
1	A	130	ILE	N-CA-C	5.11	115.33	110.53
1	A	101	VAL	N-CA-C	-5.09	105.43	110.62
3	C	247	SER	N-CA-C	5.07	121.60	110.80
4	D	505	CYS	N-CA-C	5.06	118.06	109.76
4	D	564	ALA	N-CA-C	5.01	119.47	112.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	246	SER	Peptide
3	C	273	ARG	Peptide
4	D	444	ARG	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	785	0	793	43	0
2	B	599	0	627	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1636	0	1637	68	0
4	D	1321	0	1260	55	0
All	All	4341	0	4317	169	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 20.

All (169) 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)
3:C:308:GLN:HE21	3:C:312:MET:HE2	1.40	0.85
1:A:120:MET:HG2	2:B:47:SER:HB3	1.59	0.83
1:A:40:ARG:HH12	1:A:42:ARG:HH22	1.27	0.80
4:D:469:SER:H	4:D:556:ASP:HB3	1.46	0.80
3:C:201:GLU:OE1	3:C:204:ARG:NH1	2.19	0.76
1:A:106:ASP:OD1	1:A:131:ARG:NH1	2.22	0.72
4:D:386:VAL:HG21	4:D:513:ARG:HH11	1.54	0.72
4:D:562:SER:H	4:D:565:GLU:HG2	1.55	0.70
2:B:82:THR:HG22	2:B:84:MET:H	1.58	0.69
3:C:308:GLN:NE2	3:C:312:MET:HE2	2.08	0.69
3:C:189:GLN:HA	3:C:192:GLU:HG3	1.76	0.67
2:B:72:TYR:OH	2:B:92:ARG:NH2	2.27	0.66
4:D:479:LEU:HD22	4:D:492:MET:HE3	1.76	0.66
4:D:466:LEU:HD21	4:D:551:LEU:HD11	1.78	0.65
3:C:274:LEU:H	3:C:274:LEU:HD23	1.63	0.64
1:A:111:ALA:O	1:A:112:ILE:HD13	1.97	0.64
1:A:66:PRO:HB3	2:B:29:ILE:HG22	1.78	0.64
1:A:111:ALA:C	1:A:112:ILE:HD13	2.23	0.63
1:A:121:PRO:HG2	2:B:49:LEU:HD11	1.79	0.63
1:A:104:PHE:HA	1:A:107:THR:HG22	1.82	0.61
4:D:391:GLY:O	4:D:567:MET:HE3	1.99	0.61
1:A:64:LYS:HB2	3:C:223:LEU:HD21	1.81	0.61
4:D:440:SER:O	4:D:511:THR:HB	2.01	0.61
1:A:53:ARG:HG3	3:C:335:ASN:HB3	1.82	0.61
4:D:388:TYR:CG	4:D:388:TYR:O	2.54	0.60
3:C:295:LYS:HE3	3:C:299:ARG:CZ	2.31	0.60
4:D:390:TYR:CE2	4:D:547:PRO:HA	2.37	0.60
3:C:266:GLU:CD	3:C:266:GLU:H	2.09	0.59
3:C:274:LEU:HG	3:C:275:ILE:N	2.17	0.59
1:A:40:ARG:HH21	3:C:250:GLY:H	1.49	0.59
4:D:394:LEU:HD22	4:D:464:LEU:HD22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:230:ARG:HB3	3:C:234:ARG:HH21	1.68	0.58
1:A:40:ARG:HH21	3:C:250:GLY:N	2.02	0.58
3:C:277:LYS:O	3:C:282:THR:HG21	2.06	0.56
4:D:497:SER:O	4:D:501:LEU:HB3	2.06	0.56
4:D:391:GLY:H	4:D:545:THR:HG23	1.71	0.56
4:D:505:CYS:SG	4:D:507:ASN:HB2	2.46	0.56
3:C:259:TYR:CZ	3:C:261:GLY:HA3	2.41	0.56
4:D:392:HIS:H	4:D:545:THR:HG22	1.70	0.56
3:C:243:LYS:O	3:C:244:ASP:HB2	2.07	0.55
4:D:392:HIS:N	4:D:545:THR:HG22	2.22	0.55
3:C:345:ARG:HB2	3:C:348:VAL:HG23	1.89	0.55
3:C:304:LEU:HD21	3:C:308:GLN:HB3	1.90	0.54
2:B:72:TYR:HE1	3:C:350:PRO:HD2	1.73	0.54
