



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:41 AM UTC

PDB ID : 5HEK / pdb_00005hek
Title : crystal structure of M1.HpyAVI
Authors : Ma, B.; Zhang, H.; Liu, W.
Deposited on : 2016-01-06
Resolution : 3.00 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

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	:	4-5-2 with Phenix2.0
Xtriage (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

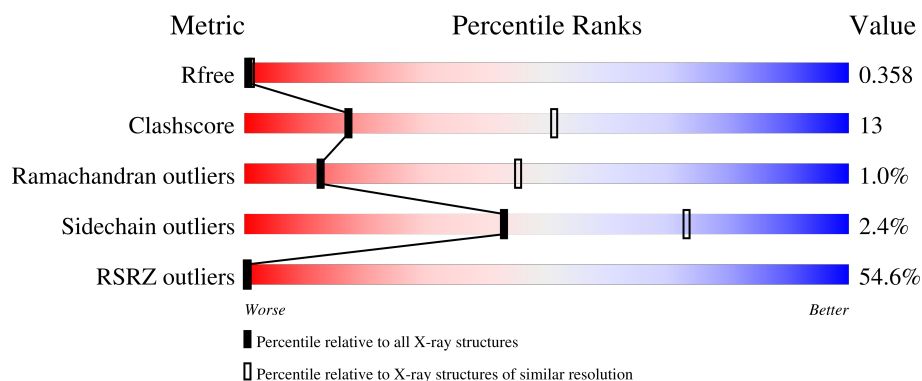
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 ≥ 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	240	45% 59% 19% • • 18%
1	B	240	41% 49% 25% • • 23%
1	C	240	48% 54% 19% • 23%
1	D	240	35% 51% 21% • 26%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6166 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 Adenine specific DNA methyltransferase (DpnA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1638	1074	274	282	8			
1	B	185	Total	C	N	O	S	0	0	0
			1532	1004	254	266	8			
1	C	185	Total	C	N	O	S	0	0	0
			1533	1004	257	265	7			
1	D	177	Total	C	N	O	S	0	0	0
			1463	962	243	251	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	233	LEU	-	expression tag	UNP O24891
A	234	GLU	-	expression tag	UNP O24891
A	235	HIS	-	expression tag	UNP O24891
A	236	HIS	-	expression tag	UNP O24891
A	237	HIS	-	expression tag	UNP O24891
A	238	HIS	-	expression tag	UNP O24891
A	239	HIS	-	expression tag	UNP O24891
A	240	HIS	-	expression tag	UNP O24891
B	233	LEU	-	expression tag	UNP O24891
B	234	GLU	-	expression tag	UNP O24891
B	235	HIS	-	expression tag	UNP O24891
B	236	HIS	-	expression tag	UNP O24891
B	237	HIS	-	expression tag	UNP O24891
B	238	HIS	-	expression tag	UNP O24891
B	239	HIS	-	expression tag	UNP O24891
B	240	HIS	-	expression tag	UNP O24891
C	233	LEU	-	expression tag	UNP O24891
C	234	GLU	-	expression tag	UNP O24891
C	235	HIS	-	expression tag	UNP O24891
C	236	HIS	-	expression tag	UNP O24891
C	237	HIS	-	expression tag	UNP O24891

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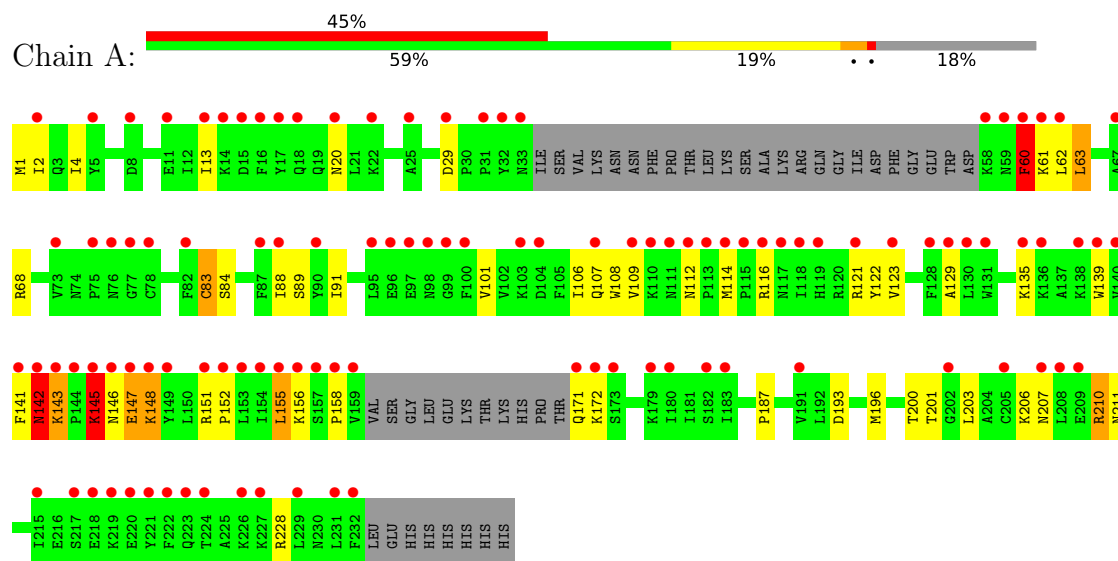
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Chain	Residue	Modelled	Actual	Comment	Reference
C	238	HIS	-	expression tag	UNP O24891
C	239	HIS	-	expression tag	UNP O24891
C	240	HIS	-	expression tag	UNP O24891
D	233	LEU	-	expression tag	UNP O24891
D	234	GLU	-	expression tag	UNP O24891
D	235	HIS	-	expression tag	UNP O24891
D	236	HIS	-	expression tag	UNP O24891
D	237	HIS	-	expression tag	UNP O24891
D	238	HIS	-	expression tag	UNP O24891
D	239	HIS	-	expression tag	UNP O24891
D	240	HIS	-	expression tag	UNP O24891

