Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 07:52 PM EDT

PDB ID	:	3K26
Title	:	Complex structure of EED and trimethylated H3K4
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Deposited on	:	2009-09-29
Resolution	:	1.58 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 (i) 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 (i)) were used in the production of this report:

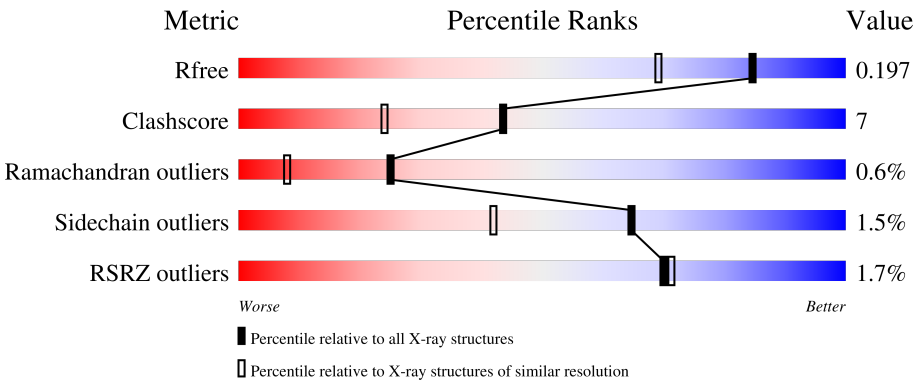
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.58 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}	130704	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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 <=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	366	% 83% 13% • • •
2	B	12	8% 8% 8% 83%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3315 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 Polycomb protein EED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	360	2925	1851	512	541	21	0	1	0

- Molecule 2 is a protein called HISTONE PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	2	21	14	4	3	0	0	0

- Molecule 3 is water.

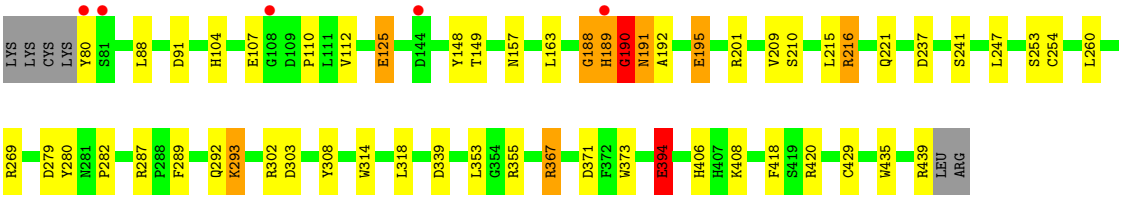
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	367	367	367	0	0
3	B	2	2	2	0	0

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.

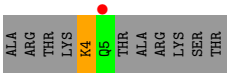
• Molecule 1: Polycomb protein EED

Chain A:



• Molecule 2: HISTONE PEPTIDE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.92Å 85.31Å 91.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.81 – 1.58 19.81 – 1.58	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.81-1.58) 97.5 (19.81-1.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.162 , 0.197 0.164 , 0.197	Depositor DCC
R_{free} test set	3057 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	12.3	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3315	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: M3L

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	1.84	28/3000 (0.9%)	1.53	29/4064 (0.7%)
2	B	1.04	0/9	0.91	0/12
All	All	1.83	28/3009 (0.9%)	1.53	29/4076 (0.7%)