4:D:444:ARG:NH1	4:D:447:GLY:HA3	2.22	0.54
4:D:556:ASP:OD1	4:D:561:VAL:HG23	2.08	0.53
3:C:343:ASP:OD2	4:D:461:LYS:NZ	2.41	0.53
4:D:388:TYR:CD2	4:D:460:PRO:HD2	2.44	0.53
2:B:39:ARG:HH22	2:B:44:LYS:HD2	1.73	0.53
3:C:252:VAL:HG22	3:C:331:ASP:HB2	1.90	0.53
4:D:388:TYR:CE2	4:D:460:PRO:HD2	2.44	0.53
1:A:41:TYR:OH	3:C:192:GLU:OE2	2.27	0.53
4:D:562:SER:N	4:D:565:GLU:HG2	2.22	0.53
4:D:459:VAL:HG21	4:D:464:LEU:HD11	1.91	0.53
1:A:85:GLN:NE2	2:B:82:THR:HG23	2.24	0.52
3:C:296:ALA:O	3:C:300:HIS:HB3	2.10	0.52
2:B:53:GLU:HG3	3:C:379:TYR:CG	2.44	0.52
2:B:29:ILE:HD12	2:B:29:ILE:O	2.09	0.52
4:D:392:HIS:H	4:D:545:THR:CG2	2.23	0.52
3:C:257:ILE:H	3:C:275:ILE:HD12	1.75	0.51
4:D:469:SER:N	4:D:556:ASP:HB3	2.22	0.51
3:C:189:GLN:O	3:C:193:GLN:HG2	2.11	0.51
4:D:443:ALA:HB3	4:D:458:LEU:HD13	1.92	0.51
1:A:45:THR:HB	3:C:196:ALA:HB2	1.93	0.50
1:A:40:ARG:HH12	1:A:42:ARG:NH2	2.03	0.50
1:A:63:ARG:HH22	3:C:230:ARG:HH12	1.60	0.50
2:B:91:LYS:HE2	2:B:100:PHE:O	2.12	0.50
1:A:74:ILE:O	1:A:77:ASP:HB3	2.12	0.50
3:C:280:PRO:O	3:C:281:ASP:HB2	2.10	0.50
1:A:54:TYR:O	1:A:58:THR:HG23	2.11	0.50
1:A:73:GLU:O	1:A:77:ASP:HB2	2.13	0.49
2:B:31:LYS:HG3	2:B:32:PRO:HD3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:SER:HB3	2:B:58:LEU:HD21	1.95	0.49
3:C:257:ILE:HG13	3:C:275:ILE:HG21	1.93	0.49
4:D:528:LEU:O	4:D:532:CYS:HB2	2.11	0.49
4:D:466:LEU:HD21	4:D:551:LEU:CD1	2.43	0.49
3:C:257:ILE:N	3:C:275:ILE:HD12	2.27	0.49
4:D:424:GLN:O	4:D:428:GLU:HG3	2.13	0.49
4:D:392:HIS:CE1	4:D:513:ARG:HB2	2.48	0.48
1:A:109:LEU:HD21	3:C:321:GLY:HA3	1.95	0.48
2:B:39:ARG:O	2:B:39:ARG:HD3	2.13	0.48
4:D:489:GLY:O	4:D:492:MET:HG2	2.13	0.48
2:B:31:LYS:HG3	2:B:32:PRO:CD	2.44	0.48
2:B:32:PRO:HB3	2:B:35:ARG:HH21	1.78	0.48
4:D:388:TYR:HH	4:D:545:THR:HG1	1.62	0.48
1:A:49:ARG:HH11	1:A:49:ARG:HB2	1.79	0.48
2:B:56:GLY:O	2:B:60:VAL:HG23	2.14	0.47
3:C:227:ARG:CZ	3:C:230:ARG:HH21	2.27	0.47
2:B:67:ARG:HD2	3:C:364:ASN:HB3	1.97	0.47
1:A:83:ARG:HB2	2:B:80:THR:HG23	1.96	0.47
2:B:32:PRO:HB3	2:B:35:ARG:NH2	2.30	0.47
3:C:195:LEU:HG	3:C:232:LEU:HD11	1.97	0.47
4:D:451:VAL:HG23	4:D:503:PRO:O	2.15	0.46
4:D:429:LEU:HD21	4:D:534:MET:HE2	1.98	0.46
4:D:562:SER:H	4:D:565:GLU:CG	2.27	0.46
1:A:103:LEU:HD12	1:A:103:LEU:HA	1.75	0.46
1:A:63:ARG:C	1:A:66:PRO:HD2	2.40	0.46
4:D:396:MET:HE3	4:D:509:PHE:CE2	2.50	0.46
3:C:227:ARG:HA	3:C:227:ARG:HD3	1.72	0.46
3:C:249:THR:O	3:C:251:ARG:HG2	2.16	0.46
4:D:425:THR:HG22	4:D:535:ALA:HB1	1.97	0.46
3:C:274:LEU:HG	3:C:275:ILE:HG23	1.97	0.45