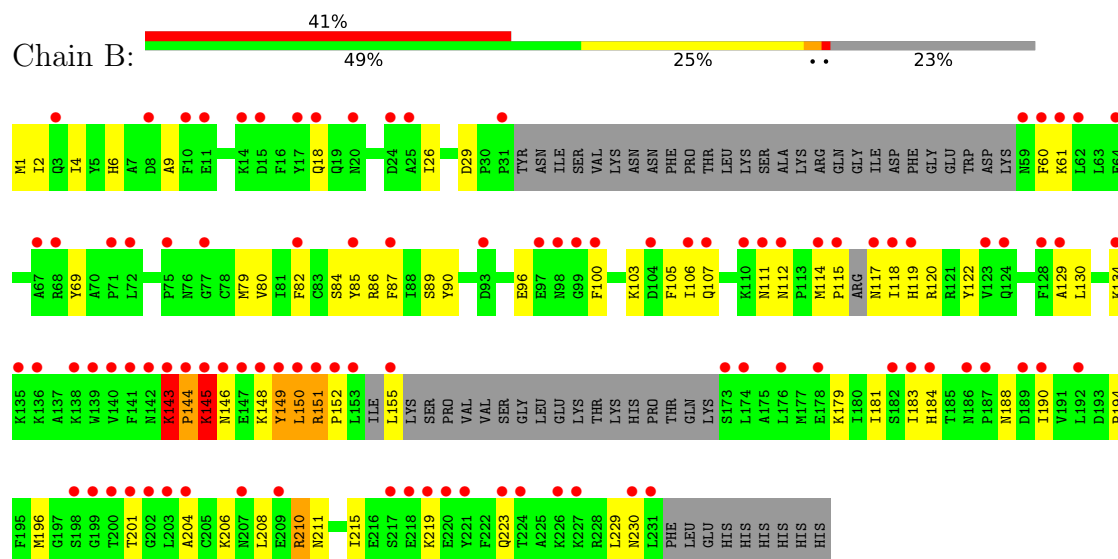
3 Residue-property plots

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.

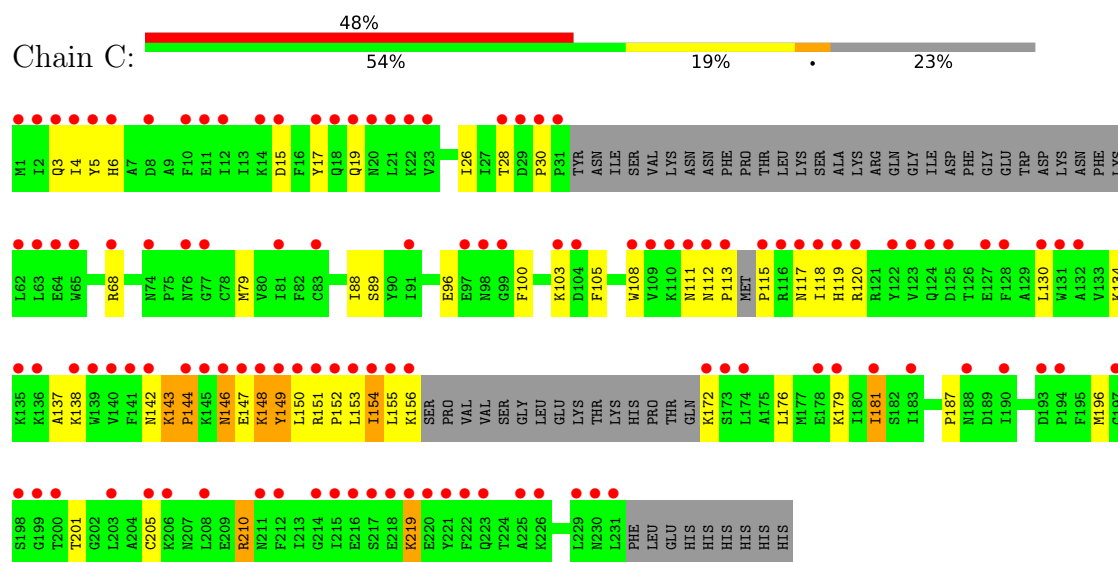
- Molecule 1: Adenine specific DNA methyltransferase (DpnA)



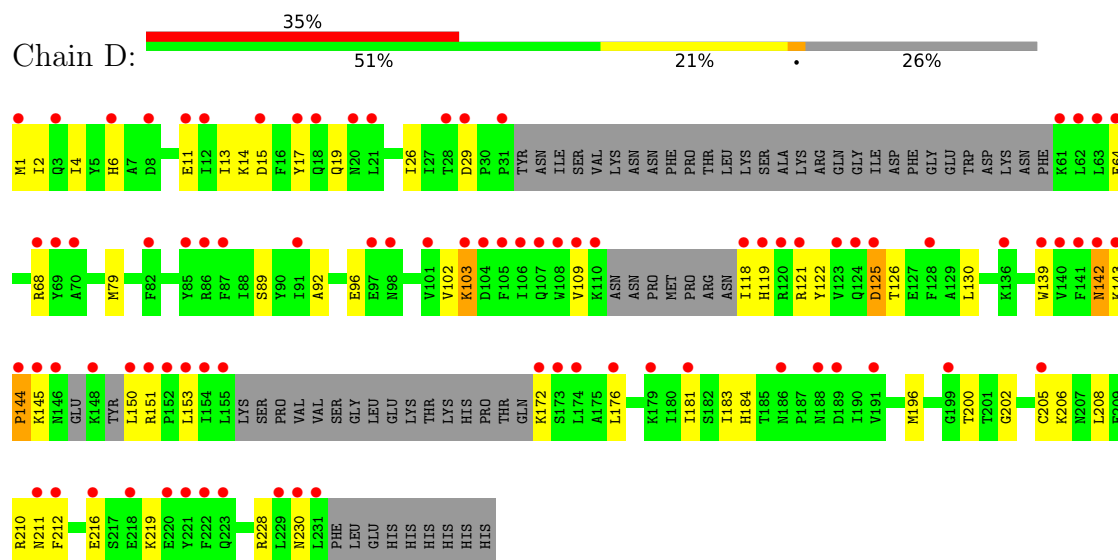
- Molecule 1: Adenine specific DNA methyltransferase (DpnA)