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	1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195[A]	GLU	CD-OE2	36.30	1.65	1.25
1	A	195[B]	GLU	CD-OE2	36.30	1.65	1.25
1	A	195[A]	GLU	CD-OE1	-16.73	1.07	1.25
1	A	195[B]	GLU	CD-OE1	-16.73	1.07	1.25
1	A	195[A]	GLU	CB-CG	-12.47	1.28	1.52
1	A	195[B]	GLU	CB-CG	-12.47	1.28	1.52
1	A	195[A]	GLU	C-N	8.27	1.53	1.34
1	A	195[B]	GLU	C-N	8.27	1.53	1.34
1	A	394	GLU	CD-OE2	8.19	1.34	1.25
1	A	125	GLU	CB-CG	-7.41	1.38	1.52
1	A	190	GLY	N-CA	6.64	1.56	1.46
1	A	280	TYR	CE2-CZ	6.62	1.47	1.38
1	A	107	GLU	CG-CD	6.13	1.61	1.51
1	A	289	PHE	CG-CD2	6.09	1.47	1.38
1	A	429	CYS	CB-SG	-6.07	1.72	1.82
1	A	373	TRP	CE3-CZ3	5.92	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195[A]	GLU	CA-CB	-5.69	1.41	1.53
1	A	195[B]	GLU	CA-CB	-5.69	1.41	1.53
1	A	418	PHE	CD1-CE1	5.51	1.50	1.39
1	A	195[A]	GLU	N-CA	5.47	1.57	1.46
1	A	195[B]	GLU	N-CA	5.47	1.57	1.46
1	A	435	TRP	CE3-CZ3	5.44	1.47	1.38
1	A	149	THR	CA-CB	5.38	1.67	1.53
1	A	420	ARG	CG-CD	-5.26	1.38	1.51
1	A	91	ASP	CB-CG	5.11	1.62	1.51
1	A	308	TYR	CD2-CE2	5.09	1.47	1.39
1	A	192	ALA	N-CA	5.07	1.56	1.46
1	A	314	TRP	CZ3-CH2	5.04	1.48	1.40

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	195[A]	GLU	OE1-CD-OE2	-24.51	93.89	123.30
1	A	195[B]	GLU	OE1-CD-OE2	-24.51	93.89	123.30
1	A	195[A]	GLU	CG-CD-OE1	22.39	163.08	118.30
1	A	195[B]	GLU	CG-CD-OE1	22.39	163.08	118.30
1	A	195[A]	GLU	CA-C-O	10.28	141.69	120.10
1	A	195[B]	GLU	CA-C-O	10.28	141.69	120.10
1	A	339	ASP	CB-CG-OD2	8.89	126.30	118.30
1	A	420	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	A	195[A]	GLU	N-CA-C	-7.84	89.84	111.00
1	A	195[B]	GLU	N-CA-C	-7.84	89.84	111.00
1	A	371	ASP	CB-CG-OD2	7.77	125.29	118.30
1	A	195[A]	GLU	CG-CD-OE2	-7.64	103.02	118.30
1	A	195[B]	GLU	CG-CD-OE2	-7.64	103.02	118.30
1	A	195[A]	GLU	CA-CB-CG	-7.62	96.63	113.40
1	A	195[B]	GLU	CA-CB-CG	-7.62	96.63	113.40
1	A	216	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	353	LEU	CA-CB-CG	-6.79	99.68	115.30
1	A	195[A]	GLU	CA-C-N	-6.37	103.19	117.20
1	A	195[B]	GLU	CA-C-N	-6.37	103.19	117.20
1	A	355	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	237	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	A	318	LEU	CB-CG-CD1	-5.88	101.00	111.00
1	A	191	ASN	N-CA-CB	-5.79	100.17	110.60
1	A	163	LEU	CB-CG-CD2	-5.64	101.40	111.00
1	A	293	LYS	CD-CE-NZ	-5.56	98.91	111.70
1	A	287	ARG	NE-CZ-NH2	-5.50	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	420	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	367	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	308	TYR	CB-CG-CD2	-5.09	117.95	121.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	189	HIS	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	2925	0	2831	38	0
2	B	21	0	28	2	0
3	A	367	0	0	16	1
3	B	2	0	0	1	0
All	All	3315	0	2859	39	1

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 7.