1:A:78:PHE:C	1:A:80:THR:H	2.24	0.45
1:A:41:TYR:HE1	3:C:243:LYS:HD3	1.82	0.45
1:A:116:ARG:HD3	2:B:44:LYS:HG3	1.98	0.45
2:B:30:THR:HG22	2:B:32:PRO:N	2.32	0.45
4:D:396:MET:HE2	4:D:507:ASN:CG	2.40	0.45
1:A:41:TYR:CE1	3:C:243:LYS:HD3	2.52	0.45
4:D:396:MET:HE3	4:D:509:PHE:CZ	2.52	0.45
4:D:479:LEU:HD23	4:D:479:LEU:HA	1.72	0.45
4:D:466:LEU:HA	4:D:543:GLY:HA3	1.99	0.44
3:C:277:LYS:HD2	3:C:277:LYS:HA	1.73	0.44
3:C:376:ILE:HD13	3:C:376:ILE:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:388:TYR:OH	4:D:459:VAL:HG13	2.17	0.44
1:A:53:ARG:HG3	3:C:335:ASN:CB	2.48	0.44
2:B:95:ARG:HH11	2:B:95:ARG:HG3	1.82	0.44
3:C:236:PHE:CD1	3:C:236:PHE:C	2.96	0.44
4:D:490:PRO:O	4:D:493:GLN:HB3	2.18	0.44
1:A:64:LYS:HB2	3:C:223:LEU:CD2	2.47	0.44
3:C:291:ARG:O	3:C:295:LYS:HB2	2.18	0.44
4:D:444:ARG:N	4:D:445:PRO:HD3	2.33	0.44
2:B:64:ASN:HA	2:B:67:ARG:HE	1.83	0.44
2:B:39:ARG:NH2	2:B:44:LYS:HD2	2.33	0.43
3:C:201:GLU:OE2	3:C:204:ARG:HD3	2.17	0.43
3:C:304:LEU:CD2	3:C:308:GLN:HB3	2.48	0.43
2:B:97:LEU:HA	2:B:97:LEU:HD12	1.72	0.43
4:D:433:LEU:HD23	4:D:531:ALA:HB2	2.00	0.43
1:A:104:PHE:O	1:A:107:THR:HG22	2.18	0.43
2:B:68:ASP:OD1	3:C:361:LEU:HD22	2.19	0.43
4:D:475:VAL:HG21	4:D:500:PHE:HE1	1.84	0.43
2:B:35:ARG:HH22	2:B:36:ARG:NH2	2.16	0.43
3:C:329:HIS:O	3:C:332:LEU:HB3	2.19	0.43
4:D:384:ASP:HB3	4:D:437:PRO:HB3	2.01	0.43
2:B:72:TYR:CE1	3:C:350:PRO:HD2	2.52	0.43
3:C:243:LYS:HE2	3:C:243:LYS:HB3	1.72	0.43
4:D:569:ASP:O	4:D:570:PHE:HB2	2.18	0.43
1:A:105:GLU:OE1	3:C:325:GLN:HG3	2.19	0.42
3:C:324:LEU:HD12	3:C:324:LEU:HA	1.75	0.42
1:A:48:LEU:HD22	1:A:48:LEU:HA	1.62	0.42
2:B:92:ARG:O	2:B:92:ARG:HG3	2.19	0.42
1:A:125:GLN:HG3	3:C:376:ILE:HG22	2.02	0.42
3:C:257:ILE:HG23	3:C:327:ARG:HH11	1.85	0.42
1:A:67:PHE:CZ	1:A:93:GLN:HA	2.54	0.42
3:C:275:ILE:H	3:C:275:ILE:HG12	1.70	0.42
4:D:388:TYR:O	4:D:388:TYR:CD2	2.72	0.42
1:A:101:VAL:O	1:A:105:GLU:HG3	2.19	0.42
4:D:471:LEU:HD22	4:D:500:PHE:CZ	2.55	0.42
4:D:555:ASN:HB2	4:D:573:PHE:CE1	2.55	0.42
2:B:90:LEU:HD23	2:B:90:LEU:HA	1.83	0.42
3:C:252:VAL:HG13	4:D:569:ASP:HB3	2.01	0.41
4:D:573:PHE:O	4:D:574:PHE:HB3	2.20	0.41
1:A:107:THR:HA	1:A:127:ALA:HB2	2.01	0.41
3:C:220:SER:O	3:C:224:GLN:HG3	2.20	0.41
1:A:56:LYS:O	1:A:59:GLU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:349:ASP:HA	3:C:350:PRO:HD3	1.91	0.41
3:C:210:LEU:HA	3:C:214:GLU:OE1	2.20	0.41
3:C:208:LYS:HD3	3:C:208:LYS:HA	1.77	0.41
3:C:230:ARG:O	3:C:234:ARG:HG2	2.20	0.41
3:C:259:TYR:HD2	3:C:271:ILE:HG21	1.86	0.41
1:A:70:LEU:O	1:A:74:ILE:HG13	2.20	0.41
3:C:223:LEU:HA	3:C:223:LEU:HD23	1.65	0.41