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• Molecule 1: Adenine specific DNA methyltransferase (DpnA)



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	69.72Å 69.72Å 532.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.09 – 3.00 49.09 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.09-3.00) 98.9 (49.09-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.251 , 0.308 0.302 , 0.358	Depositor DCC
R_{free} test set	1275 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.69	EDS
Total number of atoms	6166	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.51	0/1680	1.08	16/2268 (0.7%)
1	B	0.47	0/1569	0.99	10/2117 (0.5%)
1	C	0.47	0/1570	1.00	7/2118 (0.3%)
1	D	0.47	0/1495	0.97	3/2012 (0.1%)
All	All	0.48	0/6314	1.01	36/8515 (0.4%)

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
1	A	0	4

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	143	LYS	CA-C-N	7.93	129.75	119.84
1	C	143	LYS	C-N-CA	7.93	129.75	119.84
1	A	210	ARG	N-CA-C	7.89	122.62	112.92
1	A	29	ASP	CA-C-N	7.88	128.50	120.38
1	A	29	ASP	C-N-CA	7.88	128.50	120.38
1	A	148	LYS	N-CA-C	7.60	122.03	109.95
1	C	153	LEU	N-CA-C	7.43	120.75	109.23
1	B	145	LYS	N-CA-C	7.40	121.22	111.75
1	A	63	LEU	N-CA-C	-7.32	104.37	113.38
1	D	151	ARG	CA-C-N	7.13	127.45	119.32
1	D	151	ARG	C-N-CA	7.13	127.45	119.32
1	D	230	ASN	N-CA-C	7.10	121.46	111.52
1	A	151	ARG	CA-C-N	6.97	127.27	119.32
1	A	151	ARG	C-N-CA	6.97	127.27	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ASP	CA-C-N	6.92	126.89	119.28
1	A	193	ASP	C-N-CA	6.92	126.89	119.28
1	B	143	LYS	CA-C-N	6.79	128.33	119.84
1	B	143	LYS	C-N-CA	6.79	128.33	119.84
1	C	210	ARG	N-CA-C	6.77	121.24	112.92
1	A	114	MET	C-N-CD	-6.75	105.76	120.60
1	C	201	THR	N-CA-C	-6.34	103.89	111.69
1	A	114	MET	N-CA-C	6.05	121.75	113.16
1	B	190	ILE	N-CA-C	5.72	116.34	107.99
1	B	149	TYR	N-CA-C	5.72	122.98	110.80
1	B	210	ARG	N-CA-C	5.70	119.92	112.92
1	B	201	THR	N-CA-C	-5.50	104.93	111.69
1	B	151	ARG	CA-C-N	5.50	125.59	119.32
1	B	151	ARG	C-N-CA	5.50	125.59	119.32
1	B	150	LEU	N-CA-CB	-5.34	108.76	114.10
1	C	148	LYS	CA-C-N	5.17	131.42	121.54
1	C	148	LYS	C-N-CA	5.17	131.42	121.54
1	A	83	CYS	N-CA-C	5.15	115.33	108.38
1	A	142	ASN	N-CA-CB	-5.14	105.83	114.27
1	A	60	PHE	CA-C-N	5.10	130.88	121.70
1	A	60	PHE	C-N-CA	5.10	130.88	121.70
1	A	201	THR	N-CA-C	-5.06	105.47	111.69

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	142	ASN	Peptide
1	A	145	LYS	Peptide
1	A	147	GLU	Peptide
1	A	60	PHE	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	1638	0	1662	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1532	0	1544	52	0
1	C	1533	0	1559	46	0
1	D	1463	0	1496	39	0
All	All	6166	0	6261	157	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 13.

