wwPDB X-ray Structure Validation Summary Report (i)

May 13, 2020 – 08:03 pm BST

PDB ID	:	3QBR
Title	:	BakBH3 in complex with sjA
Authors	:	Lee, E.F.; Clarke, O.B.; Fairlie, W.D.; Colman, P.M.; Evangelista, M.; Feng, Z.; Speed, T.P.; Tchoubrieva, E.; Strasser, A.; Kalinna, B.
Deposited on	:	2011-01-13
Resolution	:	2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (1)) were used in the production of this report:

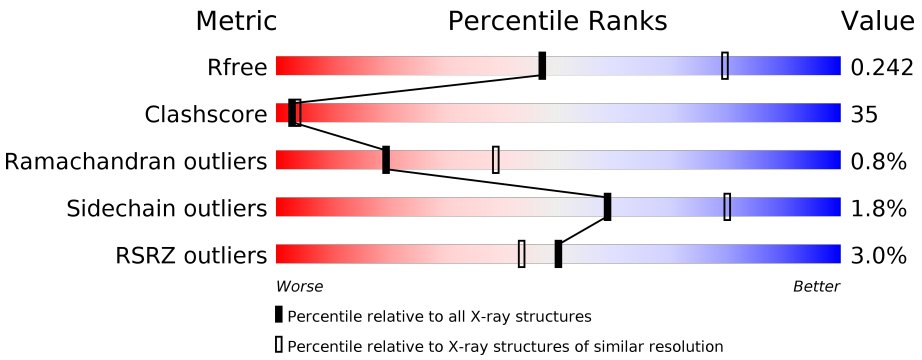
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	179	% 53% 36% • 9%
1	X	179	3% 48% 40% • 10%
2	B	34	6% 35% 35% 29%
2	Y	34	3% 44% 24% 32%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NHE	X	170	-	X	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3129 atoms, of which 10 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 SJCHGC06286 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	163	1307	835	219	249	4	0	0	0
1	X	161	1285	823	215	243	4	0	0	0

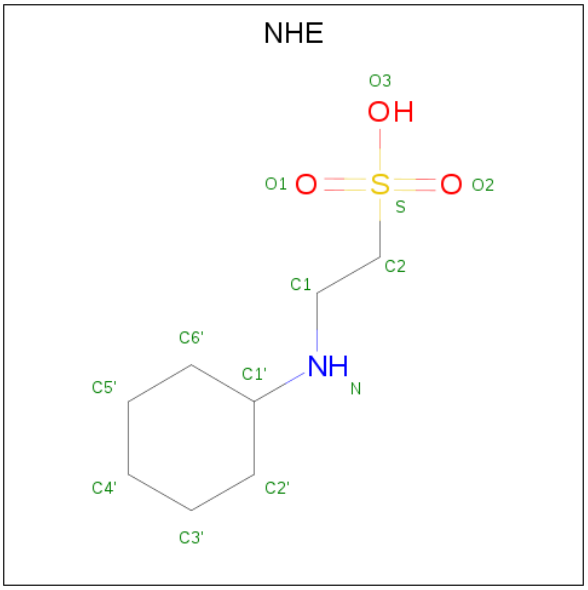
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	HIS	-	EXPRESSION TAG	UNP Q5BWX6
A	-8	HIS	-	EXPRESSION TAG	UNP Q5BWX6
A	-7	HIS	-	EXPRESSION TAG	UNP Q5BWX6
A	-6	HIS	-	EXPRESSION TAG	UNP Q5BWX6
A	-5	HIS	-	EXPRESSION TAG	UNP Q5BWX6
A	-4	HIS	-	EXPRESSION TAG	UNP Q5BWX6
A	-3	SER	-	EXPRESSION TAG	UNP Q5BWX6
A	-2	GLN	-	EXPRESSION TAG	UNP Q5BWX6
A	-1	ASP	-	EXPRESSION TAG	UNP Q5BWX6
A	0	PRO	-	EXPRESSION TAG	UNP Q5BWX6
X	-9	HIS	-	EXPRESSION TAG	UNP Q5BWX6
X	-8	HIS	-	EXPRESSION TAG	UNP Q5BWX6
X	-7	HIS	-	EXPRESSION TAG	UNP Q5BWX6
X	-6	HIS	-	EXPRESSION TAG	UNP Q5BWX6
X	-5	HIS	-	EXPRESSION TAG	UNP Q5BWX6
X	-4	HIS	-	EXPRESSION TAG	UNP Q5BWX6
X	-3	SER	-	EXPRESSION TAG	UNP Q5BWX6
X	-2	GLN	-	EXPRESSION TAG	UNP Q5BWX6
X	-1	ASP	-	EXPRESSION TAG	UNP Q5BWX6
X	0	PRO	-	EXPRESSION TAG	UNP Q5BWX6

- Molecule 2 is a protein called Bcl-2 homologous antagonist/killer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	24	187	111	36	39	1	0	0	0
			Total	C	N	O	S			
2	Y	23	181	108	35	37	1	0	0	0

- Molecule 3 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (three-letter code: NHE) (formula: $C_8H_{17}NO_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
3	X	1	23	8	10	1	3	1	0	0

- Molecule 4 is water.