4:D:439:ILE:HG23	4:D:510:ILE:HG23	2.03	0.41
4:D:444:ARG:HH11	4:D:447:GLY:HA3	1.85	0.41
3:C:259:TYR:O	3:C:268:ASN:HB3	2.21	0.41
1:A:99:TYR:HE1	1:A:134:ARG:HA	1.86	0.40
3:C:286:TYR:OH	3:C:310:GLN:HG2	2.21	0.40
1:A:107:THR:HA	1:A:127:ALA:CB	2.52	0.40
3:C:320:VAL:O	3:C:324:LEU:HB2	2.21	0.40
4:D:523:THR:H	4:D:526:GLN:HB2	1.85	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	97/135 (72%)	92 (95%)	5 (5%)	0	100	100
2	B	75/102 (74%)	69 (92%)	6 (8%)	0	100	100
3	C	203/212 (96%)	194 (96%)	9 (4%)	0	100	100
4	D	174/219 (80%)	160 (92%)	14 (8%)	0	100	100
All	All	549/668 (82%)	515 (94%)	34 (6%)	0	100	100

There are no Ramachandran outliers to report.

### 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	77/109 (71%)	68 (88%)	9 (12%)	5	24
2	B	59/78 (76%)	51 (86%)	8 (14%)	3	19
3	C	172/187 (92%)	147 (86%)	25 (14%)	3	17
4	D	137/178 (77%)	114 (83%)	23 (17%)	2	13
All	All	445/552 (81%)	380 (85%)	65 (15%)	3	17

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	45	THR
1	A	48	LEU
1	A	49	ARG
1	A	53	ARG
1	A	64	LYS
1	A	100	LEU
1	A	116	ARG
1	A	118	THR
2	B	31	LYS
2	B	32	PRO
2	B	46	ILE
2	B	50	ILE
2	B	58	LEU
2	B	64	ASN
2	B	80	THR
2	B	95	ARG
3	C	191	LEU
3	C	210	LEU
3	C	217	ASP
3	C	219	ASP
3	C	227	ARG
3	C	238	ARG
3	C	239	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	C	240	CYS
3	C	242	LEU
3	C	247	SER
3	C	248	LEU
3	C	255	GLN
3	C	257	ILE
3	C	271	ILE
3	C	275	ILE
3	C	290	LEU
3	C	304	LEU
3	C	308	GLN
3	C	324	LEU
3	C	335	ASN
3	C	348	VAL
3	C	365	ARG
3	C	372	LEU
3	C	381	MET
3	C	384	ASP
4	D	387	ARG
4	D	400	PHE
4	D	425	THR
4	D	442	TYR
4	D	444	ARG
4	D	454	HIS
4	D	455	LEU
4	D	465	LEU
4	D	466	LEU
4	D	469	SER
4	D	473	ASP
4	D	488	THR
4	D	498	SER
4	D	501	LEU
4	D	505	CYS
4	D	520	ASN
4	D	523	THR
4	D	530	ARG
4	D	532	CYS
4	D	546	VAL
4	D	551	LEU
4	D	554	VAL
4	D	567	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
3	C	255	GLN
3	C	308	GLN
3	C	314	GLN
3	C	325	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 oligosaccharides 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	99/135 (73%)	-0.18	1 (1%) 79 56	103, 121, 164, 193	0
2	B	77/102 (75%)	-0.22	0 100 100	105, 122, 149, 178	0
3	C	205/212 (96%)	-0.14	0 100 100	102, 129, 192, 206	0
4	D	180/219 (82%)	-0.04	3 (1%) 69 43	96, 121, 160, 179	0
All	All	561/668 (83%)	-0.12	4 (0%) 84 63	96, 124, 178, 206	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	488	THR	2.8
4	D	400	PHE	2.2
4	D	480	GLY	2.2
1	A	114	ALA	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.