All (157) 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:229:LEU:O	1:B:230:ASN:ND2	2.14	0.81
1:C:146:ASN:OD1	1:C:147:GLU:N	2.14	0.79
1:B:29:ASP:HB2	1:B:82:PHE:HD2	1.46	0.79
1:B:119:HIS:HA	1:D:143:LYS:HE3	1.66	0.76
1:C:6:HIS:CE1	1:C:219:LYS:HD2	2.21	0.76
1:C:156:LYS:H	1:C:156:LYS:HD2	1.50	0.76
1:A:83:CYS:SG	1:A:88:ILE:HG22	2.25	0.75
1:D:26:ILE:HD12	1:D:79:MET:HE2	1.68	0.74
1:B:89:SER:HB2	1:D:89:SER:HB2	1.69	0.73
1:B:149:TYR:HB3	1:D:122:TYR:HD1	1.52	0.73
1:C:111:ASN:ND2	1:C:155:LEU:O	2.22	0.73
1:A:171:GLN:HB2	1:A:172:LYS:HG2	1.73	0.70
1:B:117:ASN:N	1:B:118:ILE:HA	2.07	0.70
1:C:26:ILE:HD12	1:C:79:MET:HE2	1.72	0.70
1:D:118:ILE:HD12	1:D:121:ARG:HD3	1.77	0.67
1:A:2:ILE:HD11	1:A:206:LYS:HB2	1.77	0.67
1:A:89:SER:HB2	1:C:89:SER:HB2	1.79	0.65
1:A:61:LYS:N	1:A:62:LEU:HA	2.11	0.65
1:C:147:GLU:HB3	1:C:148:LYS:HG3	1.78	0.64
1:B:144:PRO:HD2	1:B:149:TYR:OH	1.97	0.64
1:B:181:ILE:HD12	1:B:204:ALA:HB3	1.80	0.64
1:D:109:VAL:HG13	1:D:125:ASP:HB3	1.80	0.63
1:B:151:ARG:NH1	1:D:126:THR:OG1	2.26	0.63
1:A:145:LYS:HB2	1:A:146:ASN:HA	1.81	0.63
1:A:60:PHE:HB3	1:A:61:LYS:HB2	1.81	0.63
1:B:26:ILE:HD12	1:B:79:MET:HE2	1.82	0.62
1:A:121:ARG:NH2	1:C:103:LYS:O	2.32	0.62
1:C:143:LYS:HD2	1:C:147:GLU:HA	1.81	0.62
1:C:152:PRO:HB3	1:C:179:LYS:HD2	1.82	0.60
1:A:4:ILE:HB	1:A:196:MET:HE1	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:MET:SD	1:B:115:PRO:HD2	2.41	0.60
1:D:200:THR:OG1	1:D:228:ARG:NH1	2.32	0.59
1:A:146:ASN:N	1:A:147:GLU:HA	2.18	0.59
1:C:113:PRO:HG2	1:C:115:PRO:HD3	1.85	0.58
1:A:123:VAL:HG11	1:C:148:LYS:HD2	1.86	0.57
1:A:101:VAL:HG23	1:A:135:LYS:HA	1.86	0.56
1:D:14:LYS:HA	1:D:17:TYR:HD2	1.71	0.56
1:D:145:LYS:N	1:D:145:LYS:HD3	2.21	0.55
1:D:4:ILE:HB	1:D:196:MET:HE1	1.86	0.55
1:B:29:ASP:HB2	1:B:82:PHE:CD2	2.35	0.55
1:A:147:GLU:OE1	1:A:147:GLU:N	2.40	0.54
1:B:149:TYR:HB3	1:D:122:TYR:CD1	2.39	0.54
1:A:116:ARG:HG2	1:A:116:ARG:HH11	1.73	0.54
1:C:105:PHE:CZ	1:C:150:LEU:HD21	2.43	0.53
1:C:134:LYS:HB3	1:C:137:ALA:HB2	1.89	0.53
1:A:61:LYS:HA	1:A:62:LEU:HD23	1.89	0.53
1:A:139:TRP:H	1:C:120:ARG:HH22	1.56	0.53
1:A:141:PHE:O	1:A:142:ASN:HB3	2.09	0.53
1:C:4:ILE:HB	1:C:196:MET:HE1	1.88	0.53
1:C:112:ASN:ND2	1:C:156:LYS:O	2.42	0.53
1:C:181:ILE:HG22	1:C:210:ARG:HD3	1.90	0.53
1:A:145:LYS:CB	1:A:146:ASN:HA	2.39	0.53
1:A:108:TRP:CE3	1:A:155:LEU:HD13	2.44	0.52
1:C:17:TYR:OH	1:C:68:ARG:O	2.21	0.52
1:D:29:ASP:OD2	1:D:172:LYS:NZ	2.35	0.51
1:C:3:GLN:OE1	1:C:5:TYR:OH	2.16	0.51
1:A:112:ASN:HB2	1:A:158:PRO:HB3	1.92	0.51
1:B:103:LYS:O	1:D:121:ARG:NH2	2.44	0.51
1:B:179:LYS:O	1:B:183:ILE:HG12	2.10	0.51
1:B:84:SER:HB3	1:B:87:PHE:HD2	1.77	0.50
1:B:143:LYS:HB2	1:B:149:TYR:HE2	1.76	0.50
1:C:117:ASN:OD1	1:C:117:ASN:N	2.44	0.50
1:A:13:ILE:HG12	1:A:68:ARG:HG3	1.93	0.50
1:B:2:ILE:HD11	1:B:206:LYS:HB2	1.93	0.50
1:C:26:ILE:HB	1:C:79:MET:HG2	1.94	0.50
1:C:108:TRP:CZ3	1:C:155:LEU:HD21	2.46	0.50
1:A:146:ASN:OD1	1:A:148:LYS:HB3	2.11	0.50
1:C:108:TRP:HZ3	1:C:155:LEU:HD21	1.77	0.50
1:B:111:ASN:ND2	1:B:155:LEU:O	2.33	0.50
1:B:4:ILE:HB	1:B:196:MET:HE1	1.94	0.50
1:B:107:GLN:O	1:B:152:PRO:HD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ILE:CG2	1:C:210:ARG:HD3	2.43	0.49
1:D:142:ASN:HB3	1:D:183:ILE:O	2.13	0.49
1:A:109:VAL:HG21	1:C:151:ARG:HH12	1.77	0.49
1:A:20:ASN:HB2	1:B:18:GLN:NE2	2.27	0.48
1:B:150:LEU:HD23	1:B:151:ARG:HH22	1.78	0.48
1:A:147:GLU:HB3	1:C:118:ILE:HG21	1.93	0.48
1:D:64:GLU:OE2	1:D:68:ARG:NH1	2.43	0.48
1:C:105:PHE:CE2	1:C:150:LEU:HD21	2.48	0.48
1:B:208:LEU:HB3	1:B:210:ARG:NH1	2.29	0.48
1:C:6:HIS:HE1	1:C:219:LYS:HD2	1.77	0.48