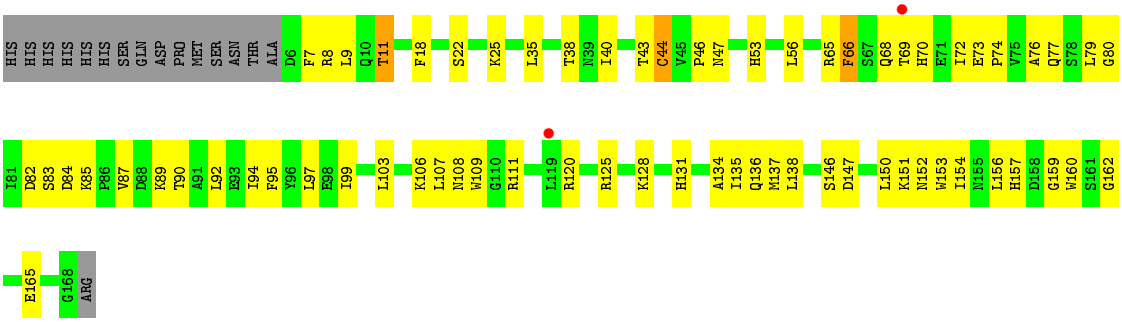
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	64	64	64	0	0
			Total	O		
4	B	8	8	8	0	0
			Total	O		
4	X	61	61	61	0	0
			Total	O		
4	Y	13	13	13	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

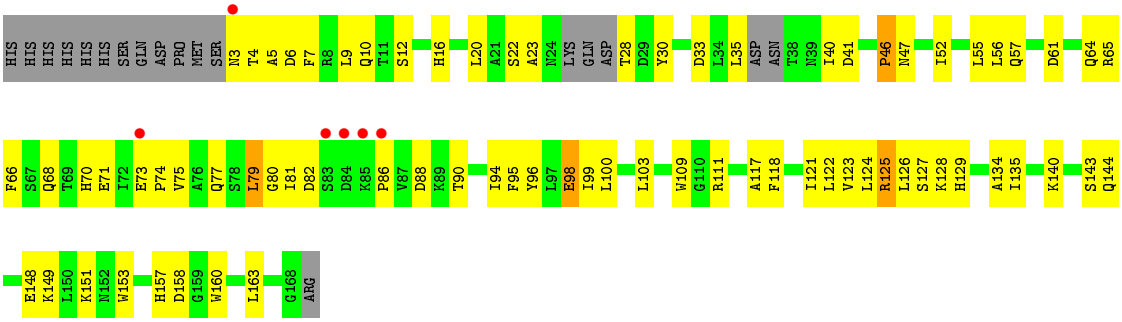
- Molecule 1: SJCHGC06286 protein

Chain A:



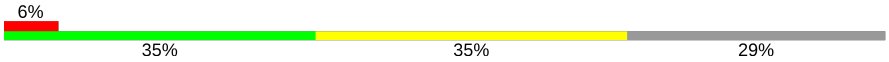
- Molecule 1: SJCHGC06286 protein

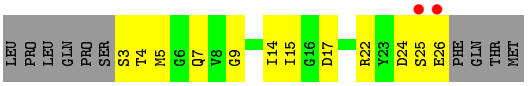
Chain X:



- Molecule 2: Bcl-2 homologous antagonist/killer

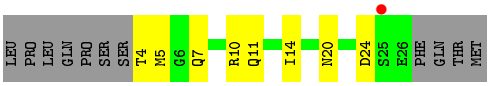
Chain B:





- Molecule 2: Bcl-2 homologous antagonist/killer

Chain Y:


LEU
PRO
LEU
GLN
PRO
SER
SER
T4
M5
G6
Q7
R10
Q11
I14
N20
D24
S25
E26
PHE
GLN
THR
MET

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	148.62Å 148.62Å 148.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.15 – 2.60 29.15 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.4 (29.15-2.60) 100.0 (29.15-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.171 , 0.234 0.181 , 0.242	Depositor DCC
R_{free} test set	1698 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å^2)	60.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 77.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.038 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3129	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: NHE