All (39) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195[A]:GLU:OE2	1:A:195[A]:GLU:CD	1.65	1.30
1:A:189:HIS:CD2	3:A:714:HOH:O	2.12	1.03
1:A:303:ASP:HB3	3:A:717:HOH:O	1.63	0.99
1:A:303:ASP:CB	3:A:717:HOH:O	2.18	0.92
1:A:394:GLU:HG3	3:A:24:HOH:O	1.76	0.85
1:A:269:ARG:HE	1:A:292:GLN:HE21	1.24	0.85
1:A:190:GLY:HA3	3:A:530:HOH:O	1.78	0.84
1:A:189:HIS:O	1:A:191:ASN:ND2	2.10	0.84
1:A:303:ASP:CG	3:A:717:HOH:O	2.16	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:HIS:C	1:A:191:ASN:H	1.80	0.83
1:A:406:HIS:HD2	1:A:408:LYS:H	1.27	0.82
1:A:367:ARG:HD3	3:A:675:HOH:O	1.80	0.80
1:A:279:ASP:HB3	3:A:725:HOH:O	1.82	0.78
1:A:104:HIS:HD2	3:A:727:HOH:O	1.68	0.76
1:A:195[A]:GLU:OE2	1:A:195[A]:GLU:OE1	2.03	0.74
1:A:279:ASP:CB	3:A:725:HOH:O	2.34	0.74
1:A:201:ARG:NH2	1:A:247:LEU:HD22	2.11	0.65
1:A:188:GLY:HA3	1:A:216:ARG:NH2	2.11	0.64
1:A:406:HIS:CD2	1:A:408:LYS:H	2.13	0.62
1:A:80:TYR:HB3	3:A:702:HOH:O	2.01	0.61
1:A:110:PRO:HB2	1:A:125:GLU:HG2	1.81	0.61
1:A:195[A]:GLU:OE2	1:A:195[A]:GLU:CG	2.51	0.58
1:A:302:ARG:NH1	3:A:630:HOH:O	2.36	0.57
1:A:189:HIS:CE1	1:A:216:ARG:HD2	2.40	0.57
1:A:190:GLY:CA	3:A:530:HOH:O	2.45	0.57
1:A:195[B]:GLU:HB3	1:A:209:VAL:HG22	1.88	0.55
1:A:269:ARG:HE	1:A:292:GLN:NE2	1.99	0.52
1:A:189:HIS:C	1:A:191:ASN:N	2.58	0.50
1:A:189:HIS:CE1	1:A:210:SER:HB2	2.49	0.48
1:A:279:ASP:CG	3:A:725:HOH:O	2.51	0.48
1:A:157:ASN:HD21	1:A:221:GLN:HE22	1.62	0.46
1:A:215:LEU:HD21	1:A:253:SER:HB3	1.98	0.44
1:A:195[B]:GLU:OE2	1:A:195[B]:GLU:HA	2.18	0.44
1:A:190:GLY:N	3:A:530:HOH:O	2.50	0.44
1:A:148:TYR:CD1	2:B:4:M3L:HM21	2.53	0.44
2:B:4:M3L:HM12	3:B:368:HOH:O	2.18	0.42
1:A:112:VAL:HG22	1:A:125:GLU:HG3	2.01	0.41
1:A:241:SER:HB3	1:A:254:CYS:SG	2.61	0.41
1:A:282:PRO:O	3:A:655:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:488:HOH:O	3:A:655:HOH:O[4_555]	1.89	0.31

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	359/366 (98%)	344 (96%)	13 (4%)	2 (1%)	25 8

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	GLY
1	A	188	GLY

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	324/329 (98%)	319 (98%)	5 (2%)	65 42
2	B	1/9 (11%)	1 (100%)	0	100 100
All	All	325/338 (96%)	320 (98%)	5 (2%)	65 42

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	LEU
1	A	260	LEU
1	A	293	LYS
1	A	394	GLU
1	A	439	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	GLN
1	A	104	HIS
1	A	157	ASN
1	A	194	ASN
1	A	283	ASN
1	A	292	GLN
1	A	295	HIS
1	A	374	GLN
1	A	406	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	M3L	B	4	2	10,11,12	1.30	1 (10%)	9,14,16	1.27	1 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	M3L	B	4	2	-	6/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	M3L	CA-N	3.12	1.56	1.48

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	4	M3L	CM2-NZ-CE	-2.03	101.85	109.91

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4	M3L	N-CA-CB-CG
2	B	4	M3L	C-CA-CB-CG
2	B	4	M3L	CD-CE-NZ-CM2
2	B	4	M3L	CD-CE-NZ-CM3
2	B	4	M3L	CD-CE-NZ-CM1
2	B	4	M3L	CG-CD-CE-NZ

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	M3L	2	0

5.5 Carbohydrates (i)

There are no monosaccharides 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(Å^2)	Q<0.9
1	A	360/366 (98%)	-0.42	5 (1%) 75 77	6, 12, 26, 54	0
2	B	1/12 (8%)	4.22	1 (100%) 0 0	49, 49, 49, 49	0
All	All	361/378 (95%)	-0.41	6 (1%) 70 71	6, 12, 26, 54	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	TYR	9.2
1	A	81	SER	5.3
2	B	5	GLN	4.2
1	A	189	HIS	3.1
1	A	108	GLY	2.7
1	A	144	ASP	2.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	M3L	B	4	12/13	0.66	0.20	33,38,43,43	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.