1:C:181:ILE:HD12	1:C:205:CYS:SG	2.54	0.48
1:B:82:PHE:CD1	1:B:129:ALA:HB2	2.49	0.47
1:A:122:TYR:HD1	1:C:149:TYR:O	1.97	0.47
1:B:112:ASN:OD1	1:B:112:ASN:N	2.46	0.47
1:B:208:LEU:HB3	1:B:210:ARG:HH11	1.80	0.47
1:C:108:TRP:CD2	1:C:176:LEU:HD22	2.50	0.47
1:D:103:LYS:HD2	1:D:103:LYS:HA	1.74	0.47
1:B:148:LYS:O	1:B:149:TYR:CG	2.68	0.47
1:B:219:LYS:HE3	1:B:223:GLN:OE1	2.14	0.46
1:A:63:LEU:HD21	1:A:91:ILE:HA	1.96	0.46
1:D:1:MET:O	1:D:211:ASN:HA	2.15	0.46
1:A:203:LEU:O	1:A:207:ASN:ND2	2.49	0.46
1:B:85:TYR:CZ	1:B:86:ARG:HD3	2.50	0.46
1:A:107:GLN:O	1:A:152:PRO:HD2	2.16	0.46
1:A:109:VAL:HG21	1:C:151:ARG:NH1	2.31	0.45
1:A:139:TRP:N	1:C:120:ARG:HH22	2.15	0.45
1:C:88:ILE:HG13	1:C:130:LEU:HG	1.98	0.45
1:D:208:LEU:HB3	1:D:210:ARG:HH11	1.81	0.45
1:A:60:PHE:C	1:A:63:LEU:H	2.24	0.45
1:C:28:THR:HG23	1:C:30:PRO:HD3	1.99	0.45
1:D:142:ASN:HD22	1:D:142:ASN:C	2.24	0.45
1:D:13:ILE:HG13	1:D:17:TYR:CE2	2.52	0.45
1:B:9:ALA:O	1:B:69:TYR:OH	2.26	0.45
1:B:84:SER:HB3	1:B:87:PHE:CD2	2.52	0.45
1:B:60:PHE:CD2	1:B:61:LYS:HG2	2.52	0.44
1:D:92:ALA:HB2	1:D:130:LEU:HD11	1.98	0.44
1:B:194:PRO:HA	1:B:215:ILE:CD1	2.47	0.44
1:B:96:GLU:HA	1:B:100:PHE:O	2.17	0.44
1:B:150:LEU:HD22	1:D:125:ASP:H	1.83	0.44
1:B:120:ARG:HH22	1:D:139:TRP:C	2.26	0.44
1:B:151:ARG:NH2	1:D:125:ASP:OD2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LYS:HE2	1:C:118:ILE:HG22	1.99	0.44
1:A:145:LYS:HB2	1:A:145:LYS:HE2	1.63	0.44
1:D:2:ILE:HD11	1:D:206:LYS:HB2	2.00	0.44
1:B:6:HIS:CE1	1:B:219:LYS:HD3	2.54	0.43
1:B:106:ILE:HG13	1:B:129:ALA:HB3	2.00	0.43
1:D:15:ASP:O	1:D:19:GLN:HG3	2.19	0.43
1:A:200:THR:HG1	1:A:228:ARG:HH12	1.61	0.43
1:D:153:LEU:HD12	1:D:176:LEU:HB2	2.01	0.43
1:C:144:PRO:HG2	1:C:146:ASN:HB3	2.01	0.43
1:A:155:LEU:HD23	1:A:156:LYS:N	2.34	0.43
1:B:145:LYS:HG2	1:B:146:ASN:N	2.30	0.42
1:D:202:GLY:HA2	1:D:212:PHE:CG	2.54	0.42
1:A:146:ASN:H	1:A:147:GLU:HA	1.83	0.42
1:C:143:LYS:HA	1:C:144:PRO:HD2	1.70	0.42
1:A:143:LYS:HD2	1:C:119:HIS:HA	2.02	0.42
1:B:87:PHE:O	1:B:90:TYR:N	2.51	0.42
1:B:184:HIS:CE1	1:D:122:TYR:HH	2.34	0.42
1:C:187:PRO:O	1:C:210:ARG:HA	2.19	0.42
1:A:1:MET:O	1:A:211:ASN:HA	2.19	0.42
1:A:84:SER:O	1:A:88:ILE:HG23	2.20	0.42
1:A:60:PHE:HB3	1:A:61:LYS:CB	2.49	0.42
1:A:106:ILE:HG13	1:A:129:ALA:HB3	2.02	0.42
1:A:155:LEU:CG	1:A:156:LYS:H	2.33	0.42
1:B:122:TYR:OH	1:D:184:HIS:NE2	2.49	0.41
1:D:17:TYR:OH	1:D:68:ARG:O	2.27	0.41
1:B:143:LYS:HZ1	1:D:119:HIS:HA	1.86	0.41
1:C:15:ASP:O	1:C:19:GLN:HG3	2.20	0.41
1:D:96:GLU:HG3	1:D:102:VAL:HG23	2.02	0.41
1:C:108:TRP:HZ3	1:C:155:LEU:HD11	1.86	0.41
1:D:143:LYS:HA	1:D:144:PRO:HD3	1.94	0.41
1:B:1:MET:O	1:B:211:ASN:HA	2.20	0.41
1:B:188:ASN:OD1	1:B:211:ASN:ND2	2.53	0.41
1:C:148:LYS:HE3	1:C:148:LYS:HB2	1.93	0.41
1:B:105:PHE:HZ	1:D:126:THR:HB	1.86	0.41
1:C:96:GLU:HA	1:C:100:PHE:O	2.20	0.41
1:D:26:ILE:HB	1:D:79:MET:HG2	2.02	0.41
1:A:20:ASN:HB2	1:B:18:GLN:CD	2.46	0.40
1:D:181:ILE:HD13	1:D:205:CYS:SG	2.61	0.40
1:B:80:VAL:HA	1:B:130:LEU:O	2.21	0.40
1:B:106:ILE:CG1	1:B:129:ALA:HB3	2.50	0.40
1:C:154:ILE:H	1:C:154:ILE:HG13	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ILE:HD12	1:B:204:ALA:CB	2.50	0.40
1:A:171:GLN:HA	1:A:172:LYS:HA	1.92	0.40
1:A:187:PRO:HD3	1:A:210:ARG:NH2	2.36	0.40
1:D:6:HIS:HD2	1:D:216:GLU:O	2.04	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	191/240 (80%)	169 (88%)	20 (10%)	2 (1%)	12	45
1	B	176/240 (73%)	155 (88%)	20 (11%)	1 (1%)	21	56
1	C	177/240 (74%)	159 (90%)	15 (8%)	3 (2%)	7	32
1	D	166/240 (69%)	152 (92%)	13 (8%)	1 (1%)	21	56
All	All	710/960 (74%)	635 (89%)	68 (10%)	7 (1%)	12	45