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	0.49	0/1333	0.59	0/1806
1	X	0.46	0/1309	0.60	1/1772 (0.1%)
2	B	0.39	0/187	0.56	0/249
2	Y	0.44	0/181	0.66	0/241
All	All	0.47	0/3010	0.60	1/4068 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	33	ASP	CB-CG-OD2	5.20	122.98	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1307	0	1291	95	0
1	X	1285	0	1272	95	0
2	B	187	0	180	14	0
2	Y	181	0	175	14	0
3	X	13	10	16	3	0
4	A	64	0	0	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	8	0	0	1	0
4	X	61	0	0	29	0
4	Y	13	0	0	3	0
All	All	3119	10	2934	207	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 35.

The worst 5 of 207 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:7:PHE:O	1:A:11:THR:HG23	1.69	0.93
1:A:11:THR:HG22	1:A:160:TRP:HE1	1.30	0.92
1:X:140:LYS:HB2	1:X:140:LYS:NZ	1.85	0.90
1:X:160:TRP:HD1	4:X:219:HOH:O	1.57	0.87
2:B:24:ASP:HB3	4:B:87:HOH:O	1.74	0.87

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	161/179 (90%)	150 (93%)	11 (7%)	0	100 100
1	X	155/179 (87%)	134 (86%)	18 (12%)	3 (2%)	8 15
2	B	22/34 (65%)	20 (91%)	2 (9%)	0	100 100
2	Y	21/34 (62%)	20 (95%)	1 (5%)	0	100 100
All	All	359/426 (84%)	324 (90%)	32 (9%)	3 (1%)	19 39

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	86	PRO
1	X	46	PRO
1	X	128	LYS

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	147/162 (91%)	144 (98%)	3 (2%)	55	78
1	X	144/162 (89%)	141 (98%)	3 (2%)	53	77
2	B	20/30 (67%)	20 (100%)	0	100	100
2	Y	19/30 (63%)	19 (100%)	0	100	100
All	All	330/384 (86%)	324 (98%)	6 (2%)	59	80

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	PHE
1	X	125	ARG
1	X	79	LEU
1	A	44	CYS
1	X	98	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	X	3	ASN
2	Y	20	ASN
1	X	157	HIS
1	A	157	HIS
2	Y	11	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)

1 ligand 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	$\#\|Z\| > 2$
3	NHE	X	170	-	13,13,13	3.93	8 (61%)	16,17,17	3.30	11 (68%)

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
3	NHE	X	170	-	-	6/7/15/15	0/1/1/1

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	170	NHE	C2-S	-7.13	1.67	1.77
3	X	170	NHE	C2'-C1'	-5.39	1.39	1.52
3	X	170	NHE	C3'-C2'	-5.13	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	170	NHE	C6'-C1'	-5.10	1.40	1.52
3	X	170	NHE	C5'-C6'	-5.00	1.40	1.53

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	X	170	NHE	C3'-C2'-C1'	5.23	120.94	111.11
3	X	170	NHE	C5'-C6'-C1'	5.16	120.83	111.11
3	X	170	NHE	C1-N-C1'	4.70	123.36	114.14
3	X	170	NHE	C6'-C1'-C2'	4.42	118.48	110.82
3	X	170	NHE	C4'-C3'-C2'	4.34	120.26	111.42

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	X	170	NHE	C6'-C1'-N-C1
3	X	170	NHE	N-C1-C2-S
3	X	170	NHE	C1-C2-S-O2
3	X	170	NHE	C1-C2-S-O3
3	X	170	NHE	C2-C1-N-C1'

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	170	NHE	3	0

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	163/179 (91%)	-0.26	2 (1%)	79	76	39, 57, 96, 120	1 (0%)
1	X	161/179 (89%)	0.06	6 (3%)	41	34	40, 67, 136, 176	4 (2%)
2	B	24/34 (70%)	0.09	2 (8%)	11	8	61, 76, 112, 125	0
2	Y	23/34 (67%)	0.08	1 (4%)	35	28	50, 61, 91, 113	0
All	All	371/426 (87%)	-0.08	11 (2%)	50	43	39, 63, 119, 176	5 (1%)

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	83	SER	4.2
1	X	85	LYS	3.4
1	X	86	PRO	3.2
1	A	69	THR	2.8
1	X	84	ASP	2.6

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)

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
3	NHE	X	170	13/13	0.75	0.32	104,125,166,169	0

6.5 Other polymers (i)

There are no such residues in this entry.