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	149	TYR
1	A	155	LEU
1	C	144	PRO
1	D	144	PRO
1	B	144	PRO
1	C	146	ASN
1	A	143	LYS

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	179/218 (82%)	178 (99%)	1 (1%)	78	88
1	B	167/218 (77%)	164 (98%)	3 (2%)	51	77
1	C	167/218 (77%)	161 (96%)	6 (4%)	31	65
1	D	159/218 (73%)	153 (96%)	6 (4%)	29	63
All	All	672/872 (77%)	656 (98%)	16 (2%)	43	73

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	LYS
1	B	134	LYS
1	B	143	LYS
1	B	145	LYS
1	C	138	LYS
1	C	142	ASN
1	C	154	ILE
1	C	172	LYS
1	C	181	ILE
1	C	219	LYS
1	D	11	GLU
1	D	103	LYS
1	D	125	ASP
1	D	142	ASN
1	D	150	LEU
1	D	219	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	HIS
1	B	142	ASN
1	B	223	GLN

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Mol	Chain	Res	Type
1	C	6	HIS
1	C	112	ASN
1	C	119	HIS
1	D	142	ASN

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

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, 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(Å ²)	Q<0.9
1	A	197/240 (82%)	2.34	108 (54%) 0 0	33, 56, 99, 142	0
1	B	185/240 (77%)	2.29	98 (52%) 0 0	33, 56, 93, 140	0
1	C	185/240 (77%)	2.52	116 (62%) 0 0	37, 61, 103, 145	0
1	D	177/240 (73%)	2.06	84 (47%) 0 0	36, 59, 90, 108	0
All	All	744/960 (77%)	2.31	406 (54%) 0 0	33, 58, 99, 145	0

All (406) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	146	ASN	7.0
1	A	33	ASN	6.8
1	B	115	PRO	6.7
1	C	153	LEU	6.5
1	B	117	ASN	6.2
1	B	149	TYR	6.1
1	A	62	LEU	6.0
1	C	155	LEU	5.9
1	A	148	LYS	5.7
1	C	110	LYS	5.6
1	B	153	LEU	5.5
1	A	117	ASN	5.5
1	C	156	LYS	5.5
1	C	199	GLY	5.4
1	A	115	PRO	5.4
1	A	32	TYR	5.3
1	C	117	ASN	5.3
1	C	188	ASN	5.3
1	A	157	SER	5.3
1	A	154	ILE	5.3
1	C	113	PRO	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	3	GLN	5.2
1	D	20	ASN	5.2
1	C	109	VAL	5.1
1	B	60	PHE	5.1
1	B	31	PRO	5.1
1	C	231	LEU	5.0
1	B	141	PHE	5.0
1	A	147	GLU	5.0
1	C	223	GLN	5.0
1	A	114	MET	4.9
1	A	59	ASN	4.9
1	C	149	TYR	4.9
1	D	155	LEU	4.9
1	B	218	GLU	4.8
1	C	115	PRO	4.8
1	C	104	ASP	4.8
1	D	110	LYS	4.8
1	C	217	SER	4.8
1	B	146	ASN	4.7
1	B	111	ASN	4.7
1	C	118	ILE	4.6
1	D	125	ASP	4.6
1	A	116	ARG	4.6
1	B	231	LEU	4.6
1	B	151	ARG	4.6
1	D	154	ILE	4.5
1	A	149	TYR	4.4
1	D	118	ILE	4.4
1	C	154	ILE	4.4
1	C	119	HIS	4.4
1	C	112	ASN	4.4
1	A	17	TYR	4.4
1	B	143	LYS	4.3
1	D	153	LEU	4.2
1	B	114	MET	4.2
1	B	112	ASN	4.2
1	B	142	ASN	4.2
1	C	31	PRO	4.2
1	B	119	HIS	4.2
1	B	62	LEU	4.1
1	B	128	PHE	4.1
1	A	158	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	159	VAL	4.1
1	A	18	GLN	4.1
1	C	148	LYS	4.0
1	A	173	SER	4.0
1	D	104	ASP	4.0
1	D	124	GLN	4.0
1	C	124	GLN	4.0
1	A	60	PHE	4.0
1	A	142	ASN	4.0
1	B	147	GLU	3.9
1	C	147	GLU	3.9
1	A	145	LYS	3.9
1	C	220	GLU	3.9
1	C	152	PRO	3.9
1	A	110	LYS	3.9
1	C	145	LYS	3.9
1	B	11	GLU	3.9
1	C	4	ILE	3.8
1	C	128	PHE	3.8
1	D	231	LEU	3.8
1	C	142	ASN	3.8
1	C	146	ASN	3.8
1	A	58	LYS	3.8
1	A	25	ALA	3.8
1	D	119	HIS	3.8
1	A	220	GLU	3.8
1	B	18	GLN	3.7
1	D	18	GLN	3.7
1	C	97	GLU	3.7
1	D	62	LEU	3.7
1	B	140	VAL	3.7
1	A	103	LYS	3.7
1	A	155	LEU	3.6
1	C	138	LYS	3.6
1	D	64	GLU	3.6
1	B	17	TYR	3.6
1	D	221	TYR	3.6
1	A	223	GLN	3.6
1	A	151	ARG	3.6
1	A	221	TYR	3.6
1	C	198	SER	3.6
1	C	150	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	143	LYS	3.5
1	B	118	ILE	3.5
1	A	61	LYS	3.5
1	C	108	TRP	3.5
1	B	104	ASP	3.5
1	A	171	GLN	3.5
1	C	140	VAL	3.5
1	B	59	ASN	3.5
1	C	98	ASN	3.5
1	B	189	ASP	3.5
1	A	218	GLU	3.4
1	A	98	ASN	3.4
1	B	155	LEU	3.4
1	D	223	GLN	3.4
1	B	135	LYS	3.4
1	D	11	GLU	3.4
1	D	97	GLU	3.4
1	D	107	GLN	3.4
1	B	220	GLU	3.4
1	D	128	PHE	3.4
1	C	221	TYR	3.4
1	C	1	MET	3.4
1	D	105	PHE	3.4
1	C	103	LYS	3.4
1	C	111	ASN	3.4
1	D	146	ASN	3.4
1	A	141	PHE	3.3
1	B	227	LYS	3.3
1	C	6	HIS	3.3
1	C	218	GLU	3.3
1	B	124	GLN	3.3
1	B	87	PHE	3.3
1	A	123	VAL	3.3
1	B	3	GLN	3.2
1	C	172	LYS	3.2
1	C	17	TYR	3.2
1	C	219	LYS	3.2
1	D	172	LYS	3.2
1	D	142	ASN	3.2
1	A	156	LYS	3.2
1	A	172	LYS	3.2
1	C	226	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	11	GLU	3.2
1	A	222	PHE	3.2
1	C	123	VAL	3.2
1	D	145	LYS	3.1
1	C	197	GLY	3.1
1	B	209	GLU	3.1
1	A	87	PHE	3.1
1	C	29	ASP	3.1
1	B	178	GLU	3.1
1	A	31	PRO	3.1
1	B	20	ASN	3.1
1	D	148	LYS	3.1
1	A	208	LEU	3.1
1	B	8	ASP	3.1
1	C	125	ASP	3.1
1	C	5	TYR	3.1
1	C	2	ILE	3.1
1	C	179	LYS	3.1
1	C	131	TRP	3.1
1	A	104	ASP	3.1
1	A	113	PRO	3.1
1	B	182	SER	3.1
1	D	140	VAL	3.1
1	D	17	TYR	3.1
1	D	21	LEU	3.0
1	D	109	VAL	3.0
1	A	88	ILE	3.0
1	B	173	SER	3.0
1	B	24	ASP	3.0
1	A	227	LYS	3.0
1	C	19	GLN	3.0
1	C	20	ASN	3.0
1	A	96	GLU	3.0
1	A	153	LEU	3.0
1	A	78	CYS	3.0
1	D	63	LEU	2.9
1	B	14	LYS	2.9
1	C	116	ARG	2.9
1	A	138	LYS	2.9
1	B	219	LYS	2.9
1	A	207	ASN	2.9
1	A	128	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	182	SER	2.9
1	D	121	ARG	2.9
1	B	186	ASN	2.9
1	B	77	GLY	2.9
1	A	2	ILE	2.9
1	B	82	PHE	2.9
1	C	22	LYS	2.9
1	D	218	GLU	2.8
1	C	203	LEU	2.8
1	B	71	PRO	2.8
1	C	28	THR	2.8
1	D	15	ASP	2.8
1	C	135	LYS	2.8
1	D	141	PHE	2.8
1	B	68	ARG	2.8
1	B	187	PRO	2.8
1	D	123	VAL	2.8
1	A	118	ILE	2.8
1	C	215	ILE	2.8
1	B	144	PRO	2.8
1	D	103	LYS	2.8
1	A	8	ASP	2.8
1	B	190	ILE	2.8
1	D	12	ILE	2.8
1	D	108	TRP	2.8
1	A	5	TYR	2.8
1	B	221	TYR	2.8
1	C	14	LYS	2.8
1	D	152	PRO	2.8
1	B	98	ASN	2.7
1	D	188	ASN	2.7
1	B	226	LYS	2.7
1	B	10	PHE	2.7
1	B	134	LYS	2.7
1	D	144	PRO	2.7
1	A	232	PHE	2.7
1	C	141	PHE	2.7
1	C	178	GLU	2.7
1	A	217	SER	2.7
1	D	176	LEU	2.7
1	B	100	PHE	2.7
1	B	97	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	22	LYS	2.7
1	C	200	THR	2.7
1	A	131	TRP	2.7
1	D	230	ASN	2.7
1	D	151	ARG	2.6
1	A	179	LYS	2.6
1	A	139	TRP	2.6
1	A	75	PRO	2.6
1	B	61	LYS	2.6
1	D	1	MET	2.6
1	D	31	PRO	2.6
1	D	179	LYS	2.6
1	B	99	GLY	2.6
1	B	204	ALA	2.6
1	A	100	PHE	2.6
1	A	144	PRO	2.6
1	D	8	ASP	2.6
1	C	127	GLU	2.6
1	C	21	LEU	2.6
1	B	110	LYS	2.6
1	C	30	PRO	2.6
1	C	193	ASP	2.6
1	A	20	ASN	2.6
1	C	11	GLU	2.6
1	A	119	HIS	2.6
1	B	198	SER	2.6
1	C	144	PRO	2.6
1	B	192	LEU	2.6
1	C	216	GLU	2.6
1	A	140	VAL	2.6
1	B	148	LYS	2.6
1	A	202	GLY	2.5
1	A	226	LYS	2.5
1	C	212	PHE	2.5
1	A	231	LEU	2.5
1	D	229	LEU	2.5
1	A	97	GLU	2.5
1	D	186	ASN	2.5
1	A	180	ILE	2.5
1	C	181	ILE	2.5
1	B	200	THR	2.5
1	A	82	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	151	ARG	2.5
1	C	10	PHE	2.5
1	D	28	THR	2.5
1	C	174	LEU	2.5
1	D	199	GLY	2.5
1	B	217	SER	2.5
1	D	61	LYS	2.5
1	D	143	LYS	2.5
1	A	95	LEU	2.5
1	A	77	GLY	2.5
1	B	107	GLN	2.5
1	C	132	ALA	2.4
1	B	139	TRP	2.4
1	B	152	PRO	2.4
1	B	199	GLY	2.4
1	C	18	GLN	2.4
1	D	173	SER	2.4
1	B	145	LYS	2.4
1	D	98	ASN	2.4
1	A	215	ILE	2.4
1	D	106	ILE	2.4
1	A	135	LYS	2.4
1	B	174	LEU	2.4
1	B	230	ASN	2.4
1	C	211	ASN	2.4
1	D	29	ASP	2.4
1	A	129	ALA	2.4
1	A	183	ILE	2.4
1	D	68	ARG	2.4
1	B	201	THR	2.3
1	A	14	LYS	2.3
1	B	106	ILE	2.3
1	C	8	ASP	2.3
1	A	16	PHE	2.3
1	C	229	LEU	2.3
1	B	123	VAL	2.3
1	D	191	VAL	2.3
1	B	67	ALA	2.3
1	B	129	ALA	2.3
1	C	122	TYR	2.3
1	B	15	ASP	2.3
1	C	15	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	173	SER	2.3
1	D	181	ILE	2.3
1	B	25	ALA	2.3
1	C	225	ALA	2.3
1	D	69	TYR	2.3
1	B	183	ILE	2.3
1	C	130	LEU	2.3
1	A	107	GLN	2.3
1	D	189	ASP	2.3
1	A	219	LYS	2.3
1	A	121	ARG	2.3
1	A	191	VAL	2.3
1	C	64	GLU	2.3
1	C	81	ILE	2.3
1	C	77	GLY	2.3
1	D	150	LEU	2.3
1	A	136	LYS	2.3
1	D	211	ASN	2.3
1	A	109	VAL	2.3
1	B	64	GLU	2.2
1	B	184	HIS	2.2
1	D	87	PHE	2.2
1	B	136	LYS	2.2
1	B	223	GLN	2.2
1	A	205	CYS	2.2
1	D	220	GLU	2.2
1	C	190	ILE	2.2
1	A	224	THR	2.2
1	D	136	LYS	2.2
1	C	68	ARG	2.2
1	D	205	CYS	2.2
1	C	62	LEU	2.2
1	D	174	LEU	2.2
1	C	65	TRP	2.2
1	D	82	PHE	2.2
1	B	224	THR	2.2
1	C	183	ILE	2.2
1	A	111	ASN	2.2
1	A	209	GLU	2.2
1	A	99	GLY	2.2
1	B	202	GLY	2.2
1	C	214	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	29	ASP	2.2
1	B	138	LYS	2.2
1	D	120	ARG	2.2
1	D	70	ALA	2.2
1	A	152	PRO	2.2
1	D	6	HIS	2.2
1	A	73	VAL	2.1
1	A	229	LEU	2.1
1	B	72	LEU	2.1
1	C	208	LEU	2.1
1	D	3	GLN	2.1
1	C	74	ASN	2.1
1	C	222	PHE	2.1
1	A	15	ASP	2.1
1	C	23	VAL	2.1
1	C	205	CYS	2.1
1	A	90	TYR	2.1
1	D	85	TYR	2.1
1	C	120	ARG	2.1
1	C	194	PRO	2.1
1	D	216	GLU	2.1
1	C	230	ASN	2.1
1	A	130	LEU	2.1
1	B	93	ASP	2.1
1	C	206	LYS	2.1
1	C	63	LEU	2.1
1	A	112	ASN	2.1
1	B	207	ASN	2.1
1	B	176	LEU	2.1
1	B	203	LEU	2.1
1	D	91	ILE	2.1
1	C	83	CYS	2.1
1	B	75	PRO	2.1
1	D	212	PHE	2.1
1	D	222	PHE	2.1
1	A	13	ILE	2.0
1	A	76	ASN	2.0
1	B	150	LEU	2.0
1	C	12	ILE	2.0
1	C	139	TRP	2.0
1	A	67	ALA	2.0
1	C	136	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	76	ASN	2.0
1	D	139	TRP	2.0
1	B	85	TYR	2.0
1	C	99	GLY	2.0
1	D	86	ARG	2.0
1	D	101	VAL	2.0
1	C	91	ILE	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 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.